Causal clustering: design of cluster experiments under network interference*

Davide Viviano[†] Lihua Lei[‡] Guido Imbens[§] Brian Karrer[¶] Okke Schrijvers[‡] Liang Shi**

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Abstract

This paper studies the design of cluster experiments to estimate the global treatment effect in the presence of network spillovers. We provide a framework to choose the clustering that minimizes the worst-case mean-squared error of the estimated global effect. We show that optimal clustering solves a novel penalized min-cut optimization problem computed via off-the-shelf semi-definite programming algorithms. Our analysis also characterizes simple conditions to choose between any two cluster designs, including choosing between a cluster or individual-level randomization. We illustrate the method's properties using unique network data from the universe of Facebook's users and existing data from a field experiment.

Keywords: Experimental Design, Spillover Effects, Causal Inference, Cluster Designs. JEL Codes: C10, C14, C31, C54

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[†]Department of Economics, Harvard University. Email: dviviano@fas.harvard.edu

[‡]Graduate School of Business, Stanford University. Email: lihualei@stanford.edu

[§]Graduate School of Business and Department of Economics, Stanford University. Email: imbens@stanford.edu

[¶]FAIR, Meta. Email: briankarrer@meta.com

Central Applied Science, Meta. Email: okke@meta.com.

^{**}Central Applied Science, Meta. Email: liangshi@meta.com.

1 Introduction

Consider a (large) population of n individuals connected under a single observed network. Researchers are interested in conducting an experiment to estimate the global average treatment effect, i.e., the difference between the average effect of treating all versus none of the individuals in the population. Treating an individual may generate spillovers to her friends in the network. To capture such effects, researchers conduct a cluster experiment. Individuals are first partitioned into clusters. Within a cluster, either all units are assigned to the treatment or all units are assigned to the control group. Finally, researchers estimate treatment effects by taking a difference between the average outcomes of treated and control units (possibly adjusting for baseline covariates). The cluster design does not require modeling the dependence of individual outcomes on neighbors' assignments, but it requires a choice of clusters and some assumptions on the extent of the spillovers along the network. For example, cluster experiments on online platforms require choosing a partition of the social network, and field experiments require choosing the unit of randomization, such as villages or regions. This raises the question of how many and which clusters to use in experiments.

Typical approaches in economic research assume prior knowledge of many independent clusters. There are many settings where this information is not available, and instead, units in the population have different degrees of connections. This paper provides an econometric framework to choose when and how to design the *clusters* in cluster experiments. Different from existing clustering algorithms geared towards community detection, we motivate the choice of clusters based on the task of estimating global treatment effects. The choice of clustering must balance two competing objectives: the larger the clusters (and the smaller the number of clusters), the smaller the bias of the estimated global effect, but the larger its variance. We introduce an algorithmic procedure – entitled *Causal Clustering* – to choose the clustering that minimizes a weighted combination of the worst-case bias and variance as a function of the network and clusters. The worst-case approach encodes uncertainty over the dependence of individual outcomes on neighbors' assignments. We study (i) *whether* to run a cluster-level instead of individual-level randomization; (ii) *how* to cluster individuals (and how many clusters to use).

We focus on a class of models where spillover effects are small relative to the outcomes' variance but possibly non-negligible for inference. This is formalized in a novel framework of local asymptotics where individual outcomes depend arbitrarily on neighbors' treatments, and, as n grows, spillovers from neighbors (and possibly also direct effects) converge to

¹For example, when using villages as clusters, individuals may interact in the same and nearby villages. See Egger et al. (2022) for an empirical example.

zero, but at an arbitrary slow rate (e.g., slower than $n^{-1/2}$). This framework encodes the researchers' uncertainty on the presence (and magnitude) of spillover effects by modeling first-order neighbors' effect local to zero, with the convergence rate capturing the expected magnitude of spillovers.² The local asymptotic framework we study is consistent with settings with small (but non-negligible) treatment and spillover effects, typical, for instance, in online experiments (e.g., Karrer et al., 2021). We characterize optimal clustering as a function of the expected magnitude of the largest spillover effects that the experiment can generate. The largest size of the spillover effects is a key input in our algorithms, whose characterization, in practice, is necessary for the design of the experiment but can be challenging. This parameter can be informed by previous experiments, in the same spirit of minimum detectable effects used in power analysis (e.g. Baird et al., 2018), or using some particular modeling assumptions. We provide guidance to practitioners in Section 7.

Our analysis proceeds as follows. First, we provide a formal characterization of the worst-case bias and variance. We show that the worst-case bias is closely related to a particular notion of between-clusters connectedness, defined as the per-individual average number of friends in other clusters. The worst-case variance can potentially be an arbitrary function of within-clusters covariances and between-clusters covariances: individuals in the same cluster have identical assignments and in different clusters may share common neighbors. We show that the variance only depends on the average squared cluster size, up to an asymptotically negligible error. This result formalizes the intuition that a larger number of clusters, with a small variance in cluster size, decreases the variance of the estimator.

We draw the implications of these results for choosing between a cluster experiment (for a given clustering) or assigning treatments independently between individuals (i.e., Bernoulli design or completely randomized design). Suppose the magnitude of the spillover effects is smaller than the square root of the number of clusters. In that case, the variance component dominates the bias, and a Bernoulli design is preferred (where a Bernoulli design is a special case of a cluster design with clusters containing a single unit). Vice-versa, a cluster design is preferred if the bias dominates the variance. Intuitively, because our objective trades off the bias and variance of the estimator, whenever the number of clusters is small, it is best to run a Bernoulli design for any value of spillover effects local to zero. On the other hand, if the number of clusters is sufficiently large and the cluster design appropriately controls the bias of the estimator, a cluster design is preferred. We provide practitioners with a simple and explicit decision rule between cluster and Bernoulli designs that can be easily implemented in practice.

²The assumption of spillovers within first-order neighbors can be relaxed here by assuming that higher-order spillovers are an order of magnitude smaller than first-order spillovers.

We then turn to the design of optimal clustering, where the choice is not whether to run a cluster or Bernoulli design but rather which clustering to use. The choice of optimal clustering reduces to a novel penalized minimum cut optimization problem, with a penalty that depends on the cluster size variation. The program admits a convenient formulation as a sequence of trace-optimization problems, each solved via off-the-shelf semidefinite programming algorithms.

We provide an empirical application using unique network data from the universe of Facebook users. We show that our procedure provides an explicit ranking between different clustering algorithms implemented at scale at Facebook. We also illustrate trade-offs in the choice of the clustering algorithm and properties of the graph. A second application using network data from Cai et al. (2015) illustrates the method's advantages for choosing clusters in field experiments. We show that the choice of the clusters based on village identity is sub-optimal in this application because the number of village clusters is too small relative to the optimal clustering, and provide an explicit choice of the clustering. These results illustrate the applicability of the method in choosing the clustering and number of clusters.

This paper connects to the literature on experimental design, causal inference with spillover effects, and clustering. Existing methods for experimental designs with spillover effects include cluster and saturation designs, studied in Baird et al. (2018); Basse and Feller (2016); Cai et al. (2022); Karrer et al. (2021); Pouget-Abadie (2018); Taylor and Eckles (2018); Viviano (2020b), among others. These papers provide an analysis of the properties of particular designs for a given clustering or clustering algorithm. Different from the current paper, these references either do not study the question of the optimal clustering algorithm for experimental design or only provide heuristic comparisons of different clustering methods.

A particular class of clustering algorithms is ε -net clustering algorithms – which consist of assigning sequentially individuals in the same neighborhood to the same cluster (Eckles et al., 2017; Ugander et al., 2013). Variants of these algorithms have been recently studied in Leung (2022) (and more recently in contemporaneous work by Leung, 2023) for spatial spillovers, and Faridani and Niehaus (2022) in general non-Euclidean spaces. These papers provide an optimal rate of the clusters' size as a function of how interference decays in space for asymptotically unbiased estimators. Here, instead, we provide an explicit trade-off and novel characterization of the bias and variance, leveraging local asymptotics. It allows us to characterize the optimal clustering as the solution of a novel and simple trace-optimization program (different from the algorithms studied in the previous references). The comparison of a cluster and Bernoulli designs through local asymptotics is also a novel contribution.

Additional references of experiments with networks in the *absence* of cluster experiments are Basse and Airoldi (2018b), and Jagadeesan et al. (2020) for estimating direct instead of

global average treatment effects studied here; Kang and Imbens (2016) who study encouragement designs, without focusing on the problem of mean-squared error optimal designs; Viviano (2020a) for experiments on networks using information from a pilot study; Basse and Airoldi (2018a) discuss limitations of design-based causal inference under interference. None of these papers study (optimal) cluster designs.

The literature on treatment effects under network interference includes Aronow and Samii (2017), Hudgens and Halloran (2008), Manski (2013), Leung (2020), Athey et al. (2018), Goldsmith-Pinkham and Imbens (2013), Sävje et al. (2021), Ogburn et al. (2017), Manresa (2013), Li and Wager (2022), often focusing on first-order degree interference.³ None of the above references study experimental designs. Finally, we relate more broadly to the literature on clustering in economics – see Wooldridge (2003), Abadie et al. (2017) and references therein – with the difference that here we focus on optimal clustering, rather than taking the clusters as given – and the literature on graph clustering, including Von Luxburg (2007), Newman (2013a,b), Lei (2019), Lei et al. (2020), Li et al. (2022), and references therein. Different from this last set of papers on graph clustering, this paper focuses on treatment effect estimation instead of community detection.

The remainder of the paper is organized as follows: Section 2 presents the setup; Section 3 characterizes the bias and variance and contrast cluster and Bernoulli designs; Section 4 formalizes the optimization problem for the optimal clustering; Section 5 presents two applications and numerical studies, Section 6 presents several extensions, and Section 7 contains recommendations for practice.

2 Setup

We consider a setting with $i \in \{1, \dots, n\}$ units. Let $Y_i \in \mathbb{R}$ denote the observed outcome of interest for individual $i, D_i \in \{0, 1\}$ denote a binary treatment assignment, and $\mathbf{D} \in \{0, 1\}^n$ the vector of treatment assignments of each unit. Define \mathbf{A} a symmetric adjacency matrix with $\mathbf{A}_{i,j} \in \{0, 1\}$, and $Y_i(\mathbf{d}), \mathbf{d} \in \{0, 1\}^n$ the potential outcome as a function of the entire vector of treatment assignments, with $Y_i = Y_i(\mathbf{D})$. We implicitly condition on \mathbf{A} , observed to the researchers, and (unobserved) potential outcomes $Y(\mathbf{d})$, unless otherwise specified (see Remark 7 for an extension with unobserved \mathbf{A}). We define $\mathcal{N}_i = \{j : \mathbf{A}_{i,j} = 1\}$ the set of individuals connected to i. Let $\mathcal{N}_{n,\max} = \max_{i \in \{1,\dots,n\}} |\mathcal{N}_i|$, the maximum degree. When $|\mathcal{N}_i| = 0$ for all nodes, we define $\mathcal{N}_{n,\max} = 1$ for notational convenience.

³Our local asymptotic framework extends to settings with higher order dependence, assuming that higher order neighbors generate spillovers of smaller order compared to first order neighbors, and the network is sufficiently sparse.

Our primary focus is on estimating the global average treatment effect,

$$\tau_n = \frac{1}{n} \sum_{i=1}^n \left[Y_i(\mathbf{1}) - Y_i(\mathbf{0}) \right]. \tag{1}$$

The overall effect defines the effect if all units had received the treatment compared to none of the individuals receiving the treatment. This is a target estimand in many economic applications when researchers are interested in implementing the policy on all individuals in the population, e.g., Egger et al. (2022), Muralidharan and Niehaus (2017), Karrer et al. (2021) (see Remark 9 for a discussion on other estimands). Table 4 summarizes the notation.

2.1 Potential outcomes and spillover effects

Next, we impose restrictions on the spillover effects.

Assumption 1 (First-order local interference). For $i \in \{1, \dots, n\}$,

$$Y_i(\mathbf{d}) = \mu_i(\mathbf{d}_i, \mathbf{d}_{\mathcal{N}_i}), \quad \forall \mathbf{d} \in \{0, 1\}^n,$$

for some functions $\mu_i(1,\cdot) \in \mathcal{M}_{1,i}, \mu_i(0,\cdot) \in \mathcal{M}_{0,i}$ for some set of functions $\mathcal{M}_{1,i}, \mathcal{M}_{0,i}$

Assumption 1 states that spillovers occur between neighbors and allows for arbitrary dependence of potential outcomes with neighbors' assignments. One-degree neighborhood is consistent with models often used in applications, e.g., Cai et al. (2015), Sinclair et al. (2012), Muralidharan and Niehaus (2017). Athey et al. (2018) provide a framework for testing Assumption 1. Higher-order interference can be accommodated, although higher-order effects are often small and difficult to detect (see Remark 2). With a slight abuse of notation, we occassionally write $\mu_i(\mathbf{d})$ for $\mu_i(\mathbf{d}_i, \mathbf{d}_{\mathcal{N}_i})$ for notational convenience.

We will refer to $\tau_{n,\mu}$ as the overall effect in Equation (1) to make the dependence of τ_n on (μ_1, \dots, μ_n) explicit. We do not assume that we know or can estimate consistently μ_i . (The functions μ_i and their classes $\mathcal{M}_{0,i}, \mathcal{M}_{1,i}$ are indexed by i, and therefore they cannot be consistently estimated.) Instead, we allow for arbitrary classes $\mathcal{M}_{1,i}, \mathcal{M}_{0,i}$ of potential outcome functions, as long as such classes satisfy the conditions below. These classes have to be sufficiently large to accommodate rich structures in the data, as well as satisfy some restrictions to be able to estimate features of causal effects.

Assumption 2 (Class of potential outcome functions). The potential outcomes $\mu = (\mu_1, \dots, \mu_n) \in \mathcal{M} = \bigotimes_{i=1}^n \mathcal{M}_i$ where \mathcal{M}_i is the set such that $\mu_i(1,\cdot) \in \mathcal{M}_{1,i}, \mu_i(0,\cdot) \in \mathcal{M}_{0,i}$. For all $i \in \{1, \dots, n\}, d \in \{0, 1\}$, the function classes $\mathcal{M}_{d,i}$ contains all functions satisfying

- (i) $\mu_i(d,\cdot) \in [\psi_L, \psi_R], \forall \mu_i(d,\cdot) \in \mathcal{M}_{d,i}$ for some constants $-\infty < \psi_L < \psi_R < \infty$ that do not vary with n;
- (ii) for all $\mathbf{d} \in \{0, 1\}^{|\mathcal{N}_i|}$,

$$\sup_{\mu_{i}(0,\cdot)\in\mathcal{M}_{0,i}} \left| \mu_{i}(0,\mathbf{d}) - \mu_{i}(0,\mathbf{0}) \right| = \frac{\bar{\phi}_{n}}{|\mathcal{N}_{i}|} \sum_{k\in\mathcal{N}_{i}} \mathbf{d}_{k},$$

$$\sup_{\mu_{i}(1,\cdot)\in\mathcal{M}_{1,i}} \left| \mu_{i}(1,\mathbf{d}) - \mu_{i}(1,\mathbf{1}) \right| = \frac{\bar{\phi}_{n}}{|\mathcal{N}_{i}|} \sum_{k\in\mathcal{N}_{i}} \left(1 - \mathbf{d}_{k} \right),$$
(2)

for some $\bar{\phi}_n \leq \psi_R - \psi_L$.

Assumption 2 imposes two restrictions. Condition (i) states that potential outcomes are uniformly bounded.⁴ Condition (ii) is our main restriction on the exposure mapping. Condition (ii) is attained if $\mathcal{M}_{1,i}$, $\mathcal{M}_{0,i}$ are Lipschitz function classes in the share of treated neighbors. Condition (ii) states that potential outcomes vary in the share of neighbors' treatments by at most $\bar{\phi}_n$. Here $\bar{\phi}_n$ captures the magnitude of (largest) spillovers. The condition that $\bar{\phi}_n \leq \psi_R - \psi_L$ is a regularity assumption that guarantees that (ii) is consistent with the boundedness restriction in (i). In Section 6.1, we relax Assumption 2, by imposing (ii) only on the expected value of the potential outcomes (instead of the realized potential outcomes). In Section 6.2, we relax Assumption 2 by allowing for heterogeneity in the range of potential outcomes and the spillover effects.

The component $\bar{\phi}_n$ depends on n and will play an important role in our asymptotic analysis as $n \to \infty$. We focus on settings where $\bar{\phi}_n$ is small (i.e., $\bar{\phi}_n = o(1)$ as $n \to \infty$), in the spirit of a local asymptotic framework (e.g. Hirano and Porter, 2009), but its convergence rate can be arbitrarily slow. These scenarios formalize the idea that spillover effects (and possibly but not necessarily also overall treatment effects τ_n) are local to zero. For example, in an information campaign, we might expect spillover (and direct) effects to be small but non-negligible for inference. Small treatment and spillover effects are common in many experimental setups. In experiments conducted on online platforms, individual (and spillover) effects are often statistically small, whereas the sum of all such effects can be economically significant with a large target population. Our asymptotic framework allows for such scenario, where $\bar{\phi}_n$, while local to zero, can be of order slower than $n^{-1/2}$. Empirical relevant examples include Athey et al. (2023), Karrer et al. (2021), among others.

We show how different magnitudes of spillover effects justify different designs.

Assumption 3 (Local and sparse network asymptotics). We consider asymptotic scenarios with a sequence of $(\mathbf{A}, (Y_i(\cdot))_{i=1}^n)$, indexed by n, where $\bar{\phi}_n \min\{n, \mathcal{N}_{n,\max}^2\} = o(1)$.

⁴This restriction is common in the literature, e.g., Kitagawa and Wang (2021), and can be relaxed by assuming random sub-gaussian potential outcomes.

Assumption 3 formalizes the local asymptotic framework considered here: spillovers converge to zero, but the rate can be arbitrarily slow up to a term that depends on the squared maximum degree. Assumption 3 holds for arbitrary rates of convergence of the spillover effects $\bar{\phi}_n$ for networks with bounded degree (e.g. De Paula et al., 2018, where $\mathcal{N}_{n,\text{max}}$ is bounded), and requires faster rates of $\bar{\phi}_n$ (smaller spillover effects), for dense networks.

Example 2.1 (Linear exogenous peer effects). Consider a class of functions of the form $\mu_i(\mathbf{d}) = \mu(T_i(\mathbf{d})) + \varepsilon_i$, with $T_i(\mathbf{d}) = \left[\mathbf{d}_i, (1 - \mathbf{d}_i) \times \frac{\sum_{j \neq i} \mathbf{A}_{i,j} \mathbf{d}_j}{\sum_{j \neq i} \mathbf{A}_{i,j}}, \mathbf{d}_i \times \frac{\sum_{j \neq i} \mathbf{A}_{i,j} \mathbf{d}_j}{\sum_{j \neq i} \mathbf{A}_{i,j}}\right]$, and $\mu(t) = t^{\top}\beta$ for $\beta \in [-\bar{\Delta}_n, \bar{\Delta}_n] \times [-\bar{\phi}_n, \bar{\phi}_n]^2$, for some arbitrary $\bar{\Delta}_n, \bar{\phi}_n$, and ε_i that is not a function of \mathbf{d} . Then Assumption 2 holds.

Remark 1 (Weaker conditions on the degree). Assumption 3 can be sharpened by imposing restrictions on the *average* second-order degree instead of maximum degree; see Equation (33) in the proof of Lemma C.2. We state this version for expositional convenience. \Box

Remark 2 (Higher order interference and endogenous peer effects). Our setting generalizes to higher-order interference in two scenarios.

First, suppose that friends up to degree $d < \infty$ generate spillovers in magnitude similar to first-degree friends. Our results extend after we define the set of friends as the set of friends up to degree d, and $\bar{\phi}_n$ the largest effect that such friends generate. Sparsity restrictions on the largest degree in Assumption 3 are with respect to the number of friends up to degree d.

In the second scenario, suppose that the assumption of first-order effects approximates higher-order effects up to a term of smaller order than first-order effects. Specifically, suppose that $Y_i(\mathbf{d}) = \mu_i(\mathbf{d}_i, \mathbf{d}_{\mathcal{N}_i}) + \mathcal{O}(h_n)$, for some $h_n \to 0$. Our results hold if $h_n = o(1/n)$, capturing the idea that first-order effects $\bar{\phi}_n$ are larger than second-order effects. In Appendix B we provide an example and sufficient conditions for the approximation error due to higher order interference being of order o(1/n) in the presence of endogenous peer effects (Bramoullé et al., 2009; Manski, 1993), where the individual outcome depends on other units' outcomes.

In practice, higher-order effects can be small, leading to underpowered studies, especially when individuals have many friends and first-order effects capture most of the spillovers.

This motivates our focus on first-order effects.

Remark 3 (Local asymptotics and direct effect). Our local asymptotic framework also allows direct treatment effects (and global effects) to be local to zero. Specifically, it is possible that $\tau_n = o(1)$ at arbitrary rate, e.g., at the *same* rate as $\bar{\phi}_n$. Therefore, our local asymptotic assumption does not require that spillover effects are local to the global effect (since τ_n can also converge to zero). Instead, our local asymptotics formalizes settings where the noise-to-signal ratio decreases slower than $n^{-1/2}$ (for example, common in experiments on online platforms, Karrer et al. (2021)).

2.2 Experimental design and estimation

Next, we turn to the class of designs and estimators considered here. Define a clustering of size K_n as a set of sets of indicators satisfying

$$C_n = \left\{ c_k \subseteq \{1, \dots, n\}, k \in \{1, \dots, K_n\}, \bigcup_k c_k = \{1, \dots, n\}, c_k \bigcap c_{k'} = \emptyset \text{ for } k \neq k' \right\}.$$

Here, C_n denotes a particular partition of the units in the population with K_n exclusive clusters. With an abuse of notation, let $c(i) \subseteq \{1, \dots, n\}$ denote the cluster assigned to unit i, and $|c_k| = n_k$ the number of individuals in cluster k. For ease of exposition, we focus our discussion and assumptions below in the presence of a given clustering C_n and return to choosing the optimal clustering in Section 4.

Assumption 4 (Cluster designs). C_n is measurable with respect to \mathbf{A} and is such that the number of units in cluster k is $n_k = \gamma_k \frac{n}{K_n}$ with $\max_k \gamma_k \leq \bar{\gamma} < \infty$, for some $\bar{\gamma} < \infty$. Assume that $D_i = \tilde{D}_{c(i)}$ almost surely, where $\tilde{D}_{c(i)}|\mathbf{A}, \{Y_i(\mathbf{d})\}_{i \in \{1, \dots, n\}} \mathbf{d} \in \{0, 1\}^N \sim \text{Bern}(0.5)$ are independent across clusters.

Assumption 4 states the clustering is constructed using information from the adjacency matrix only (i.e., it is independent of potential outcomes), clusters are proportional in size⁵, and individuals in a given cluster are all assigned either treatment or control with equal probability. Assumption 4 restricts the class of designs to cluster designs, motivated by our focus on overall treatment effects and empirical practice.

Motivated by standard practice both in industrial applications and in field experiments with clusters (Baird et al., 2018), we consider estimators obtained by simple differences in means between treated and control clusters. Because $P(D_i = 1) = 1/2$, we construct a (biased) estimator of treatment effects as

$$\hat{\tau}_n(\mathcal{C}_n) = \frac{2}{n} \sum_{i=1}^n \left[D_i Y_i - (1 - D_i) Y_i \right] = \frac{2}{n} \sum_{i=1}^n (2D_i - 1) Y_i.$$
 (3)

The estimator $\hat{\tau}_n(C_n)$ is a simple difference in means between treated and control units that normalizes by the probability of treatment. Therefore, $\hat{\tau}_n(C_n)$ depends on the clustering C_n only because the distribution of the treatments depends on the clusters under Assumption 4. Studying the estimator in Equation (18) is a natural starting point for the analysis of cluster experiments. Variants of difference in means estimators (possibly also with regression adjustments discussed in Remark 4) are often used or studied in practice (Holtz et al., 2020;

⁵This restriction is sufficient but not necessary for our analysis, and it is imposed for expositional convenience. It is possible to relax such an assumption by assuming that $\sum_{k=1}^{K_n} \gamma_k^2 / K_n = \mathcal{O}(1)$.

Karrer et al., 2021; Sävje et al., 2021). One could also normalize each sum in Equation (18) by the number of treated and control units (instead of using knowledge about the treatment probability). This would improve the stability of the estimator but complicate the analysis when the number of treated units is stochastic (e.g., when clusters have different sizes).

Remark 4 (Covariate adjustment). Our framework generalizes to settings that use covariate adjustment. Denote $\bar{\mu}_i$ an arbitrary predictor for $\mu_i(\mathbf{0})$ that only uses information from some arbitrary baseline observable characteristics (i.e., does not depend on the treatments or endline outcomes in the experiment). The estimator with such an adjustment takes the form

$$\frac{2}{n}\sum_{i=1}^{n}(Y_i - \bar{\mu}_i)(2D_i - 1). \tag{4}$$

Note that $Y_1 - \bar{\mu}_1, \dots, Y_n - \bar{\mu}_n$ typically have different ranges ex ante even under Assumption 2. To account for this, we can apply the more general result in Section 6.2.

Remark 5 (Alternative estimators). Alternative estimators studied in the literature are inverse probability weights estimators (e.g., Aronow and Samii, 2017; Ugander et al., 2013) (these estimators reweight by the probability that the treatment of all friends being either zero or one). Unless researchers impose additional restrictions on the exposure mapping, in the network context, these estimators can be subject to the instability of the propensity score because they reweight by the inverse probability that all friends of a given individual are either under treatment or control. An alternative are model-based estimators, which are subject to model misspecification. A third class of estimators are trimming estimators, which trim observations based on their position in the network. We show how our framework generalizes for such estimators in Section 6.3.

Remark 6 (Saturation designs). It is possible to consider designs where treatments are assigned with different cluster-level probabilities. Our main insights for the bias and variance characterization follow similarly to what we present for cluster experiments, with appropriate modifications presented in Section 6.4.

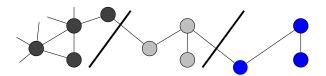


Figure 1: Example of clustering design with a single network. The network is partitioned into three clusters. Elements in a given cluster are assigned the same color.

3 (When) should you cluster?

This section studies when a given clustering C_n should be chosen over a simple Bernoulli design where treatments are randomized independently across individuals. This is often a central question in experiments (e.g. Holtz et al., 2020). To study this question, we first characterize the bias and variance of the estimator $\hat{\tau}_n(C_n)$.

We denote a Bernoulli design as a special cluster design with clusters $C_{B,n} = \{c_k = \{k\}, k \in \{1, \dots, n\}\}$. Denote $\mathbb{E}_{\mu}[\cdot]$ the expectation for given potential outcome functions μ (conditional on \mathbf{A}). The components $\mathcal{O}(\cdot)$, $o(\cdot)$ in the following lemmas and theorems hold uniformly over all cluster designs with K_n many clusters that satisfy Assumption 4.

Our goal is to design experiments that minimize the worst-case variance, while controlling the worst-case bias. For a given clustering C_n , the dual of the optimization problem is:

$$\mathcal{B}_{n}(\mathcal{C}_{n},\lambda) = \sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} [\hat{\tau}_{n}(\mathcal{C}_{n})] \right)^{2} \right] + \lambda \sup_{\mu \in \mathcal{M}} \left(\tau_{n,\mu} - \mathbb{E}_{\mu} [\hat{\tau}_{n}(\mathcal{C}_{n})] \right)^{2}, \tag{5}$$

where the supremum is intended over $(\mu_i)_{i=1}^n$, and \mathcal{M} is the product space of potential outcome functions as in Assumption 2. The parameter λ is user-specific and denotes the relative importance weight assigned to the worst-case bias. For $\lambda = 1$, Theorem 3.4 below shows that $\mathcal{B}_n(\mathcal{C}_n, \lambda)$ coincides in the limit with the worst-case mean-squared error.

3.1 Worst-case bias, variance, and MSE

As a first step, we characterize the worst-case bias of the estimator $\hat{\tau}_n(\mathcal{C}_n)$. Let

$$b_n(\mathcal{C}_n) = \frac{1}{n} \sum_{i=1}^n \frac{1}{|\mathcal{N}_i|} \Big| \mathcal{N}_i \bigcap \Big\{ j : c(i) \neq c(j) \Big\} \Big|$$
 (6)

and $\{j: c(i) \neq c(j)\}$ denotes the set of units j in a different cluster from unit i.

Lemma 3.1 (Worst-case bias). Let Assumptions 1, 2, 4 hold. Then

$$\sup_{\mu \in \mathcal{M}} \left| \tau_{n,\mu} - \mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)] \right| = \bar{\phi}_n b_n(\mathcal{C}_n).$$

Proof. See Appendix C.2.

Lemma 3.1 shows that the worst-case bias can be expressed as the number of friends of i in a different cluster from i, appropriately reweighted by the overall number of friends of i. The size of the worst-case bias also depends on the magnitude of spillover effects $\bar{\phi}_n$. Lemma

3.1 provides a formal justification to notions of between clusters connectedness based on the worst-case bias of the treatment effect estimator.

To derive the worst-case variance, we define

$$\bar{\psi}^{1/2} = 2 \max\{|\psi_R|, |\psi_L|\}. \tag{7}$$

By Assumption 2 (i), $\bar{\psi}$ can also be expressed as $\max_{\mu_i \in \mathcal{M}_i} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0}))^2$ for every i.

Lemma 3.2 (Worst-case variance). Let Assumptions 1, 2, 3, 4 hold. Then as $K_n \to \infty$

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}[\hat{\tau}_n(\mathcal{C}_n)] \right)^2 \right] = \frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2 \times \left[\bar{\psi} + o(1) \right].$$

Proof. See Appendix C.5.

Lemma 3.2 characterizes the worst-case variance as the number of clusters K_n grows (at an arbitrary rate). Such bounds depend on the variance in cluster sizes, $\frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2$, times a positive constant $\bar{\psi}$. In Section 7 we provide practical recommendations for the choice of $\bar{\psi}$. By leveraging the local asymptotic framework in Assumption 3, a key insight is that the variance is (asymptotically) driven by the within-cluster correlations instead of cross-cluster connections. This intuition formalizes the idea that a larger variation in clusters' size increases the variance of the estimator. To our knowledge, these characterizations of the worst-case bias and variance are novel to the literature on spillover effects.

Combining Lemma 3.1 and Lemma 3.2, we obtain the expression of $\mathcal{B}_n(\mathcal{C}_n,\lambda)$.

Theorem 3.3. Suppose that Assumptions 1, 2, 3, 4 hold. Then as $K_n \to \infty$

$$\mathcal{B}_n(\mathcal{C}_n, \lambda) = \mathcal{B}_n^*(\mathcal{C}_n, \lambda)(1 + o(1)),$$

where

$$\mathcal{B}_n^*(\mathcal{C}_n, \lambda) = \bar{\psi} \cdot \frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2 + (\lambda \bar{\phi}_n^2) \cdot b_n^2(\mathcal{C}_n). \tag{8}$$

Proof of Theorem 3.3. Theorem 3.3 is a direct corollary of Lemmas 3.1, 3.2. \Box

An alternative quality measure of the estimator is the worst-case mean square error (MSE), defined as

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} [(\hat{\tau}_n(\mathcal{C}_n) - \tau_{n,\mu})^2]$$
(9)

Since the MSE is obtained by adding up the square of bias and variance, it is evidence that the worst-case MSE is upper bounded by $\mathcal{B}_n(\mathcal{C}_n, 1)$. Here, we can also show that they coincide as $K_n \to \infty$.

Theorem 3.4. Suppose that Assumptions 1, 2, 3, 4 hold. Then as $K_n \to \infty$,

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu}[(\hat{\tau}_n(\mathcal{C}_n) - \tau_{n,\mu})^2] = \mathcal{B}_n^*(\mathcal{C}_n, 1)(1 + o(1)).$$

Proof. See Appendix C.6.

Remark 7 (Unobserved **A**). Suppose that **A** is unobserved or *partially* observed, and researchers have a prior over **A**. In this case, the worst-case variance does not change, the worst-case bias is replaced by $\bar{\phi}_n \mathbb{E}_{\mathbf{A}}[b_n(\mathcal{C}_n)]$, and $b_n^2(\mathcal{C}_n)$ in $\mathcal{B}_n^*(\mathcal{C}_n, \lambda)$ is replaced by $\mathbb{E}_{\mathbf{A}}[b_n^2(\mathcal{C}_n)]$, where the expectation may depend on partial network information (Breza et al., 2020).

3.2 Comparison with a Bernoulli design

We now compare a given class of clustering designs to a Bernoulli design $\mathcal{C}_{B,n}$.

Theorem 3.5. Suppose that Assumptions 1, 2, 3, 4 hold. Then for any $\lambda \in (0, \infty)$, bounded away from zero and infinity, as $K_n \to \infty$, for arbitrary constants $\delta \in [0, 1)$, $\kappa < 1$ independent of n,

$$\liminf_{n \to \infty} \frac{\mathcal{B}_n(\mathcal{C}_n, \lambda)}{\mathcal{B}_n(\mathcal{C}_{B,n}, \lambda)} > 1 \quad \text{if } \sqrt{K_n} \bar{\phi}_n \to 0 \text{ and } K_n/n \le \kappa,
\limsup_{n \to \infty} \frac{\mathcal{B}_n(\mathcal{C}_n, \lambda)}{\mathcal{B}_n(\mathcal{C}_{B,n}, \lambda)} < 1 \quad \text{if } \sqrt{K_n} \bar{\phi}_n \to \infty, \text{ and } b_n(\mathcal{C}_n) \le \delta,$$
(10)

where $b_n(\mathcal{C}_n)$ is defined in (6).

Proof. See Appendix C.7. \Box

Theorem 3.5 compares a Bernoulli design and a cluster design. Theorem 3.5 states that we should not run a cluster experiment if the size of the spillover effects $\bar{\phi}_n$ goes to zero at an order faster than $1/\sqrt{K_n}$, where K_n denotes the number of clusters, and the number of clusters is sufficiently smaller than the sample size (at an arbitrary rate). We should instead run a cluster design if spillover effects are larger in magnitude than $1/\sqrt{K_n}$. The assumption that $b_n(\mathcal{C}_n) \leq \delta$ is equivalent to assuming that $\sum_{i=1}^n \frac{1}{|\mathcal{N}_i|} |\mathcal{N}_i \cap \{j : c(j) \neq c(i)\}| \leq \delta$, for some $\delta \in [0, 1)$, i.e., the clustering decreases the bias of the Bernoulli design (since $b_n(\mathcal{C}_{B,n}) = 1$).

⁶The worst-case MSE has been considered as the criterion in other settings for design of randomized experiments (Wu, 1981).

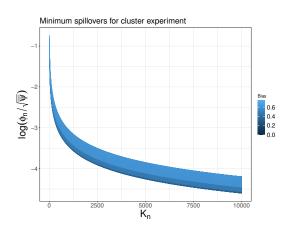
The choice of the Bernoulli design must depend on (i) the number of clusters and (ii) the size of spillovers. Table 1 provides explicit recommendations for researchers. Suppose that spillovers are of order $n^{-1/3}$ or smaller, therefore of slower order than $n^{-1/2}$. Then we should not run a cluster design if K_n is smaller than $n^{2/3}$. Therefore, even if spillovers are "not very small", cluster designs are sub-optimal if the number of clusters is "not very large", formally characterized by the rates of convergence. If, instead, spillovers are of order $n^{-1/3}$, and the number of clusters is of order n (e.g., clusters contain few individuals each), the cluster design is preferred over a Bernoulli design.

Table 1: Implications of Theorem 3.5 and examples of rates.

Description	Formulation	Implication: Run	Examples of Rates
Small spillovers small $\#$ of clusters	$\sqrt{K_n}\bar{\phi}_n = o(1)$	Bernoulli design	$K_n = n^{1/2}, \bar{\phi}_n = n^{-1/2}$
Not that small spillovers very small $\#$ of clusters	$\sqrt{K_n}\bar{\phi}_n = o(1)$	Bernoulli design	$\bar{\phi}_n = o(n^{-1/3}), K_n = \mathcal{O}(n^{2/3})$
Non-negligible spillovers large $\#$ of clusters	$\sqrt{K_n}\bar{\phi}_n\to\infty$	Cluster design	$K_n \propto n, \bar{\phi} = n^{-1/3}$

Table 2: Minimum spillover effects' size that justifies running a cluster experiment instead of a Bernoulli design in the presence of equally sized clusters ($\gamma_k = 1$ for all $k \in \{1, \dots, K_n\}$). The bias denotes $\frac{1}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_i|} |j \in \mathcal{N}_i : c(i) \neq c(j)| \in [0, 1]$. The table on the left-hand side reports the value of $\bar{\phi}_n$ for different values of the bias and number of clusters, fixing $\bar{\psi} = 4$ (e.g., valid when outcomes are bounded between [-1, 1]). In the figure on the right-hand side, the y-axis reports in log-scale the minimum size of the spillover effects $\bar{\phi}_n/\sqrt{\bar{\psi}}$ to run a cluster experiment as in Theorem 3.6. The x-axis reports the number of clusters. Different colors report different values of the bias.

Bias	K_n	$\bar{\psi}$	$ar{\phi}_n$
0.25	100	4	0.21
0.5	100	4	0.23
0.75	100	4	0.3
0.25	200	4	0.15
0.5	200	4	0.16
0.75	200	4	0.21
0.25	500	4	0.09
0.5	500	4	0.10
0.75	500	4	0.14



To complement the properties as a function of rates of convergence, in the following

theorem, we provide an explicit rule of thumb for a cluster design. It will be useful to define

$$\xi_n = (\lambda \bar{\phi}_n^2 / \bar{\psi})^{-1},\tag{11}$$

denoting the ratio of the largest deviation $\bar{\psi}$ over the magnitude of the spillovers squared times the weight λ on the bias. Our algorithm and explicit recommendations will require researchers to specify ξ_n as a tuning parameter (see Section 7 for recommendations for ξ_n).

Theorem 3.6 (Rule of thumb). Suppose that Assumptions 1, 2, 3, 4 hold. Let $\underline{\gamma} = \frac{1}{K_n} \sum_{k=1}^{K_n} \gamma_k^2$, where $\gamma_k = n_k K_n / n$. Then for some N > 0, n > N

$$\frac{\mathcal{B}_n^*(\mathcal{C}_{B,n},\lambda)}{\mathcal{B}_n^*(\mathcal{C}_n,\lambda)} \ge 1 \quad \text{if} \quad \xi_n \le \frac{K_n(1-b_n(\mathcal{C}_n)^2)}{\gamma}.$$

Proof of Theorem 3.6. See Appendix C.8.

Theorem 3.6 provides a rule of thumb for choosing a cluster design with given clusters C_n over a Bernoulli design $C_{B,n}$, using the approximate objective $\mathcal{B}_n^*(C_n,\lambda)$. The right-hand side depends on three *observables*: (i) $\underline{\gamma}$, (ii) the expected bias of the clustering method (as a function of \mathbf{A}), and (iii) the number of clusters K_n . The left-hand side depends on ξ_n . For $\lambda = 1$, known $\overline{\psi}$, the rule of thumb provides the smallest spillover effects that would guarantee that the cluster design dominates the Bernoulli design. When clusters are equally sized, the minimum size of the spillover effects to run a cluster experiment is $\overline{\phi}_n \geq \sqrt{\frac{\overline{\psi}}{(1-b_n(C_n)^2)K_n}}$, where $b_n(C_n)$ is defined in (6).

For example, assume (i) equally sized clusters, (ii) the bias of the clustering is at most 50% as a conservative upper bound, and (iii) outcomes are bounded between zero and one (in which case $\bar{\psi} \leq 4$). In this setting, researchers should run a cluster experiment when $\bar{\phi}_n \sqrt{K_n}$ is larger than 2.3. Figure 2 illustrates the exact threshold for the minimum size of spillovers that justifies conducting a cluster experiment. In our empirical application in Section 5 we find $\bar{\phi}_n \geq 0.003$ would motivate conducting a cluster experiment.⁷

4 Choosing the clusters

In this section, we turn to designing the optimal clustering. Theorem 3.3 characterizes the objective function. After simple re-arrangement, Theorem 3.3 provides a simple-to-compute

⁷This magnitude is constistent with typical magnitudes of treatment and spillover effects obtained from information campaigns on online platforms (Athey et al., 2023; Karrer et al., 2021).

metric for ranking (a few) given clusters (with ξ_n as in Equation 11)

$$\frac{\xi_n}{n^2} \sum_{k=1}^{K_n} n_k^2 + \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{|\mathcal{N}_i|} \middle| j \in \mathcal{N}_i : c(i) \neq c(j) \middle| \right)^2.$$
 (12)

When practitioners must choose between a few different clusters, we recommend drawing the frontier in Equation (12) as a function of the bias $\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{|\mathcal{N}_i|}\Big|j\in\mathcal{N}_i:c(i)\neq c(j)\Big|\right)^2$ and the variance $\frac{1}{n^2}\sum_{k=1}^{K_n}n_k^2$, with multiplier over the variance $\xi_n=(\lambda\bar{\phi}_n^2/\bar{\psi})^{-1}$. Clusters that perform reasonably well compared to other clusters for a large set of values of ξ_n should be preferred for implementation.

4.1 Causal clustering: algorithm

Equation (12) is computationally difficult to optimize over a *large* space of clusters. In particular, the task of estimating the best clustering over a large class is challenging because the number of connections between different clusters enters non-linearly in Equation (12). First, we consider an objective as a function of the absolute (instead of squared) bias.

Corollary 4.1. Suppose that the conditions in Theorem 3.3 hold. Then as $K_n \to \infty$

$$\mathcal{B}_n(\mathcal{C}_n, \lambda) \le \lambda \bar{\phi}_n^2 \left(\frac{\xi_n}{n^2} \sum_{k=1}^{K_n} n_k^2 \left[1 + o(1) \right] + \frac{1}{n} \sum_{i=1}^n \frac{1}{|\mathcal{N}_i|} \left| \mathcal{N}_i \bigcap \left\{ j : c(i) \ne c(j) \right\} \right| \right). \tag{13}$$

Corollary 4.1 shows that Equation (13) with ξ_n as in Equation (11), as a function of the absolute instead of squared bias, is a surrogate (upper bound) loss of the objective function.

We interpret the objective in Equation (12) as minimizing the worst-case variance under constraints on the squared worst-case bias (whose dual depends on the multiplier λ). Whenever we are interested in the frontier that trade-offs the bias and variance over different values of ξ_n , Equation (12) or (13) have the same dual representation for (different) values of the multipliers ξ_n in each equation. Corollary 4.1 shows that we can choose the same ξ_n to obtain an upper bound on the original objective.

Following Corollary 4.1, we optimize over $(K_n, c(\cdot))$ as a function of a constant ξ_n ,

$$\frac{\xi_n}{n^2} \sum_{k=1}^{K_n} n_k^2 + \frac{1}{n} \sum_{i=1}^n \frac{1}{|\mathcal{N}_i|} \Big| j \in \mathcal{N}_i : c(i) \neq c(j) \Big|.$$
 (14)

Equation (14) solves a weighted min-cut problem with an additional *penalization* term that depends on the variance of the clusters' size. The optimization problem in Equation (14) is similar in spirit to, though different from, the minimum normalized-cut problem (e.g., Ling

and Strohmer, 2020; Shi and Malik, 2000), whose objective is $\sum_{k=1}^{K} \sum_{i:c(i)=k} |j \in \mathcal{N}_i : c(i) \neq c(j)|/\sum_{i:c(i)=k} |\mathcal{N}_i|$. Different from our proposal, standard min-cut problems use a different denominator (since the objective is not motivated by the bias of treatment effect estimators), and do not account for the additional variance component. Here, researchers should balance the bias and variance in the choice of the clusters. To the best of our knowledge, the problem in Equation (14) has not been studied before.

In the following lines we exploit Corollary 4.1 to find the clustering that minimizes Equation (14) over a large space of clusters. Let $\mathbf{V} = \operatorname{diag}(\mathbf{A}\mathbf{1}_n) = \operatorname{diag}(|\mathcal{N}_1(1)|, \dots, |\mathcal{N}_n(1)|)$. Define the left-normalized Laplacian

$$\mathbf{L} = \mathbf{V}^{-1} \mathbf{A}. \tag{15}$$

Given a set of K clusters (i.e., fixing the number of clusters), for any cluster mapping $c: \{1, \dots, n\} \mapsto \{1, \dots, K\}$, let $\mathbf{M}_c(K) \in \mathbb{R}^{n \times K}$ with

$$\mathbf{M}_{c,ik}(K) = 1\{c(i) = k\}, \quad i \in \{1, \dots, n\}, \quad k \in \{1, \dots, K\},$$

where $\mathbf{M}_{c}(K)$'s dimension depends on K. Here, $\mathbf{M}_{c,ik}(K) = 1$ if unit i is in cluster k.

Theorem 4.1. Let $tr(\cdot)$ denote the trace operator. c^* minimizes Equation (14) if and only if

$$c^{\star} \in \arg\max_{c:\{1,\dots,n\}\mapsto\{1,\dots,K\}} \operatorname{tr}\Big((n\mathbf{L} - \xi_n \mathbf{1}_n \mathbf{1}_n^T)\mathbf{M}_c(K)\mathbf{M}_c^T(K)\Big).$$

Proof of Theorem 4.1. See Appendix C.9.

Theorem 4.1 formalizes the optimization problem as a trace-optimization program for a fixed number of clusters K. Theorem 4.1 does not characterize a convex optimization program, but it provides a natural starting point to study convex relaxations of the proposed optimization problem. To obtain a convex relaxation, we relax the constraint on the matrix $\mathbf{X}(K) = \mathbf{M}_c(K)\mathbf{M}_c^T(K)$. We propose solving the following semi-definite programming (SDP) problem (for a given number of clusters K):

$$\max_{\mathbf{X}(K)} \operatorname{tr}(\mathbf{L}_{\xi_n} \mathbf{X}(K)), \quad \text{s.t.} \quad \operatorname{diag}(\mathbf{X}(K)) = \mathbf{1}_n, \ \mathbf{X}(K) \succeq 0, \quad \mathbf{L}_{\xi_n} = n\mathbf{L} - \xi_n \mathbf{1}_n \mathbf{1}_n^T.$$
 (16)

where Equation (16) defines a sequence of semi-definite optimization programs, each indexed by the number of clusters K. The main distinction between Equation (14), and Equation (16) is that the matrix $\mathbf{X}(K)$ must be positive-definite instead of a matrix with binary entries. Let $\hat{\mathbf{X}}(K)$ be the solution of (16), for given K, that can be obtained using off-the-shelf optimization routines. We then apply the K-means algorithm on the first K eigenvectors of $\hat{\mathbf{X}}(K)$ to retrieve the mapping c, whose properties are well studied in the literature (Von Luxburg, 2007). Finally, we compare solutions for different values of K and choose the clustering with the largest objective.

In summary, the complete algorithm (Algorithm 1) solves a sequence of semi-definite trace-optimization problems, each indexed by a different value of K, and reports the clustering (and corresponding number of clusters) that leads to the largest objective.

Equation (16) is a convex relaxation of the problem in Theorem 4.1 because it substitutes the original constraint on \mathbf{X} to contain binary entries with a semi-definite constraint. Such convex relaxations, together with K-means algorithm to retrieve the clusters, are common in the clustering literature and have been widely studied both from theoretical and numerical perspectives; see Hong et al. (2021) for a review.

Remark 8 (Spectral relaxation). Unlike the minimum normalized cut, there is no simple *spectral* relaxation of the optimization problem in Theorem 4.1, unless all clusters are equally sized. For the special case where all clusters are equal-sized, (16) can be relaxed to

$$\max_{\mathbf{U}} \operatorname{tr}(\mathbf{L}_{\xi_n} \mathbf{U}(K) \mathbf{U}^T(K)), \quad \text{s.t. } \mathbf{U}^T(K) \mathbf{U}(K) = \mathbf{I}_K,$$

where \mathbf{I}_{K} denotes the identity matrix of dimension K. We first symmetrize

$$\operatorname{tr}(\mathbf{L}_{\xi_n}\mathbf{U}(K)\mathbf{U}^T(K)) = \operatorname{tr}\left(\frac{\mathbf{L}_{\xi_n} + \mathbf{L}_{\xi_n}^T}{2}\mathbf{U}\mathbf{U}^T\right)$$

The solution to the above problem $\hat{\mathbf{U}}(K) \in \mathbb{R}^{n \times K}$ is given by the matrix of top-K eigenvectors of $(\mathbf{L}_{\xi_n} + \mathbf{L}_{\xi_n}^T)/2$. Then we can perform a constrained K-means algorithm with equal-sized clusters to recover the clusters (Bradley et al., 2000).

Algorithm 1 Causal Clustering

Require: Adjacency matrix \mathbf{A} , \underline{K} , \overline{K} smallest and largest number of clusters, ξ_n .

- 1: for $K \in \{\underline{K}, \cdots, K\}$ do
 - a: Solve Equation (16) and obtain $\hat{\mathbf{X}}(K)$ as the minimized of Equation (16)
 - b: Retrive the clusters c_K via K-means algorithm on the first K eigenvectors of $\hat{\mathbf{X}}(K)$
 - c: Compute the objective function corresponding to the chosen clustering in (14)
- 2: end for
- 3: **return** Clustering with the lowest objective function in (14).

5 Empirical illustration and numerical studies

In this section, we illustrate the properties of the procedure in two empirical applications, one using unique data from the Facebook friendship and messaging graphs and one using data from an experiment conducted in rural China by Cai et al. (2015). We provide further evidence supporting our theoretical analysis using simulated networks in Section 5.3.

5.1 Clustering on Facebook graphs

We evaluate our procedure on the universe of users using Facebook and Messenger.

5.1.1 Clustering algorithms, bias and variance

We consider two clustering algorithms implemented at scale on social networks owned by Meta: Louvain algorithm (Blondel et al., 2008), and Balanced Partitioning (Kabiljo et al., 2017). Louvain and Balanced Partitioning clustering produces a hierarchical clustering structure with a growing number of clusters. We consider three "types" of such algorithms, corresponding to three levels in the clustering structure hierarchy (i.e., different numbers of clusters), defined as Type 1, 2, and 3, respectively. For Louvain, higher-order types denote more clusters, whereas it is the opposite for Balanced Partitioning. For each clustering, we also report $\log(n/K_n)$, the log ratio of the number of clusters over the population size.

We consider two graphs owned by Meta. In the first graph, edges capture the strength of the friendship in the Facebook graph, and in the second graph, they capture connections based on messaging on Facebook. In both cases, the data was aggregated and de-identified. In each graph, edges are continuous variables. For each graph, we construct three adjacency matrices by setting the edges to be zero if below the 5^{th} , 10^{th} , and 50^{th} percentile value of the edges. We will refer to these graphs obtained as dense, moderate (mod), and sparse after thresholding. We also note that all graphs have a bounded maximum degree.

We report the bias and variance, with the variance weighted by a parameter ξ_n , defined respectively as

$$\frac{1}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_i|} \Big| \mathcal{N}_i \bigcap \Big\{ j : c(i) \neq c(i) \Big\} \Big|, \quad \frac{\xi_n}{n^2} \sum_{k=1}^{K_n} n_k^2.$$

5.1.2 Comparisons between different algorithms

Table 3 collects each of these algorithms' worst-case bias and variance and the number of clusters per individual. A larger number of clusters increases the bias but decreases the variance throughout all graphs. (The bias increases for sparser networks because the denominator

 $|\mathcal{N}_i|$ decreases.) Louvain algorithm dominates Balanced Partitioning uniformly in variance and bias, suggesting that practitioners may prefer Louvain over Balanced Partitioning.

We study different types of Louvain algorithms (each having a different number of clusters) in Figure 2. Figure 2 reports the worst-case mean squared error for different graphs, Louvain algorithms, and degrees of sparsity. For $\xi_n \approx 1$, the Louvain algorithm with the largest number of clusters (Type 3) dominates the other two algorithms in all but one case.

As ξ_n increases, Louvain clustering with the largest number of clusters (Type 3) is optimal for a dense graph but sub-optimal as the graph becomes more sparse. This result is intuitive: for denser networks, a larger number of clusters may best control the estimator's bias relative to the bias induced by other clustering algorithms. However, we observe that Type 1 is the most robust in terms of variance in the mean-squared error across different values of spillover effects. This is suggestive that Louvain clustering with the largest number of clusters (Type 1) may be preferred in various applications.

5.1.3 Comparison between Bernoulli and Cluster design

To conclude, we present when a cluster design with our preferred clustering (Louvain Type 1) should be preferred over a Bernoulli design. Using Theorem, and the dense Messaging graph, 3.6 for Louvain clustering (Type 1), for any value of ξ_n such that

$$\xi_n^{1/2} \le \bar{\xi}_n^{1/2}, \quad \bar{\xi}_n^{1/2} = 706,$$

we should run a cluster experiment instead of a Bernoulli design. Because $\xi_n = \bar{\psi}/\bar{\phi}_n^2$ for $\lambda = 1$, researchers should run a Cluster design if $\bar{\phi}_n^2 \geq \bar{\psi}/\bar{\xi}_n$. This implies that the researcher should run a cluster design if spillovers are larger than $\bar{\phi}_n \geq \bar{\psi}^{1/2}/706$. This comparison is suggestive that a cluster design with a Louvain clustering may be preferred over a Bernoulli design over a wide range of values of spillover effects (and outcomes variation $\bar{\psi}$). For binary outcomes, we should prefer cluster experiments for $\bar{\phi}_n \geq 0.003$.

In summary, our results shed light on using clustering algorithms for large-scale implementation on online platforms. These results suggest that Louvain clustering with possibly many clusters performs best in practice, and may often be preferred to a Bernoulli design. It confirms heuristic arguments in Karrer et al. (2021) that recommend Louvain clustering based on AA-tests.

Friendship	Type 1			Type 2		Type 3			
	dense	mod	sparse	dense	mod	sparse	dense	mod	sparse
		Ba	lanced F	Partitioni	ng Algor	rithm			
100 Bias	38.41	38.54	39.95	55.21	55.17	55.89	69.00	68.92	69.37
10000 Variance	9.76	9.76	9.85	0.30	0.30	0.30	0.01	0.01	0.01
$\log(n/K_n)$	14.41	14.37	14.17	10.95	10.91	10.70	7.48	7.44	7.24
			Lou	vain Algo	rithm				
100 Bias	0.17	3.64	16.55	0.01	2.34	12.43	0.01	2.29	12.17
10000 Variance	0.03	0.03	0.03	0.05	0.05	0.05	0.06	0.06	0.06
$\log(n/K_n)$	2.30	2.28	2.16	4.51	4.56	4.59	5.32	5.50	6.05
	Type 1								
Messaging		Type 1			Type 2	2		Type 3	
Messaging	dense	Type 1 mod	sparse	dense	Type 2	2 sparse	dense	Type 3 mod	sparse
Messaging	dense	mod	sparse	dense Partitioni	mod	sparse	-		sparse
Messaging 100 Bias	dense 17.26	mod	sparse		mod	sparse	-		sparse 39.06
		mod Ba	sparse lanced F	Partitioni	mod ng Algor	sparse	dense	mod	
100 Bias	17.26	mod Ba 18.10	sparse lanced F 22.57	Partitioni 26.94	mod ng Algor 27.62	sparse rithm 31.00	dense 37.06	mod 37.46	39.06
100 Bias 10000 Variance	17.26 97.65	mod Ba 18.10 97.65	sparse llanced F 22.57 97.71 15.76	Partitionii 26.94 3.05	mod ng Algor 27.62 3.05 12.55	sparse rithm 31.00 3.05	37.06 0.09	mod 37.46 0.09	39.06 0.09
100 Bias 10000 Variance	17.26 97.65	mod Ba 18.10 97.65	sparse llanced F 22.57 97.71 15.76	Partitionic 26.94 3.05 12.57	mod ng Algor 27.62 3.05 12.55	sparse rithm 31.00 3.05	37.06 0.09	mod 37.46 0.09	39.06 0.09
100 Bias 10000 Variance $\log(n/K_n)$	17.26 97.65 16.04	mod Ba 18.10 97.65 16.02	sparse lanced F 22.57 97.71 15.76 Lou	Partitionic 26.94 3.05 12.57 vain Algorithms	mod ng Algor 27.62 3.05 12.55 orithm	sparse rithm 31.00 3.05 12.30	37.06 0.09 9.10	mod 37.46 0.09 9.09	39.06 0.09 8.83

Table 3: Worst-case bias and variance for Balanced Partition Clustering and Louvain clusterings, and for two different graphs owned by Meta. Different types correspond to algorithms with an increasing number of clusters for Balanced Partition and a decreasing number of clusters for Louvain. Note that for Type 1 to Type 3 of Balanced partition, the number of clusters increases, while for Louvain algorithm, the number of clusters decreases.

5.2 Clustering in the field

Next, we present an application of a field experiment where the treatment consists of informing individuals to increase insurance take-up (Cai et al., 2015).

5.2.1 Data description

Cai et al. (2015) collected network information in 185 villages in rural China from 48 larger regions. We use network data collected by Cai et al. (2015) to study the properties of the proposed method, where we assume that two individuals are connected if at least one of the two indicates the other as a friend. Because we do not require information from end-line outcomes, we construct a network using information from surveyed individuals as well as their friends. The network has a total of 7649 nodes, once we also include individuals who are friends of surveyed individuals (but do not necessarily live in their same village or were

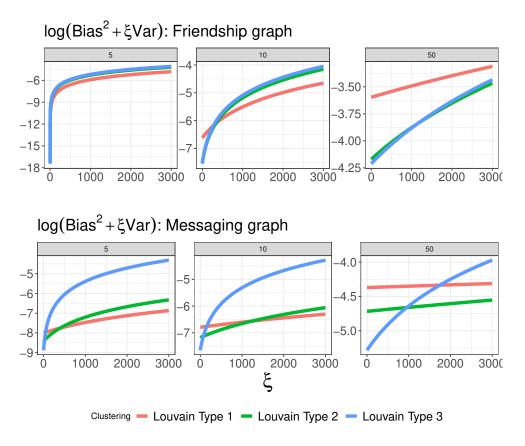


Figure 2: Clusters comparisons for Louvain clustering. Different Types correspond to different numbers of clusters (with Type 1 having the largest number of clusters). Different panels correspond to different graphs where two individuals are not connected if the connection (measured with a continuous variable) is below the 5^{th} , 10^{th} , 50^{th} percentile (dense, moderate, and sparse graph). The two graphs in the panels are Facebook friendship and Facebook messaging.

surveyed in the experiment). Individuals between villages present on average 50% of their connections *outside* their village. On the other hand, individuals in different regions (with 48 regions) have 99% of their connections within the same region. We use an adjacency matrix a "weak ties" adjacency matrix, where two individuals are connected if either indicates the other has a friend.

We construct a clustering in each of the 48 regions (since individuals are not connected between different regions). Clustering within each region is performed as in Algorithm 1, where we first estimate $\hat{\mathbf{X}}(K)$ via semi-definite programming, use K-means algorithm to retrieve the clusters from $\hat{\mathbf{X}}(K)$ and iterate to estimate the optimal number of clusters K.

5.2.2 Choosing the number of clusters

The left-hand side panel of Figure 3 reports the average number of estimated clusters, estimated by the proposed method divided by the population size in a given cluster. Different

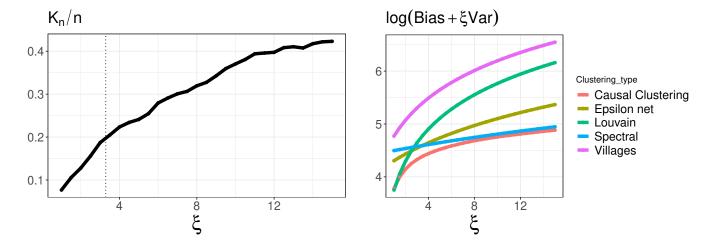


Figure 3: Example of a number of clusters as a function of ξ_n (left-panel, with dotted line corresponding to 3.2) and objective function in Theorem 4.1 for different clustering. Algorithm 1 corresponds to causal clustering. Data from Cai et al. (2015), where we report the average result across 47 regions in the dataset.

choices of ξ_n justify a different number of clusters. For $\xi_n = 1$, the number of clusters is 7% of the total population size, whereas for $\xi_n = 15$, the number of clusters is roughly half the population size.

To gain further intuition of its practical implication, take $\bar{\psi} = 0.24$ approximately equal to the outcomes' variance in Cai et al. (2015) and $\bar{\phi}_n = 0.27$ as in Table 2 in Cai et al. (2015). A conservative choice of ξ_n (i.e., a choice that favors a smaller bias) is approximately $\bar{\psi}/\bar{\phi}_n^2 = 3.29$. Even with such a conservative choice, the suggested number of clusters is large relative to the population size. In this case, the optimal number of clusters is around 15% of the overall population size, approximately 600 clusters with a surveyed sample size of 3600 individuals. This number is consistent (in scale) with the choice in the number of clusters in other applications in development, such as Egger et al. (2022), Alatas et al. (2012), but larger than the number of villages that we have in the application in Cai et al. (2015). This result is suggestive of the relevance of our method to optimally choose the number of clusters.

5.2.3 Comparison with other clustering methods

Next, we compare the procedure (denoted as "Causal Clustering") with the following alternative clustering algorithms: ε -net clustering as in Eckles et al. (2017) with $\varepsilon = 3$ as suggested in Eckles et al. (2017); spectral clustering with a fixed number of clusters equal to n/3, where n is the population size in a given region (note that spectral clustering do not optimize over the number of clusters); Louvain clustering with default parameters selected by the R-package igraph; clustering based on village identity of each individual (creating one

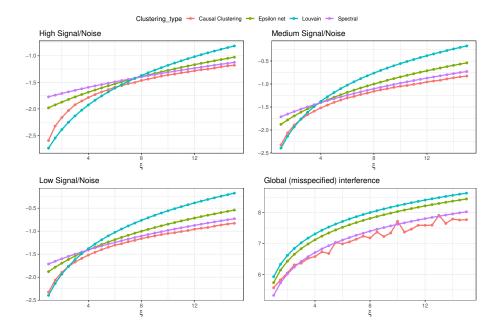


Figure 4: Mean-squared error (in logs) simulated by calibrating the model to data from Cai et al. (2015), averaged over 47 regions. The first three plots vary the variance of the residuals in the outcome model $\sigma^2 \in \{1/4, 1/2, 1\}$, and calibrating the remaining parameters to the model in Cai et al. (2015), Table 2, Column 4, where outcomes are functions of neighbors' treatments. The last plot calibrate the simulations to settings where the outcomes are functions of the neighbors' outcome violating Assumption 1, and $\sigma^2 = 1/4$.

additional cluster for those individuals whose village is missing in the data).

We contrast the objective function with alternative algorithms on the right-hand side of Figure 3. The proposed method achieves the smallest objective function across all competitors over a wide range of ξ_n , providing suggestive evidence that Algorithm 1 (with a semi-definite relaxation) works well in practice. For a smaller number of clusters, the method is closer to the Louvain clustering algorithm, while for a larger number of clusters, the objective of the algorithm is close to the objective of the spectral algorithm. Interestingly, clustering based on village identity leads to the largest loss function. This is because individuals are connected within and between villages in this application.

Finally, in Figure 4 (first three panels), we report the mean-squared error obtained by simulating the model in Cai et al. (2015) (Table 2, Column 4), which assumes that individual outcomes depend on neighbors' treatments, consistently with our Assumption 1. We vary the variance of the residuals $\sigma^2 \in \{1/4, 1/2, 1\}$ to emulate settings with high, medium, and low signal-to-noise ratios. Our method uniformly outperforms competitors regarding mean-squared error, except for a slight underperformance relative to the Louvain algorithm when the signal-to-noise ratio is particularly high, but not in the remaining settings.

In the last panel of Figure 4, we consider settings where the local interference assumption

is violated, and we calibrate our model to the specification in Cai et al. (2015) (Column 4, Table 5), where the individual outcome depends on the neighbors' outcomes. Although this is not the main specification in Cai et al. (2015), such calibration is useful to measure robustness to misspecification. We fix the residuals' variance to be $\sigma^2 = 1/4$, whereas the results are robust as we increase σ^2 . In this setup, we observe a larger mean-squared error of all methods, with the proposed method achieving the lowest mean-squared error.

5.3 Clustering with simulated networks

Next, we illustrate the numerical properties of the method using simulated networks.

We consider three data-generating processes for the network formation: a geometric network formation, the Albert Barabasi network, and Erdos-Renyi graph. The geometric network takes the form $A_{i,j} = 1\{|X_{i,1} - X_{j,1}|/2 + |X_{i,2} - X_{j,2}|/2 \le r_n\}$ where $r_n = \sqrt{4/2.75n}$ similarly to simulations in Leung (2020). Here, $X_{i,1}, X_{i,2}$ are drawn independently from a uniform distribution between [-1,1]. For the Albert-Barabasi network, we first draw n/5 edges uniformly according to the Erdos-Renyi graph with probabilities p = 10/n, and second, we draw sequentially connections of the new nodes to the existing ones with probability equal to the number of connections of each pre-existing node divided by the overall number of connections. The Erdos-Renyi graph has a probability of connection p = 2/n.

The proposed procedure uniformly leads to the lowest objective function.

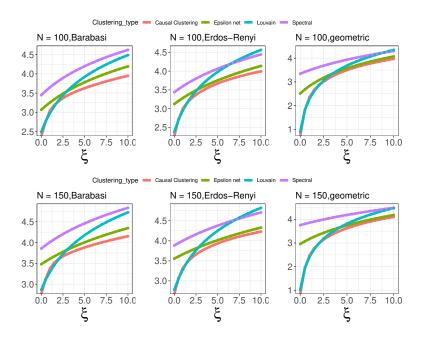


Figure 5: Objective function in Theorem 4.1 (in log scale) as a function of ξ over 100 replications for different network formation models. N denotes the size of the network.

6 Extensions

In this section, we present four main extensions. The first extension presents optimal clustering moving away from a finite population framework and allowing potential outcomes to be random variables. The second extension relaxes the ex-ante symmetry restriction on potential outcomes. The the third extension presents trimming estimators enlarging the class of estimators considered. The last extension studies designs with treatments assigned with different probabilities across clusters, possibly allowing the identification of estimands other than the global average treatment effect.

6.1 Random outcomes

While the finite population framework considered in Assumption 1 can be viewed as conditioning on potential outcomes, Assumption 2 may not be plausible for realizations of potential outcomes. For example, when the outcomes are binary, the potential outcomes can only take two values, hence violating both parts of Assumption 2. In these settings, we can re-interpret our approach by imposing Assumption 2 on the expected potential outcomes, which can take any values in [0,1].

To accommodate random outcomes, we can modify Assumption 1 by redefining $\mu_i(\mathbf{d})$.

Assumption 5 (Weaker version of Assumption 1). For $i \in \{1, \dots, n\}$,

$$\mathbb{E}[Y_i(\mathbf{d})] = \mu_i(\mathbf{d}_i, \mathbf{d}_{\mathcal{N}_i}), \quad \forall \mathbf{d} \in \{0, 1\}^n.$$

for some functions $\mu_i(1,\cdot) \in \mathcal{M}_{1,i}, \mu_i(0,\cdot) \in \mathcal{M}_{0,i}$ for some set of functions $\mathcal{M}_{1,i}, \mathcal{M}_{0,i}$.

Similarly, we can redefine the global average treatment effect as

$$\tau_{n,\mu} = \frac{1}{n} \sum_{i=1}^{n} (\mu_i(\mathbf{1}) - \mu_i(\mathbf{0})).$$

In this setting, the expression of the bias in Lemma 3.1 does not change since the potential outcomes $Y_i(\mathbf{d})$ are independent of the treatment assignments. However, the variance and MSE will be inflated due to the randomness. To make the problem tractable, we impose the following two assumption on the variance-covariance structure of potential outcomes.

Assumption 6 (Second moment of potential outcomes). For some non-decreasing and Lipschitz function $g: \mathbb{R} \to \mathbb{R}^+$, for any $i \in \{1, ..., n\}$ and $\mathbf{d} \in \{0, 1\}^n$,

$$\mathbb{E}[Y_i(\mathbf{d})^2] = g(\mathbb{E}[Y_i(\mathbf{d})])$$

Assumption 7 (Weak correlation among potential outcomes). Let $C(\mathbf{d})$ denote the correlation matrix of $(Y_1(\mathbf{d}), \ldots, Y_n(\mathbf{d}))$. Then, by letting $||\cdot||_{\text{op}}$ the operator norm,

$$\sup_{\mathbf{d} \in \{0,1\}^n} \|\mathbf{C}(\mathbf{d}) - \mathbf{I}\|_{\mathrm{op}} = o(1).$$

Assumption 6 holds for a variety of outcome distributions, including the Bernoulli distribution $(g(\mu) = \mu)$, Poisson distribution $(g(\mu) = \mu + \mu^2)$, Exponential distribution $(g(\mu) = \mu^2)$, χ^2 distribution $(g(\mu) = 2\mu + \mu^2)$, Gaussian distribution $(g(\mu) = \mu^2 + \sigma^2)$, and Log-normal distribution $(g(\mu) = \exp\{2\mu + 2\sigma^2\})$. Assumption 7 holds when $\{Y_i(\mathbf{d}) : \mathbf{d} \in \{0,1\}^n\}$ are independent or weak dependent across i. In particular, under the endogenous peer effects model (Bramoullé et al., 2009; Manski, 1993), this assumption is satisfied when the peer effect is small; see Appendix B for details.

Under these assumptions, we prove that the worst-case variance and MSE are both inflated by a constant that does not depend on the clustering. As a consequence, the objective function $\mathcal{B}_n^*(\mathcal{C}_n, \lambda)$ defined in Corollary 4.1 can be used to compare different clustering algorithms and generate optimal clustering.

Theorem 6.1. Let Assumptions 2, 3, 4, 5, 6, 7 hold, with $\mu_i(\cdot)$ as defined in Assumption 5. Further assume $|\psi_R| \ge |\psi_L|$. Then the worst-case bias is

$$\sup_{\mu \in \mathcal{M}} \left| \tau_{n,\mu} - \mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)] \right| = \bar{\phi}_n b_n(\mathcal{C}_n),$$

the worst-case variance is

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}[\hat{\tau}_n(\mathcal{C}_n)] \right)^2 \right] = \left(\frac{\bar{\psi}}{n^2} \sum_{k=1}^{K_n} n_k^2 + \frac{4g(\psi_R) - \bar{\psi}}{n} \right) (1 + o(1)),$$

and the worst-case MSE is

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu}[(\hat{\tau}_n(\mathcal{C}_n) - \tau_{n,\mu})^2] = \left(\mathcal{B}_n^*(\mathcal{C}_n, 1) + \frac{4g(\psi_R) - \bar{\psi}}{n}\right) (1 + o(1)).$$

Proof of Theorem 6.1. See Appendix C.10.

6.2 Relaxing the ex-ante symmetry

Assumption 2 imposes ex-ante symmetry in the sense that the range of potential outcomes and the size of spillover effect are identical across individuals. This excludes regression adjustment under which the range of potential outcomes differs across individuals (see Re-

mark 4) or heterogeneous spillover effects. To account for the heterogeneity, we consider the following relaxation of Assumption 2.

Assumption 8. The potential outcomes $\mu = (\mu_1, \dots, \mu_n) \in \mathcal{M} = \bigotimes_{i=1}^n \mathcal{M}_i$ where \mathcal{M}_i is the set such that $\mu_i(1,\cdot) \in \mathcal{M}_{1,i}, \mu_i(0,\cdot) \in \mathcal{M}_{0,i}$. For all $i \in \{1,\dots,n\}, d \in \{0,1\}$, the function classes $\mathcal{M}_{d,i}$ contains all functions satisfying

- (i) $\mu_i(d,\cdot) \in [\psi_{Li}, \psi_{Ri}], \forall \mu_i(d,\cdot) \in \mathcal{M}_{d,i} \text{ for some } -\infty < \psi_{Li} < \psi_{Ri} < \infty;$
- (ii) for all $\mathbf{d} \in \{0,1\}^{|\mathcal{N}_i|}$, for some (unknown) $\alpha_i \in [\underline{\alpha},1], \underline{\alpha} > 0$, with $\max_i \alpha_i = 1$,

$$\sup_{\mu_{i}(0,\cdot)\in\mathcal{M}_{0,i}} \left| \mu_{i}(0,\mathbf{d}) - \mu_{i}(0,\mathbf{0}) \right| = \bar{\phi}_{n} \frac{\alpha_{i}}{|\mathcal{N}_{i}|} \sum_{k\in\mathcal{N}_{i}} \mathbf{d}_{k},$$

$$\sup_{\mu_{i}(1,\cdot)\in\mathcal{M}_{1,i}} \left| \mu_{i}(1,\mathbf{d}) - \mu_{i}(1,\mathbf{1}) \right| = \bar{\phi}_{n} \frac{\alpha_{i}}{|\mathcal{N}_{i}|} \sum_{k\in\mathcal{N}_{i}} \left(1 - \mathbf{d}_{k} \right),$$
(17)

for some $\bar{\phi}_n \leq \min_i \{ \psi_{Ri} - \psi_{Li} \}$.

We can still derive the worst-case bias, variance, and MSE assuming the above under mild assumptions on (ψ_{Li}, ψ_{Ri}) .

Theorem 6.2. Let Assumptions 1, 3, 4, 8 hold. Further assume that $|\psi_{Ri}| \ge |\psi_{Li}|$ for all $i \in \{1, ..., n\}$, or $|\psi_{Li}| \ge |\psi_{Ri}|$ for all $i \in \{1, ..., n\}$. Let $\bar{\psi}_i = \max\{|\psi_{Ri}|, |\psi_{Li}|\}/2$ and assume that $\underline{\psi} \le (1/n) \sum_{i=1}^n \bar{\psi}_i \le \bar{\psi}$. for some constants $0 < \underline{\psi} < \bar{\psi} < \infty$ that does not vary with n. Then the worst-case bias is

$$\sup_{\mu \in \mathcal{M}} \left| \tau_{n,\mu} - \mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)] \right| = \bar{\phi}_n b_{n,\alpha}(\mathcal{C}_n),$$

where

$$b_{n,\alpha}(\mathcal{C}_n) = \frac{1}{n} \sum_{i=1}^n \frac{\alpha_i}{|\mathcal{N}_i|} \Big| \mathcal{N}_i \bigcap \Big\{ j : c(i) \neq c(i) \Big\} \Big|.$$

The worst-case variance is

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}[\hat{\tau}_n(\mathcal{C}_n)] \right)^2 \right] = \left\{ \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 \right\} (1 + o(1)),$$

and the worst-case MSE is

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} [(\hat{\tau}_n(\mathcal{C}_n) - \tau_{n,\mu})^2] = \left\{ \bar{\phi}_n^2 b_{n,\alpha}(\mathcal{C}_n)^2 + \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 \right\} (1 + o(1)).$$

Proof of Theorem 6.2. See Appendix C.11.

It is easy to show that similarly to what discussed in Section 4.1, the optimization program admits a semi-definite relaxation that depends on the values of α and $\bar{\psi}$.

6.3 Trimming estimators

To illustrate how our framework generalizes to alternative estimators, in this section we study properties of

$$\hat{\tau}_n^w(\mathcal{C}_n) = \frac{2}{\sum_{i=1}^n w_i} \sum_{i=1}^n w_i \Big[D_i Y_i - (1 - D_i) Y_i \Big], \ w_i \ge 0$$
 (18)

for arbitrary non-negative weights w as deterministic functions of the matrix \mathbf{A} and on the clustering \mathcal{C}_n (but not of the treatments or outcomes).⁸ For example, these weights may upweight units with many neighbors in the same cluster and down-weights units with few neighbors in the same cluster in the spirit of trimming estimators (Hayes and Moulton, 2017; Leung, 2023). We show how our framework extends to estimators different from the difference in means estimators, provide a characterization of their bias and variance as in previous sections, and an algorithmic procedure to optimize over the weights w and the clustering \mathcal{C}_n .

Theorem 6.3. Let Assumptions 1, 2, 3, 4 hold. Consider an estimator $\hat{\tau}_n^w$, as in Equation (18). Then as $n \to \infty$,

$$\sup_{\mu \in \mathcal{M}} \left| \tau_{n,\mu} - \mathbb{E}_{\mu} [\hat{\tau}_n^w(\mathcal{C}_n)] \right| = \left(\bar{\phi}_n b_n^w(\mathcal{C}_n) + (\psi_R - \psi_L) \sum_{i=1}^n \left| \frac{w_i}{\|w\|_1} - \frac{1}{n} \right| \right) \cdot (1 + o(1))$$

where

$$b_n^w(\mathcal{C}_n) = \sum_{i=1}^n \frac{w_i}{||w||_1} \frac{1}{|\mathcal{N}_i|} \Big| \mathcal{N}_i \bigcap \Big\{ j : c(i) \neq c(j) \Big\} \Big|.$$

If, further, $w_i \leq \bar{w}$ and $||w||_1 \geq \underline{w}n$ for some constants $0 < \underline{w} < \bar{w} < \infty$ that do not vary with n. Then, as $K_n \to \infty$,

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} [\hat{\tau}_{n}^{w}(\mathcal{C}_{n})] \right)^{2} \right] = \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} w_{i} \right)^{2} \cdot \bar{\psi}(1 + o(1)).$$

Proof of Theorem 6.3. See Appendix C.12.

⁸The restriction that the weights do not depend on the treatments is imposed for simplicity since otherwise, correlations may also depend on the correlations between the weights. The focus on difference in means estimators instead of inverse probability weights estimators is motivated by their robustness to poor overlap.

Theorem 6.3 characterizes the worst-case bias and variance of the trimming estimator. Following the discussion for the difference in means estimator, this result suggests a weighted objective function

$$\mathcal{B}_{n}^{*}(\mathcal{C}_{n}, w, \lambda) = \bar{\psi} \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} w_{i} \right)^{2} + \lambda \left(\bar{\phi}_{n} b_{n}^{w}(\mathcal{C}_{n}) + (\psi_{R} - \psi_{L}) \sum_{i=1}^{n} \left| \frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right| \right)^{2}.$$

$$(19)$$

For the difference in means estimator, the objective function $\mathcal{B}_n^*(\mathcal{C}_n, \lambda)$ defined in Theorem 3.3 can be interpreted as the worst-case MSE, up to 1 + o(1) terms, as implied by Theorem 3.4. Unfortunately, this exact equivalence no longer holds for general trimming estimators because the worst-case bias and variance are achieved by different configurations of potential outcomes. In fact, we can show that the worst-case MSE is given by the maximum of a quadractic function in the vectors $(\mu_1(\mathbf{1}), \dots, \mu_n(\mathbf{1}))$ and $(\mu_1(\mathbf{0}), \dots, \mu_n(\mathbf{0}))$ over the constraint defined by Assumption 2 (i); see Remark 10 in Appendix C.13 for details. Nevertheless, we can show that the equivalence holds up to a constant.

Theorem 6.4. Under the conditions in Theorem 6.3, with $w_i \leq \bar{w}$ and $||w||_1 \geq \underline{w}n$ for some constants $0 < \underline{w} < \bar{w} < \infty$ that do not vary with n,

$$1/4 \leq \liminf_{K_n \to \infty} \frac{\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu}[(\hat{\tau}_n^w(\mathcal{C}_n) - \tau_{n,\mu})^2]}{\mathcal{B}_n^*(\mathcal{C}_n, w, 1)} \leq \limsup_{K_n \to \infty} \frac{\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu}[(\hat{\tau}_n^w(\mathcal{C}_n) - \tau_{n,\mu})^2]}{\mathcal{B}_n^*(\mathcal{C}_n, w, 1)} \leq 1.$$

Proof of Theorem 6.3. See Appendix C.13.

Theorem 6.4 justifies that the objective function $\mathcal{B}_n^*(\mathcal{C}_n, w, 1)$ is a reasonable proxy for the worst-case MSE – its optimal solution yields a clustering whose worst-case MSE is no more than four times the optimal worst-case MSE.

As with Section 4, to obtain the frontier that trades off the worst-case bias and variance, we can remove the square in the second term and optimize the following proxy objective for a range of ξ_n :

$$\frac{\xi_n}{\|w\|_1^2} \sum_{k=1}^{K_n} \left(\sum_{i:c(i)=k} w_i \right)^2 + \sum_{i=1}^n \frac{w_i}{\|w\|_1} \frac{1}{|\mathcal{N}_i|} \left| \mathcal{N}_i \bigcap \left\{ j : c(i) \neq c(j) \right\} \right|, \tag{20}$$

where the term $(\psi_R - \psi_L) \sum_{i=1}^n \left| \frac{w_i}{\|w\|_1} - \frac{1}{n} \right|$ is not kept because it does not depend on the clustering. The program admits a semi-definite relaxation of the form

$$\max_{\mathbf{X}(K)} \operatorname{tr}(\mathbf{L}_{\xi_n}^w \mathbf{X}(K)), \quad \text{s.t.} \quad \operatorname{diag}(\mathbf{X}(K)) = \mathbf{1}_n, \ \mathbf{X}(K) \succeq 0, \quad \mathbf{L}_{\xi_n}^w = ||w||_1 \mathbf{L}^w - \xi_n w w^\top, \quad (21)$$

where $\mathbf{L}_{i,j}^w = w_i \mathbf{L}_{i,j}$.

It is possible to optimize sequentially over the weights by first, for given weights w optimizing over the clustering, and for given clustering, optimizing over the weights w. Optimization over the weights can be solved as a fractional program (Bitran and Novaes, 1973). The approximately optimal clustering for given weights w can be obtained via semi-definite programming.

Algorithm 2 presents details. In summary, Theorem 6.3 shows how our insights in the characterization of the worst-case bias and variance more broadly apply to other estimators.

Algorithm 2 Causal Clustering with trimming estimators

Require: Adjacency matrix \mathbf{A} , $\underline{\mathbf{K}}$, $\overline{\mathbf{K}}$ smallest and largest number of clusters, ξ_n , number of iterations T

- 1: Initialize $w_i^0=1$ for all $i\in\{1,\cdots,n\}$
- 2: for $t \in \{0, \cdots, T\}$ do
- 3: for $K \in \{\underline{K}, \cdots, \bar{K}\}$ do
 - a: Solve Equation (21) and obtain $\mathbf{X}(K)$ as the minimized of Equation with weights (21) under a semi-definite relaxation on $\mathbf{X}(K) \succeq 0$, with weights w^t
 - b: Retrieve the clusters c_K via K-means algorithm on the first K eigenvectors of $\hat{\mathbf{X}}(K)$
 - c: Compute the objective function corresponding to the chosen clustering in (21)
 - d: Define \mathcal{C}_n^t the clustering with lowest objective in Equation (21)
- 4: end for
- 5: Define w^* the weights with lowest objective in Eq. (19) via fractional programming
- 6: Define $w^{t+1} \leftarrow w^*$
- 7: end for

return Clustering C_n^T and weights w^{T+1}

6.4 Saturation designs

In this section, we study settings where individuals in a given cluster are assigned treatments with different probabilities across clusters, i.e., saturation experiments. For the sake of brevity, we focus on settings where the researcher must choose between two treatment probabilities only, whereas our discussion applies to more than two treatment probabilities.

Assumption 9 (Treatment assignments). Suppose that for all $i \in \{1, \dots, n\}$,

$$D_i|\mathbf{A}, \{Y_i(\mathbf{d})\}_{i\in\{1,\dots,n\},\mathbf{d}\in\{0,1\}^n} \sim \text{Bern}(p_{c(i)}), \quad P(p_{c(i)}=q_0) = P(p_{c(i)}=q_1) = 1/2$$

where for some (q_0, q_1) , $0 \le q_0 < 0.5 < q_1 \le 1, q_0 + q_1 = 1$, and p_1, \dots, p_{K_n} are independent.

Assumption 9 generalizes the cluster design to designs with arbitrary cluster-level treatment probabilities. In particular, a cluster design has $q_0 = 0$ and $q_1 = 1$. We assume that

 $q_0 + q_1 = 1$ to ensure the marginal treatment probability for each unit remains 1/2 and hence the same estimator can be used:

$$\hat{\tau}_n(\mathcal{C}_n) = \frac{2}{n} \sum_{i=1}^n \left[Y_i D_i - Y_i (1 - D_i) \right]$$

denoting a difference between treated and control units, reweighted by the individual treatment probability, similar to the difference in means estimator studied in previous sections.

Theorem 6.5. Suppose that Assumptions 1, 2, 3, 4 hold, and treatments are assigned as in Assumption 9. Then as $K_n \to \infty$, the worst-case bias is

$$\sup_{\mu \in \mathcal{M}} \left| \mathbb{E}[\hat{\tau}_n^q(\mathcal{C}_n)] - \tau_{n,\mu} \right| = \bar{\phi}_n \left\{ b_n(\mathcal{C}_n) + 4q_1 q_0 (1 - b_n(\mathcal{C}_n)) \right\}, \tag{22}$$

the worst-case variance is

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}\left[\left(\mathbb{E}[\hat{\tau}_n^q(\mathcal{C}_n)] - \hat{\tau}_n\right)^2\right] = (q_1 - q_0)^2 \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} [\bar{\psi} + o(1)], \tag{23}$$

and the worst-case MSE is the sum of the right-hand side of (22) and (23).

Theorem 6.5 characterizes the worst-case bias, variance, and MSE for estimating the global treatment effect under a saturation design. The bias depends on an additional bias component with respect to Lemma 3.1 that arises from possibly assigning individuals in the same cluster to different treatments. The bias under a saturation design increases because individuals in the same clusters are not all assigned to the same treatment status. On the other hand, the variance decreases because treatments are not necessarily perfectly correlated in the same cluster. For given treatment probabilities (q_1, q_0) with $q_1 + q_0 = 1$, and given clustering algorithms, researchers can compare such algorithms by studying their worst-case bias, variance, or MSE. In practice, if researchers are mostly concerned about the bias of the estimated overall treatment effects, cluster experiments are recommended.

In conclusion, Theorem 6.5 shows how our characterization of the bias and variance can be extended to more complex designs.

Remark 9 (Estimating spillover effects). Whereas we focus here on the overall effect for their relevance in many applications, such as online experiments (Karrer et al., 2021), saturation experiments can be useful to study other estimands of interest, such as direct and spillover effects (Baird et al., 2018). In particular, suppose researchers are interested in the estimand (with a corresponding estimator)

$$\tau_n^s = \frac{1}{n} \sum_{i=1}^n \mu_i(1, \mathbf{1}) - \mu_i(1, \mathbf{0}), \quad \hat{\tau}_n^s(\mathcal{C}_n) = \frac{2}{n} \sum_{i=1}^n \left[\frac{Y_i D_i 1\{p_c(i) = q_1\}}{q_1} - \frac{Y_i D_i 1\{p_c(i) = q_0\}}{q_0} \right] \quad (24)$$

denoting the contrast between potential outcomes under treatment when switching the treatment status of their friends from one to zero. The estimator compares average outcomes between treated units in clusters with larger and lower treatment probability. It is easy to show that the tools developed in this paper allow us to characterize the bias and variance of the estimator in Equation (24) relative to the estimand in the same equation. In particular, results similar to those in Theorem 6.5 for the overall treatment effect can also apply to other estimands (spillover effects in Equation 24, direct effects, and other forms of spillover effects) in the presence of saturation experiments discussed in the current subsection.

7 Recommendations for practice

We conclude with a summary of our method and explicit recommendations for practice.

Choice of the adjacency matrix The choice of the adjacency matrix must depend on researchers' prior knowledge of which dimension spillovers propagate over, as, for example, in Cai et al. (2015). Our framework directly extends to settings where researchers only have some prior distribution on the network as in Breza et al. (2020). In this case, researchers can compute the *expected* bias and variance over the network distribution by taking the expected value of the expressions of the bias presented in Section 3 (see Remark 7).

Choosing the range of magnitude for the spillover effects Similarly to standard power analysis (e.g. Baird et al., 2018), our method with $\lambda = 1$ also depends on the choice of $\xi_n = (\bar{\phi}_n^2/\bar{\psi})^{-1}$ (the size of spillover effects $\bar{\phi}_n$ relative to the outcomes' largest squared deviation $\bar{\psi}$). In our empirical applications, we observe that certain clustering algorithms uniformly outperform others for a large range of values of ξ_n , suggesting that studying clustering over ranges of ξ_n can be informative.

To choose such a range of values, our recommended choice for $\bar{\psi}$ is to consider values $\bar{\psi} = c\bar{\sigma}^2, c \in [1,4]$ and $\bar{\sigma}^2$ is the baseline variance of the residuals after removing the covariate adjustment, and c is a constant between one to four. Algorithm 3 presents details.

The choice of $\bar{\phi}_n$ can be based on spillover effects observed in previous experiments, in the spirit of minimum detectable effects (Baird et al., 2018), or using a priori bound on the magnitude of the spillover effects.

⁹To gain further intuition, let $\lambda = 1$. Let $\bar{\mu}_i$ be a prediction for $\mu_i(\mathbf{0})$ as in Remark 4 and consider an estimator as in Equation (4). When using regression adjusted estimators, we have $\bar{\psi} = \left(\mu_i(\mathbf{1}) - \bar{\mu}_i + \mu_i(\mathbf{0}) - \bar{\mu}_i\right)^2$. By approximating $(\mu_i(\mathbf{d}) - \bar{\mu}_i)^2 \approx \bar{\sigma}^2$, we can write $\bar{\psi} \leq 4\bar{\sigma}^2$.

Choosing between a Cluster or Bernoulli design Given the range of values of ξ_n , and the choice of the network, Theorem 3.6 provides a rule of thumb to choose between a cluster or Bernoulli design. Table 1 suggests a rule of thumb $\bar{\phi}_n \sqrt{K_n} > 2.3$ for outcomes bounded between minus one and one. Figure 2 provides a wider and specific range of values of the minimum spillover effects to run cluster experiments.

Choosing the optimal clusters Finally, once researchers decide to run a clustering experiment, Algorithm 1 provides an explicit algorithm to estimate the optimal clusters via semi-definite programming, choosing both the clustering and the number of clusters.

Algorithm 3 Practical choice of range of tuning parameter ξ_n

Require: Baseline covariates Z_1, \dots, Z_n

- 1: Estimate $\bar{\mu}_i$ by regressing baseline outcomes on covariates Z
- 2: Estimate $\bar{\sigma}^2$ the variance of the residuals from this regression
- 3: Consider the range of values $\bar{\psi} \in [\bar{\sigma}^2, 4\bar{\sigma}^2]$
- 4: if past experiments are available then
- 5: Use ϕ_n from previous experiments
- 6: else
- 7: Consider a range of values of plausible spillover effects
- 8: end if

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A Notation

Table 4: Notation.

Description	Mathematical Formulation
Estimand	$ au_{n,\mu} = \frac{1}{n} \sum_{i=1}^{n} \mu_i(1) - \mu_i(0)$
Spillovers' effects size	$ar{\phi}_n$
Neighbors	\mathcal{N}_i
Maximum degree	$\mathcal{N}_{n,\max} = \max_i \mathcal{N}_i $
Treatments	$D_1,\cdots,D_n,D_i\in\{0,1\}$
Cluster's partition and size	\mathcal{C}_n
Number of clusters	K_n
Cluster's groups	$c(i) \in \{1, \cdots, K_n\}$
Cluster's assignment	$D_i = 1\{\tilde{D}_{c(i)} = 1\}, \tilde{D}_{c(i)} \sim \text{Bern}(1/2)$
Cluster's estimator	$\hat{\tau}(\mathcal{C}_n) = \frac{2}{n} \sum_{i=1}^n Y_i(2D_i - 1)$
Cluster's bias	$\bar{\phi}_n b_n(\mathcal{C}_n) = \frac{\bar{\phi}_n}{n} \sum_{i=1}^n \frac{1}{ \mathcal{N}_i } \left \mathcal{N}_i \bigcap \{j : c(i) \neq c(j)\} \right $
Bernoulli design	$\mathcal{C}_{\mathrm{B},n}$

B Endogenous peer effects

Following models in Manski (1993), let

$$Y_i(\mathbf{d}) = \alpha + \beta_n \mathbf{d}_i + \kappa_n \frac{\sum_{j \neq i} \mathbf{A}_{i,j} \mathbf{d}_j}{\sum_{j \neq i} \mathbf{A}_{i,j}} + \gamma_n \frac{\sum_{j \neq i} \mathbf{A}_{i,j} Y_i(\mathbf{d})}{\sum_{j \neq i} \mathbf{A}_{i,j}} + \varepsilon_i, \quad \beta_n, \kappa_n, \gamma_n \in [-\bar{\phi}_n, \bar{\phi}_n], \bar{\phi}_n \in (-1, 1),$$

for some (deterministic) ε_i independent of **d**. By (15), we can rewrite it as (recall that **L** defines the left-normalized Laplacian in Equation (15))

$$Y_i(\mathbf{d}) = \alpha + \beta_n \mathbf{d}_i + \kappa_n \sum_{j \neq i} \mathbf{L}_{i,j} \mathbf{d}_j + \gamma_n \sum_{j \neq i} \mathbf{L}_{i,j} Y_i(\mathbf{d}) + \varepsilon_i.$$

Assuming **A** is connected (Eq (6) in Bramoullé et al., 2009), for arbitrary G, and letting $\bar{\mathbf{d}}_i^A = \sum_{j \neq i} \mathbf{L}_{i,j} \mathbf{d}_j$,

$$Y_{i}(\mathbf{d}) = \alpha_{n,i} + \beta_{n}\mathbf{d}_{i} + \kappa_{n}\bar{\mathbf{d}}_{i}^{A} + \gamma_{n}\left\{\sum_{g=0}^{G-1}\gamma_{n}^{g}\mathbf{L}^{g+1}(\beta_{n}\mathbf{d} + \kappa_{n}\bar{\mathbf{d}}^{A}) + \underbrace{\gamma_{n}^{G}\sum_{g=0}^{\infty}\gamma_{n}^{g}\mathbf{L}^{g+G+1}(\beta_{n}\mathbf{d} + \kappa_{n}\bar{\mathbf{d}}^{A})}_{\text{Effect of }G \text{ closest friends}} + \underbrace{\gamma_{n}^{G}\sum_{g=0}^{\infty}\gamma_{n}^{g}\mathbf{L}^{g+G+1}(\beta_{n}\mathbf{d} + \kappa_{n}\bar{\mathbf{d}}^{A})}_{\text{Approximation error from }G+1 \text{ neighbors' effects}}\right\} + \tilde{\epsilon}_{i},$$

Interference from higher order friends

where
$$\alpha_n = (\alpha_{n,1}, \dots, \alpha_{n,n})' = \alpha (\mathbf{I} - \gamma_n \mathbf{L})^{-1} \mathbf{1}$$
 and $\tilde{\epsilon} = (\tilde{\epsilon}_1, \dots, \tilde{\epsilon}_n)' = (\mathbf{I} - \gamma_n \mathbf{L})^{-1} \epsilon$.

Observe that the additional term that depends on higher order interference, multiplies by a factor $\gamma_n\beta_n+\gamma_n\kappa_n$. By letting each of these coefficients β_n , κ_n , $\gamma_n \propto \bar{\phi}_n$, Assumption 1 holds up to an order o(1/n) (see Remark 2) for an adjacency matrix \mathbf{A}_G where two individuals are connected if they are friends up to order G, provided that $\bar{\phi}_n^{G+1} \sum_{g=0}^{\infty} \bar{\phi}_n^g \mathbf{L}^{g+G+1} \mathbf{1} = o(1/n)$. This example illustrates that the approximation error due to local interference decreases exponentially fast in G as $\bar{\phi}_n = o(1)$. However, in settings where researcher use an adjacency matrix \mathbf{A}_G (G > 1), we require stronger sparsity restrictions for our local asymptotic framework to hold (Assumption 3), with $\bar{\phi}_n G \mathcal{N}_{n,\text{max}}^{2G} = o(1)$, where $\mathcal{N}_{n,\text{max}}$ is the maximum degree under the original adjacency matrix \mathbf{A} .

Finally, we show that Assumption 7 holds under this model if γ_n is small.

Lemma B.1. Assume that **A** is connected and $\epsilon_1, \ldots, \epsilon_n$ are independent with $Var(\epsilon_i) = \sigma^2 < \infty$. Then Assumption 7 holds if

$$\gamma_n \sqrt{\mathcal{N}_{n,\max}} = o(1).$$

Proof of Lemma B.1. See Appendix C.15.

C Proofs

Throughout the proofs, expectations are conditional on the adjacency matrix \mathbf{A} . Recall the notation in Table 4.

C.1 Auxiliary lemmas

In the following lines, we study the variance of the estimator $\hat{\tau}_n(\mathcal{C}_n)$. Observe that

$$\mathbb{E}_{\mu}\left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)]\right)^2\right] = \frac{4}{n^2} \sum_{i,j} \operatorname{Cov}\left(\mu_i(D_i, \mathbf{D}_{-i})[2D_i - 1], \mu_j(D_j, \mathbf{D}_{-j})[2D_j - 1]\right).$$

Lemma C.1 (Zero covariances). Suppose that Assumptions 1, 4 hold. For all $i \in \{1, \dots, n\}$

$$\operatorname{Cov}\Big(\mu_i(D_i, \mathbf{D}_{-i})\Big[2D_i - 1\Big], \mu_j(D_j, \mathbf{D}_{-j})\Big[2D_j - 1\Big]\Big) = 0, \quad \forall j \notin B_i \cup G_i,$$

where

$$B_i = \left\{ v \in \{1, \dots, n\} : \text{ either } c(v) = c(i) \text{ or } c(v) = c(v'), \text{ for some } v' \in \mathcal{N}_i \right\}.$$

$$G_i = \left\{ g \in \{1, \dots, n\} : \mathcal{N}_g \cap B_i \neq \emptyset \right\}$$

Proof of Lemma C.1. See Appendix C.3.

Lemma C.1 states that two realized outcomes have zero covariance if two individuals (i) are in two different clusters, such that none of the two clusters contains a friend of the other individual, and (ii) are not friends or share a common friend (set), and if there is no friend of j in a cluster that contains a friend of i. Lemma C.1 is equivalent to state that $\mu_i(D_i, \mathbf{D}_{-i})[2D_i - 1], \mu_j(D_j, \mathbf{D}_{-j})[2D_j - 1]$ have zero covariance if $B_i \cap B_j = \emptyset$.¹⁰ Next, we analyze the covariances for the remaining units.

Lemma C.2 (Non-zero Covariances). Suppose Assumptions 1, 2, 4 hold. Then

$$\left| \operatorname{Cov} \left(\mu_i(D_i, \mathbf{D}_{-i}) \left[2D_i - 1 \right], \mu_j(D_j, \mathbf{D}_{-j}) \left[2D_j - 1 \right] \right) \right| = \mathcal{O} \left(\bar{\phi}_n b_n(\mathcal{C}_n) \right) \quad \forall j : c(j) \neq c(i).$$
 (25)

In addition, for c(i) = c(j),

$$\operatorname{Cov}\left(\mu_{i}(D_{i}, \mathbf{D}_{-i})[2D_{i} - 1], \mu_{j}(D_{j}, \mathbf{D}_{-j})[2D_{j} - 1]\right)$$

$$= \frac{1}{4}\left(\mu_{i}(\mathbf{1}) + \mu_{i}(\mathbf{0})\right)\left(\mu_{j}(\mathbf{1}) + \mu_{j}(\mathbf{0})\right) + \mathcal{O}\left(\bar{\phi}_{n}b_{n}(\mathcal{C}_{n})\right).$$
(26)

Proof. See Appendix C.4.

Lemma C.2 characterizes the covariance between individuals in different clusters (Equation 25) and individuals in the same cluster (Equation 26). For individuals in different clusters, the covariance is of the same order of the bias, whereas for individuals in the same cluster, the covariance is $\mathcal{O}(1)$. The component $\frac{1}{4}(\mu_i(1) + \mu_i(0))(\mu_j(1) + \mu_j(0))$ captures the covariance between individuals in the same clusters up-to a factor of order $\bar{\phi}_n b_n(\mathcal{C}_n)$. The covariance between individuals in different clusters is zero if there are no individuals with neighbors in a different cluster since, in this case, the within-cluster covariance captures all the covariances between individuals.

C.2 Proof of Lemma 3.1

We prove the equality by proving inequality on both sides.

¹⁰By definition, $B_i \cap B_j \neq \emptyset$ implies the existence of $i' \in \{i\} \cup \mathcal{N}_i, j' \in \{j\} \cup \mathcal{N}_j$, and k such that c(i') = c(k) = c(j'). Thus, $j' \in B_i$. If j' = j, then $j \in B_i$; otherwise, $j' \in G_i$. For the converse, first note that $j \in B_i$ implies that $j \in B_i \cap B_j \neq \emptyset$ since $j \in B_j$ for any j. If $j \in G_i \setminus B_i$, then there exists $j' \in \mathcal{N}_j$ such that $j' \in B_i$. Since $j' \in B_j$, $j' \in B_i \cap B_j \neq \emptyset$.

Upper bound (\leq case) We have

$$\sup_{\mu \in \mathcal{M}} \left| \mathbb{E}_{\mu}[\hat{\tau}_{n}] - \tau_{n,\mu} \right| = \sup_{\mu \in \mathcal{M}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1}) | D_{i} = 1 \right] - \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{0}) | D_{i} = 0 \right] \right|$$

$$\leq \sup_{\mu(1,\cdot) \in \otimes_{i=1}^{n} \mathcal{M}_{1,i}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1}) | D_{i} = 1 \right] \right|$$

$$+ \sup_{\mu(0,\cdot) \in \otimes_{i=1}^{n} \mathcal{M}_{0,i}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{0}) | D_{i} = 0 \right] \right|.$$

The last inequality follows from the triangular inequality. By Assumption 2 (ii), we write

$$\sup_{\mu(1,\cdot)\in\otimes_{i=1}^{n}\mathcal{M}_{1,i}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1}) | D_{i} = 1 \right] \right| = \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \mathbb{E} \left[\sum_{k \in \mathcal{N}_{i}} (1 - D_{k}) \Big| | D_{i} = 1 \right]$$

$$= \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \mathbb{E} \left[|\mathcal{N}_{i}| - \sum_{k \in \mathcal{N}_{i}} D_{k} \Big| D_{i} = 1 \right]$$

$$= \frac{\bar{\phi}_{n}}{2n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \Big| j \in \mathcal{N}_{i} : c(i) \neq c(j) \Big|,$$

$$(27)$$

where the last inequality follows from the fact that each unit not assigned to the same cluster of i has treatment probability equal to 1/2 under Assumption 4. The same reasoning applies to $\sup_{\mu(0,\cdot)\in\otimes_{i=1}^n\mathcal{M}_{0,i}}\left|\frac{1}{n}\sum_{i=1}^n\mathbb{E}\left[\mu_i(D_i,\mathbf{D}_{-i})-\mu_i(\mathbf{0})|D_i=0\right]\right|$.

Lower bound (\geq case) To prove the above upper bound is achievable, we construct potential outcomes as follows:

$$\mu_i(1, \mathbf{d}_{-i}) = \mu_i(0, \mathbf{d}_{-i}) = \begin{cases} \psi_R - \bar{\phi}_n \frac{1}{|\mathcal{N}_i|} \sum_{k \in \mathcal{N}_i} (1 - \mathbf{d}_k) & \text{if } |\psi_R| \ge |\psi_L|, \\ \psi_L + \bar{\phi}_n \frac{1}{|\mathcal{N}_i|} \sum_{k \in \mathcal{N}_i} \mathbf{d}_k & \text{otherwise} \end{cases}$$
(28)

Since $0 \le \bar{\phi}_n \le \psi_R - \psi_L$, for $d \in \{0, 1\}$, $\mu_i(d, \cdot) \in [\psi_L, \psi_R]$. Thus, $\mu_i(d, \cdot) \in \mathcal{M}_i$. Note that in both cases, $\mu_i(1, \mathbf{d}_{-i}) - \mu_i(1, \mathbf{1})$ and $\mu_i(0, \mathbf{d}_{-i}) - \mu_i(0, \mathbf{0})$ have different signs. Thus, we have

$$\sup_{\mu \in \mathcal{M}} \left| \mathbb{E}_{\mu}[\hat{\tau}_{n}] - \tau_{n,\mu} \right| = \sup_{\mu \in \mathcal{M}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1}) | D_{i} = 1 \right] - \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{0}) | D_{i} = 0 \right] \right|$$

$$\geq \left| \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \mathbb{E} \left[\sum_{k \in \mathcal{N}_{i}} (D_{k} - 1) | D_{i} = 1 \right] - \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \mathbb{E} \left[\sum_{k \in \mathcal{N}_{i}} D_{k} | D_{i} = 0 \right] \right|$$

$$= \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \mathbb{E} \left[\sum_{k \in \mathcal{N}_{i}} (1 - D_{i}) | D_{i} = 1 \right] + \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \mathbb{E} \left[\sum_{k \in \mathcal{N}_{i}} D_{k} | D_{i} = 0 \right],$$

where we inverted the sign in the last expression using the absolute value in the second expression. The proof completes following the same steps for the upper bound.

C.3 Proof of Lemma C.1

Let $C_i = \{c(v) : v \in B_i\}$, and $G_i = \{g \in \{1, \dots, n\} : \mathcal{N}_g \cap B_i \neq \emptyset\}$. Observe that we can write Lemma C.1 equivalently as stating that

$$\operatorname{Cov}\left(\mu_i(D_i, \mathbf{D}_{-i}) \left[2D_i - 1 \right], \mu_j(D_j, \mathbf{D}_{-j}) \left[2D_j - 1 \right] \right) = 0, \quad \forall j \notin \{B_i \cup G_i\}.$$

We, therefore, prove the above expression. By definition of B_i , we have (a) $c(v') \in C_i$ iff $v' \in B_i$, and (b) $C_i = \{c(v) : v \in \{i\} \cup \mathcal{N}_i\}$. By the local interference assumption (Assumption 1), $\mu_i(D_i, \mathbf{D}_{-i})[2D_i - 1]$ is a function of $\{D_v : v \in \{i\} \cup \mathcal{N}_i\} = \{\tilde{D}_c : c \in C_i\}$. For any j and $v \in B_j$, property (b) implies there exists $v' \in \{j\} \cup \mathcal{N}_j$ such that c(v') = c(v). When $j \notin \{B_i \cup G_i\}$, $(\{j\} \cup \mathcal{N}_j \cap B_i = \emptyset)$ and hence $v' \notin B_i$. Property (a) then implies $c(v) = c(v') \notin C_i$. Thus, $C_i \cap C_j = \emptyset$. Since $\{\tilde{D}_c : c \in \mathcal{C}_n\}$ are independent (Assumption 4), $Cov(\mu_i(D_i, \mathbf{D}_{-i})[2D_i - 1], \mu_j(D_j, \mathbf{D}_{-j})[2D_j - 1]) = 0$.

C.4 Proof of Lemma C.2

We consider the case where two units are in the same or different clusters separately. We will refer to $\mu_i(D_i, \mathbf{D}_{-i})$ as $\mu_i(\mathbf{D})$ for notational convenience.

Unit i and j are in different clusters First, we write

$$\operatorname{Cov}\left(\mu_{i}(\mathbf{D})\left[2D_{i}-1\right], \mu_{j}(\mathbf{D})\left[2D_{j}-1\right]\right) = \operatorname{Cov}\left(\mu_{i}(1, \mathbf{D}_{-i})D_{i}, \mu_{j}(1, \mathbf{D}_{-j})D_{j}\right) - \operatorname{Cov}\left(\mu_{i}(1, \mathbf{D}_{-i})D_{i}, \mu_{j}(0, \mathbf{D}_{-j})(1-D_{j})\right) - \operatorname{Cov}\left(\mu_{i}(0, \mathbf{D}_{-i})(1-D_{i}), \mu_{j}(1, \mathbf{D}_{-j})D_{j}\right) + \operatorname{Cov}\left(\mu_{i}(0, \mathbf{D}_{-i})(1-D_{i}), \mu_{i}(0, \mathbf{D}_{-j})(1-D_{j})\right).$$

$$(29)$$

We bound the first component in the right-hand side of Equation (29).

First component in Equation (29) We can write

$$\operatorname{Cov}\left(\mu_{i}(1, \mathbf{D}_{-i})D_{i}, \mu_{j}(1, \mathbf{D}_{-j})D_{j}\right) = \operatorname{Cov}\left(\mu_{i}(1, \mathbf{D}_{-i})D_{i} - \mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(1, \mathbf{D}_{-j})D_{j}\right) + \operatorname{Cov}\left(\mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(1, \mathbf{D}_{-j})D_{j} - \mu_{j}(1, \mathbf{1})D_{j}\right) + \operatorname{Cov}\left(\mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(1, \mathbf{1})D_{j}\right).$$

$$(30)$$

We can now study each component separately. Since $\mu_i(\cdot)$ is uniformly bounded, it is easy to show that

$$\operatorname{Cov}\left(\mu_i(1, \mathbf{D}_{-i})D_i - \mu_i(1, \mathbf{1})D_i, \mu_j(1, \mathbf{D}_{-j})D_j\right) = \mathcal{O}\left(\mathbb{E}\left[|\mu_i(1, \mathbf{D}_{-i}) - \mu_i(1, \mathbf{1})| \middle| D_i = 1\right]\right).$$

By (27) in the proof of Lemma 3.1, we have

$$\mathbb{E}\Big[|\mu_i(1,\mathbf{D}_{-i}) - \mu_i(1,\mathbf{1})|\Big|D_i = 1\Big] = \frac{\bar{\phi}_n b_n(\mathcal{C}_n)}{2}.$$

Following a similar argument for the second component in Equation (30),

$$\operatorname{Cov}\left(\mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(1, \mathbf{D}_{-j})D_{j} - \mu_{j}(1, \mathbf{1})D_{j}\right) = \mathcal{O}\left(\frac{\bar{\phi}_{n}}{2n}\sum_{j=1}^{n}\frac{1}{|\mathcal{N}_{j}|}\Big|i \in \mathcal{N}_{j}: c(j) \neq c(i)\Big|\right)$$
$$= \mathcal{O}\left(\bar{\phi}_{n}b_{n}(\mathcal{C}_{n})\right),$$

where the last line is obtained by swapping i and j. Finally, for the third component in Equation (30) note that since $c(i) \neq c(j)$, we have that

$$\operatorname{Cov}\Big(\mu_i(1,\mathbf{1})D_i,\mu_j(1,\mathbf{1})D_j\Big)=0,$$

by design. Putting pieces together, we obtain that

$$\operatorname{Cov}\left(\mu_i(1, \mathbf{D}_{-i})D_i, \mu_j(1, \mathbf{D}_{-j})D_j\right) = \mathcal{O}\left(\bar{\phi}_n b_n(\mathcal{C}_n)\right).$$

Remaining components in Equation (29) We now move to the second component in Equation (29). We have

$$\operatorname{Cov}\Big(\mu_{i}(1, \mathbf{D}_{-i})D_{i}, \mu_{j}(0, \mathbf{D}_{-j})(1 - D_{j})\Big) = \operatorname{Cov}\Big(\mu_{i}(1, \mathbf{D}_{-i})D_{i} - \mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(0, \mathbf{D}_{-j})(1 - D_{j})\Big) + \operatorname{Cov}\Big(\mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(0, \mathbf{D}_{-j})(1 - D_{j}) - \mu_{j}(0, \mathbf{0})(1 - D_{j})\Big) + \operatorname{Cov}\Big(\mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(0, \mathbf{0})(1 - D_{j})\Big).$$
(31)

The same reasoning used to bound the first component in Equation (30) directly applies also to Equation (31).

Finally, we can use similar arguments for the third and fourth components in Equation (29), whose proof follows verbatim as the proof to bound the components in Equation (30).

Collecting bounds Collecting the bounds, it is easy to show that for (i, j) in different clusters

$$\operatorname{Cov}\left(\mu_i(\mathbf{D})\left[2D_i-1\right],\mu_j(\mathbf{D})\left[2D_j-1\right]\right) = \mathcal{O}\left(\bar{\phi}_n b_n(\mathcal{C}_n)\right),$$

completing the proof for when i, j are in two different clusters.

Unit i and j are in the same cluster If i and j are in the same cluster we can invoke Equation (29) similarly as above, with the only difference that for c(i) = c(j),

$$\operatorname{Cov}\left(\mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(1, \mathbf{1})D_{j}\right) = \frac{1}{4}\mu_{i}(1, \mathbf{1})\mu_{j}(1, \mathbf{1}),$$

$$\operatorname{Cov}\left(\mu_{i}(0, \mathbf{0})(1 - D_{i}), \mu_{j}(0, \mathbf{0})(1 - D_{j})\right) = \frac{1}{4}\mu_{i}(0, \mathbf{0})\mu_{j}(0, \mathbf{0}),$$

$$\operatorname{Cov}\left(\mu_{i}(0, \mathbf{0})(1 - D_{i}), \mu_{j}(1, \mathbf{1})D_{j}\right) = -\frac{1}{4}\mu_{i}(1, \mathbf{1})\mu_{j}(0, \mathbf{0}),$$

$$\operatorname{Cov}\left(\mu_{i}(1, \mathbf{1})D_{i}, \mu_{j}(0, \mathbf{0})(1 - D_{j})\right) = -\frac{1}{4}\mu_{i}(0, \mathbf{0})\mu_{j}(1, \mathbf{1}).$$
(32)

Following the same steps as for the case where i, j are in different clusters, accounting for Equation (32), the proof completes.

C.5 Proof of Lemma 3.2

We organize the proof as follows. First, we decompose the variance into sums of covariances in different sets. We then study the dominant components.

Variance decomposition into multiple components As a first step, we characterize the size of the set of units for which the covariances are not zero, but of order at most $\mathcal{O}(\bar{\phi}_n b_n(\mathcal{C}_n))$. Thus,

$$\begin{split} \mathbb{E}_{\mu} \Big[\Big(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}_{\mu} \big[\hat{\tau}_n(\mathcal{C}_n) \big] \Big)^2 \Big] &= \frac{4}{n^2} \sum_{i,j} \operatorname{Cov} \Big(\mu_i(D_i, \mathbf{D}_{-i})[2D_i - 1], \mu_j(D_j, \mathbf{D}_{-j})[2D_j - 1] \Big) \\ &= \frac{4}{n^2} \sum_{i,j:c(i) = c(j)} \operatorname{Cov} \Big(\mu_i(D_i, \mathbf{D}_{-i})[2D_i - 1], \mu_j(D_j, \mathbf{D}_{-j})[2D_j - 1] \Big) + \\ \mathcal{O} \left(\frac{\bar{\phi}_n b_n(\mathcal{C}_n)}{n^2} \cdot \sum_{i,j:c(i) \neq c(j)} I(j \in B_i \cup G_i) \right) & \text{(by Lemma C.1)} \\ &= \frac{4}{n^2} \sum_{i,j:c(i) = c(j)} \frac{1}{4} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0}))(\mu_j(\mathbf{1}) + \mu_j(\mathbf{0})) + \mathcal{O} \left(\frac{\bar{\phi}_n b_n(\mathcal{C}_n)}{n^2} \cdot \sum_{i,j:c(i) = c(j)} 1 \right) + \\ \mathcal{O} \left(\frac{\bar{\phi}_n b_n(\mathcal{C}_n)}{n^2} \cdot \sum_{i,j:c(i) \neq c(j)} I(j \in B_i \cup G_i) \right) & \text{(by Lemma C.2)} \\ &= \frac{4}{n^2} \sum_{i,j:c(i) = c(j)} \frac{1}{4} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0}))(\mu_j(\mathbf{1}) + \mu_j(\mathbf{0})) \\ \mathcal{O} \left(\frac{\bar{\phi}_n b_n(\mathcal{C}_n)}{n^2} \cdot \sum_{i,j} I(j \in B_i \cup G_i) \right) & \text{(because } c(i) = c(j) \Longrightarrow j \in B_i \cup G_i) \\ &= \frac{1}{n^2} \sum_{i=1}^{K_n} \left(\sum_{i \in \mathcal{C}_i} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0})) \right)^2 + \mathcal{O} \left(\frac{\bar{\phi}_n b_n(\mathcal{C}_n)}{n^2} \cdot \sum_{i \in \mathcal{C}_i} |B_i \cup G_i| \right). \end{split}$$

Size of the set $B_i \cup G_i$ Next, we study the size of $B_i \cup G_i$. By definition, $j \in G_i$ only if j is the neighbor of a unit in B_i . Thus,

$$|B_i \cup G_i| \le \sum_{\ell: \ell \in B_i} (|\mathcal{N}_\ell| + 1) = \sum_{\ell: c(\ell) \in C_i} (|\mathcal{N}_\ell| + 1),$$

where $C_i = \{c(v) : v \in \{i\} \cup \mathcal{N}_i\}$ is defined in the proof of Lemma C.1. Thus,

$$\sum_{i} |B_{i} \cup G_{i}| \leq \sum_{i} \sum_{\ell: c(\ell) \in C_{i}} (|\mathcal{N}_{\ell}| + 1) = \sum_{k=1}^{K_{n}} |\{i : k \in C_{i}\}| \sum_{\ell: c(\ell) = k} (|\mathcal{N}_{\ell}| + 1).$$

By definition, $k \in C_i$ only if c(i) = k or i is the neighbor of a unit in cluster k. Thus,

$$|\{i: k \in C_i\}| \le \sum_{\ell: c(\ell)=k} (|\mathcal{N}_{\ell}|+1).$$

As a result,

$$\sum_{i} |B_i \cup G_i| \le \sum_{k=1}^{K_n} \left(\sum_{\ell: c(\ell)=k} (|\mathcal{N}_{\ell}| + 1) \right)^2.$$

By Cauchy-Schwarz inequality and Assumption 4,

$$\sum_{i} |B_{i} \cup G_{i}| \leq \sum_{k=1}^{K_{n}} n_{k} \sum_{\ell: c(\ell) = k} (|\mathcal{N}_{\ell}| + 1)^{2} \leq \bar{\gamma} \frac{n}{K_{n}} \sum_{i} (|\mathcal{N}_{i}| + 1)^{2}.$$

On the other hand, $|B_i \cup G_i| \leq n$ implies that

$$\sum_{i} |B_i \cup G_i| \le n^2.$$

Collecting all terms together Putting two pieces together, we obtain that

$$\mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} \left[\hat{\tau}_{n}(\mathcal{C}_{n}) \right] \right)^{2} \right] = \frac{1}{n^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} (\mu_{i}(\mathbf{1}) + \mu_{i}(\mathbf{0})) \right)^{2} + \mathcal{O}(\bar{\phi}_{n} b_{n}(\mathcal{C}_{n})) \cdot \min \left\{ \frac{1}{nK_{n}} \sum_{i} (|\mathcal{N}_{i}| + 1)^{2}, 1 \right\}.$$
(33)

Since $\mathcal{N}_{n,\max} = \max\{\max_i |\mathcal{N}_i|, 1\}$ and $b_n(\mathcal{C}_n) \leq 1$,

$$\mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} [\hat{\tau}_{n}(\mathcal{C}_{n})] \right)^{2} \right]$$

$$= \frac{1}{n^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} (\mu_{i}(\mathbf{1}) + \mu_{i}(\mathbf{0})) \right)^{2} + \mathcal{O} \left(\bar{\phi}_{n} \cdot \min \left\{ \mathcal{N}_{n,\max}^{2} / K_{n}, 1 \right\} \right)$$

$$= \frac{1}{n^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} (\mu_{i}(\mathbf{1}) + \mu_{i}(\mathbf{0})) \right)^{2} + \mathcal{O} \left(\bar{\phi}_{n} / K_{n} \cdot \min \left\{ \mathcal{N}_{n,\max}^{2}, n \right\} \right).$$

$$(34)$$

By Assumption 3 and the fact that $K_n \leq n$,

$$\mathbb{E}_{\mu} \Big[\Big(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}_{\mu} [\hat{\tau}_n(\mathcal{C}_n)] \Big)^2 \Big] = \frac{1}{n^2} \sum_{k=1}^{K_n} \left(\sum_{i: c(i) = k} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0})) \right)^2 + o(1/K_n).$$
 (36)

By Assumption 2 (i),

$$\mathbb{E}_{\mu}\left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)]\right)^2\right] \leq \frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2 \cdot \bar{\psi} + o(1/K_n).$$

Conclusions by showing that the upper bound is achievable Consider the potential outcomes constructed in (28). If $|\psi_R| \ge |\psi_L|$, then it must be that $\psi_R > 0$ and

$$\mu_i(\mathbf{1}) + \mu_i(\mathbf{0}) = 2\psi_R - \bar{\phi}_n = \bar{\psi}^{1/2} - \bar{\phi}_n.$$

Similarly, when $|\psi_L| > |\psi_R|$, it must be that $\psi_L < 0$ and

$$\mu_i(\mathbf{1}) + \mu_i(\mathbf{0}) = 2\psi_L + \bar{\phi}_n = -\bar{\psi}^{1/2} + \bar{\phi}_n.$$

$$\frac{1}{n^2} \sum_{k=1}^{K_n} \left(\sum_{i:c(i)=k} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0})) \right)^2 = \frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2 \cdot (\bar{\psi}^{1/2} - \bar{\phi}_n)^2 \ge \frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2 \cdot \bar{\psi} - \frac{2\bar{\psi}\bar{\phi}_n\bar{\gamma}}{K_n}, \quad (37)$$

where the last inequality invokes Assumption 4 under which

$$\frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2 \le \frac{1}{n^2} \sum_{k=1}^{K_n} n_k \cdot \bar{\gamma} \frac{n}{K_n} = \frac{\bar{\gamma}}{K_n}.$$

Note that Assumption 3 implies $\bar{\phi}_n = o(1)$, we obtain that

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}_{\mu} [\hat{\tau}_n(\mathcal{C}_n)] \right)^2 \right] \ge \frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2 \cdot \bar{\psi} + o(1/K_n).$$

Finally, by Cauchy-Schwarz inequality,

$$\frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2 \ge 1/K_n.$$

The proof completes by recognizing that the $o(1/K_n)$ term is dominated by the first term.

C.6 Proof of Theorem 3.4

We prove the following more general result:

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \Big[\Big(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}_{\mu} [\hat{\tau}_n(\mathcal{C}_n)] \Big)^2 \Big] + \lambda \Big(\tau_{n,\mu} - \mathbb{E}_{\mu} [\hat{\tau}_n(\mathcal{C}_n)] \Big)^2 = \mathcal{B}_n^*(\mathcal{C}_n, \lambda) (1 + o(1)).$$

Clearly, the left-hand side is upper bounded by $\mathcal{B}_n(\mathcal{C}_n, \lambda)$ which, by Theorem 3.3, is equal to the right-hand side. From the proofs of Lemma 3.1 and Lemma C.2, we observe that the worst-case bias and variance are both achieved, up to 1 + o(1) factors, by the potential outcomes defined in (28). The result is then proved. In particular, when $\lambda = 1$, the left-hand side is the worst-case MSE because

$$\mathbb{E}_{\mu}[(\hat{\tau}_n(\mathcal{C}_n) - \tau_{n,\mu})^2] = \mathbb{E}_{\mu}\Big[\Big(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)]\Big)^2\Big] + \Big(\tau_{n,\mu} - \mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)]\Big)^2.$$

C.7 Proof of Theorem 3.5

We decompose the proof as follows. First, we characterize the bias and variance of the Bernoulli design. We then compare \mathcal{B}_n for the cluster and Bernoulli design, assuming that $\lambda \in (0, \infty)$ is bounded away from zero and infinity as assumed in Theorem 3.5.

Worst-case bias and variance of the Bernoulli and cluster design Note that $C_{B,n}$ satisfies Assumption 4. By Lemma C.1 and C.2, $C_{B,n}$ has worst-case bias $\bar{\phi}_n b_n(C_{B,n}) = \bar{\phi}_n$, and worst-case variance $\frac{1}{n}[\bar{\psi} + o(1)]$. Thus,

$$\mathcal{B}_n^*(\mathcal{C}_{\mathrm{B},n},\lambda) = \lambda \bar{\phi}_n^2 + \frac{1}{n}\bar{\psi},$$

and

$$\mathcal{B}_n^*(\mathcal{C}_n, \lambda) = \lambda \bar{\phi}_n^2 b_n(\mathcal{C}_n)^2 + \left(\frac{1}{n^2} \sum_{k=1}^{K_n} n_k^2\right) \bar{\psi}.$$

Case $\mathcal{B}_n(\mathcal{C}_n, \lambda) > \mathcal{B}_n(\mathcal{C}_{B,n}, \lambda)$. By Theorem 3.3, it remains to prove that $\liminf_{n\to\infty} \mathcal{B}_n^*(\mathcal{C}_n, \lambda)/\mathcal{B}_n^*(\mathcal{C}_{B,n}, \lambda) > 1$. By Cauchy-Schwarz inequality, $(1/n^2)\sum_{k=1}^{K_n} n_k^2 \geq 1/K_n$. Thus,

$$\mathcal{B}_n^*(\mathcal{C}_n,\lambda) \ge \frac{\bar{\psi}}{K_n},$$

and

$$\frac{\mathcal{B}_n^*(\mathcal{C}_n, \lambda)}{\mathcal{B}_n^*(\mathcal{C}_{\mathrm{B},n}, \lambda)} \ge \frac{1}{K_n \bar{\phi}_n^2 \cdot \lambda / \bar{\psi} + K_n / n} \ge \frac{1}{K_n \bar{\phi}_n^2 \cdot \lambda / \bar{\psi} + \kappa}.$$

If $\sqrt{K_n}\bar{\phi}_n \to 0$, $\liminf_{n\to\infty} \mathcal{B}_n^*(\mathcal{C}_n,\lambda)/\mathcal{B}_n^*(\mathcal{C}_{\mathrm{B},n},\lambda) \ge 1/\kappa > 1$. The proof is then completed.

Case $\mathcal{B}_n(\mathcal{C}_n, \lambda) < \mathcal{B}_n(\mathcal{C}_{B,n}, \lambda)$ Similarly, by Theorem 3.3, it remains to prove that $\limsup_{n\to\infty} \mathcal{B}_n^*(\mathcal{C}_n, \lambda)/\mathcal{B}_n^*(\mathcal{C}_{B,n}, \lambda) < 1$. By Assumption 4, for a finte constant $\bar{\gamma} < \infty$ (since clusters are proportional to each other) $(1/n^2) \sum_{k=1}^{K_n} n_k^2 \leq \bar{\gamma}^2/K_n$. Thus,

$$\mathcal{B}_n^*(\mathcal{C}_n, \lambda) \le \lambda \bar{\phi}_n^2 \delta^2 + \frac{\bar{\psi}\bar{\gamma}^2}{K_n},$$

and

$$\frac{\mathcal{B}_n^*(\mathcal{C}_n,\lambda)}{\mathcal{B}_n^*(\mathcal{C}_{\mathrm{B},n},\lambda)} \leq \frac{\lambda \bar{\phi}_n^2 \delta^2 + \bar{\psi} \bar{\gamma}^2 / K_n}{\lambda \bar{\phi}_n^2 + \bar{\psi} / n} \leq \delta^2 + \frac{\bar{\psi} \bar{\gamma}^2}{K_n \bar{\phi}_n^2}.$$

If $\sqrt{K_n}\bar{\phi}_n \to \infty$, $\limsup_{n\to\infty} \mathcal{B}_n^*(\mathcal{C}_n,\lambda)/\mathcal{B}_n^*(\mathcal{C}_{\mathrm{B},n},\lambda) \le \delta^2 < 1$. The proof is then completed.

C.8 Proof of Theorem 3.6

The proof follows directly the proof of Theorem 3.5 (case for $\mathcal{B}_n(\mathcal{C}_{B,n},\lambda) \geq \mathcal{B}_n(\mathcal{C}_n,\lambda)$), after noticing that the result directly holds if we replace $\bar{\gamma}^2$ in the proof of Theorem 3.5 with $\underline{\gamma}$ as defined in the statement of Theorem 3.6, and rearranging terms accordingly.

C.9 Proof of Theorem 4.1

For any $u, v \in \{1, \dots, K\}$,

$$(\mathbf{M}_c^T \mathbf{L} \mathbf{M}_c)_{uv} = \sum_{c(i)=u, c(j)=v} \mathbf{L}_{ij} = \sum_{c(i)=u} \frac{1}{|\mathcal{N}_i|} \Big| j \in \mathcal{N}_i : c(j) = v \Big|.$$

Therefore,

$$\sum_{i=1}^{n} \frac{1}{|\mathcal{N}_i|} \Big| j \in \mathcal{N}_i : c(i) \neq c(j) \Big| = \sum_{u \neq v} (\mathbf{M}_c^T \mathbf{L} \mathbf{M}_c)_{uv}.$$

Since $\mathbf{M}_c \mathbf{1}_k = \mathbf{1}_n$,

$$\sum_{u,v=1}^K (\mathbf{M}_c^T \mathbf{L} \mathbf{M}_c)_{uv} = \mathbf{1}_k^T \mathbf{M}_c^T \mathbf{L} \mathbf{M}_c \mathbf{1}_k = \mathbf{1}_n^T \mathbf{L} \mathbf{1}_n$$

which is independent of c. On the other hand,

$$\mathbf{1}_n^T(\mathbf{M}_c\mathbf{M}_c^T)\mathbf{1}_n = \sum_{k=1}^K n_k^2$$

Thus, (14) is equivalent to

$$\begin{aligned} & \min_{c:\{1,\cdots,n\}\mapsto\{1,\cdots,K\}} - \mathrm{tr}(\mathbf{M}_c^T n \mathbf{L} \mathbf{M}_c) + \xi_n (\mathbf{1}_n^T \mathbf{M}_c \mathbf{M}_c^T \mathbf{1}_n) \\ &= \min_{c:\{1,\cdots,n\}\mapsto\{1,\cdots,K\}} - \mathrm{tr}((n \mathbf{L} - \xi_n \mathbf{1}_n \mathbf{1}_n^T) \mathbf{M}_c \mathbf{M}_c^T). \end{aligned}$$

C.10 Proof of Theorem 6.1

We study the worst-case bias and variance separately. We conclude with a characterization of the MSE.

Worst-case bias Note that

$$\mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)] = \mathbb{E}_{\mu}[\mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n) \mid \mathbf{D}]] = \mathbb{E}_{\mu}\left[\frac{2}{n}\sum_{i=1}^n (2D_i - 1)\mu_i(\mathbf{D})\right].$$

The right-hand side is the expectation of the difference in means estimator with known μ_i which is studied in Lemma 3.1. Thus, the worst-case bias remains the same and the worst case is achieved when $\mu_i(\mathbf{d})$ is given by (28) in the proof of Lemma 3.1.

Worst-case variance: Part I Moving to the variance, by variance decomposition formula,

$$\mathbb{E}_{\mu}\Big[\Big(\hat{\tau}_{n}(\mathcal{C}_{n}) - \mathbb{E}[\hat{\tau}_{n}(\mathcal{C}_{n})]\Big)^{2}\Big] = \mathbb{E}_{\mu}\Big[\Big(\mathbb{E}_{\mu}[\hat{\tau}_{n}(\mathcal{C}_{n}) \mid \mathbf{D}] - \mathbb{E}[\hat{\tau}_{n}(\mathcal{C}_{n})]\Big)^{2}\Big] + \mathbb{E}_{\mu}\Big[\Big(\hat{\tau}_{n}(\mathcal{C}_{n}) - \mathbb{E}_{\mu}[\hat{\tau}_{n}(\mathcal{C}_{n}) \mid \mathbf{D}]\Big)^{2}\Big].$$
(38)

Again, the second term is the variance of the difference in means estimator with known $\mu_i(\mathbf{d})$'s. By (36) in the proof of Lemma C.2,

$$\mathbb{E}_{\mu}[(\mathbb{E}_{\mu}[\hat{\tau}_{n}(C_{n}) \mid \mathbf{D}] - \mathbb{E}[\hat{\tau}_{n}(C_{n})])^{2}] = \frac{1}{n^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} (\mu_{i}(\mathbf{1}) + \mu_{i}(\mathbf{0})) \right)^{2} + o(1/K_{n}).$$
 (39)

Worst-case variance: Part II We decompose the second term in the right-hand side of Equation (38) as

$$\mathbb{E}_{\mu}[(\hat{\tau}_{n}(C_{n}) - \mathbb{E}_{\mu}[\hat{\tau}_{n}(C_{n}) \mid \mathbf{D}])^{2}]$$

$$= \frac{4}{n^{2}} \sum_{i \neq j} \mathbb{E}_{\mu} \left[\mathbf{C}_{ij}(\mathbf{D})(2\mathbf{D}_{i} - 1)(2\mathbf{D}_{j} - 1)\sqrt{\operatorname{Var}(Y_{i}(\mathbf{D}) \mid \mathbf{D})}\sqrt{\operatorname{Var}(Y_{j}(\mathbf{D}) \mid \mathbf{D})} \right]$$

$$+ \frac{4}{n^{2}} \sum_{i=1}^{n} \mathbb{E}_{\mu}[\operatorname{Var}(Y_{i}(\mathbf{D}) \mid \mathbf{D})].$$
(40)

Since $|\psi_R| \ge |\psi_L|$, it must be that $\psi_R > 0$. Let $v(\mathbf{D}) = (v_1(\mathbf{D}), \dots, v_n(\mathbf{D}))$ where $v_i(\mathbf{D}) = (2\mathbf{D}_i - 1)\sqrt{\operatorname{Var}(Y_i(\mathbf{D} \mid \mathbf{D}))}$. Then

$$\frac{4}{n^2} \sum_{i \neq j} \mathbb{E}_{\mu} \left[\mathbf{C}_{ij}(\mathbf{D}) (2\mathbf{D}_i - 1) (2\mathbf{D}_j - 1) \sqrt{\operatorname{Var}(Y_i(\mathbf{D}) \mid \mathbf{D})} \sqrt{\operatorname{Var}(Y_j(\mathbf{D}) \mid \mathbf{D})} \right]$$

$$= \frac{4}{n^2} \mathbb{E}_{\mu} [v(\mathbf{D})'(\mathbf{C}(\mathbf{D}) - \mathbf{I}) v(\mathbf{D})]$$

$$\leq \frac{4}{n^2} \mathbb{E}_{\mu} [\|v(\mathbf{D})\|_2^2] \cdot \sup_{\mathbf{d} \in \{0,1\}^n} \|\mathbf{C}(\mathbf{d}) - \mathbf{I}\|_{\text{op}}.$$

By Assumption 6,

$$\operatorname{Var}(Y_i(\mathbf{D}) \mid \mathbf{D}) = g(\mu_i(\mathbf{D})) - \mu_i(\mathbf{D})^2 \le g(\psi_R).$$

Thus, $||v(\mathbf{D})||_2^2 \le ng(\psi_R)^2 = \mathcal{O}(n)$. By Assumption 7,

$$\frac{4}{n^2} \sum_{i \neq j} \mathbb{E}_{\mu} \left[\mathbf{C}_{ij}(\mathbf{D}) (2\mathbf{D}_i - 1) (2\mathbf{D}_j - 1) \sqrt{\operatorname{Var}(Y_i(\mathbf{D}) \mid \mathbf{D})} \sqrt{\operatorname{Var}(Y_j(\mathbf{D}) \mid \mathbf{D})} \right] = o(1/n) = o(1/K_n). \tag{41}$$

Returning to the second term of (40). By Assumption 6,

$$\frac{4}{n^2} \sum_{i=1}^{n} \mathbb{E}_{\mu}[\text{Var}(Y_i(\mathbf{D}) \mid \mathbf{D})] = \frac{4}{n^2} \sum_{i=1}^{n} \mathbb{E}_{\mu}[g(\mu_i(\mathbf{D})) - \mu_i(\mathbf{D})^2]
= \frac{2}{n^2} \sum_{i=1}^{n} \mathbb{E}_{\mu}[g(\mu_i(1, \mathbf{D}_{-i})) - \mu_i(1, \mathbf{D}_{-i})^2 \mid D_i = 1] + \mathbb{E}_{\mu}[g(\mu_i(0, \mathbf{D}_{-i})) - \mu_i(0, \mathbf{D}_{-i})^2 \mid D_i = 0]$$

By Assumption 2, and $|\psi_R| \ge |\psi_L|$,

$$|\mu_i(1, \mathbf{D}_{-i}) - \mu_i(1)| \le \bar{\phi}_n, \quad -\psi_R \le \mu_i(1, \mathbf{D}_{-i}) \le \psi_R.$$

Let L_g denote the Lipschitz constant of g. Then by Assumption 6

$$|g(\mu_{i}(1, \mathbf{D}_{-i})) - \mu_{i}(1, \mathbf{D}_{-i})^{2} - \{g(\mu_{i}(\mathbf{1})) - \mu_{i}(\mathbf{1})^{2}\}|$$

$$\leq |\mu_{i}(1, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1})| \cdot |L_{g} + \mu_{i}(1, \mathbf{D}_{-i}) + \mu_{i}(\mathbf{1})| \leq (L_{g} + 2\psi_{R})\bar{\phi}_{n}.$$

Similarly,

$$|g(\mu_i(0, \mathbf{D}_{-i})) - \mu_i(0, \mathbf{D}_{-i})^2 - \{g(\mu_i(\mathbf{0})) - \mu_i(\mathbf{0})^2\}| \le (L_g + 2\psi_R)\bar{\phi}_n.$$

Thus,

$$\frac{4}{n^2} \sum_{i=1}^{n} \mathbb{E}_{\mu}[\text{Var}(Y_i(\mathbf{D}) \mid \mathbf{D})] = \frac{2}{n^2} \sum_{i=1}^{n} \left(\mathbb{E}_{\mu}[g(\mu_i(\mathbf{1})) - \mu_i(\mathbf{1})^2] + \mathbb{E}_{\mu}[g(\mu_i(\mathbf{0})) - \mu_i(\mathbf{0})^2] \right) + \mathcal{O}\left(\bar{\phi}_n/n\right)$$

$$= \frac{2}{n^2} \sum_{i=1}^{n} \left\{ g(\mu_i(\mathbf{1})) - \mu_i(\mathbf{1})^2 + g(\mu_i(\mathbf{0})) - \mu_i(\mathbf{0})^2 \right\} + o\left(1/K_n\right),$$
(42)

where the last line uses the fact that $\mu_i(\cdot)$ is non-random and Assumption 3 that implies $\bar{\phi}_n = o(1)$.

Worst case variance: Part III, putting together bounds Putting together (39), (40), (41), and (42), we have

$$\mathbb{E}_{\mu}[(\hat{\tau}_{n}(C_{n}) - \mathbb{E}[\hat{\tau}_{n}(C_{n})])^{2}] = \frac{1}{n^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} (\mu_{i}(\mathbf{1}) + \mu_{i}(\mathbf{0})) \right)^{2} \\
+ \frac{2}{n^{2}} \sum_{i=1}^{n} \left\{ g(\mu_{i}(\mathbf{1})) - \mu_{i}(\mathbf{1})^{2} + g(\mu_{i}(\mathbf{0})) - \mu_{i}(\mathbf{0})^{2} \right\} + o(1/K_{n}) \tag{43}$$

$$= \frac{2}{n^{2}} \sum_{k=1}^{K_{n}} \sum_{i

$$= \frac{2}{n^{2}} \sum_{k=1}^{K_{n}} \sum_{i$$$$

Since $\psi_R > 0$ and $|\psi_R| \ge |\psi_L|$, $\bar{\psi} = \psi_R/2$,

$$(\mu_i(\mathbf{1}) + \mu_i(\mathbf{0}))(\mu_j(\mathbf{1}) + \mu_j(\mathbf{0})) \le 4\psi_R^2 = \bar{\psi},$$

and

$$2g(\mu_i(\mathbf{1})) + 2g(\mu_i(\mathbf{0})) - (\mu_i(\mathbf{1}) - \mu_i(\mathbf{0}))^2 \le 4g(\psi_R),$$

where both terms achieve their maximums when $\mu_i(\mathbf{1}) = \mu_i(\mathbf{0}) = \psi_R$ for all i. Thus,

$$\mathbb{E}_{\mu}[(\hat{\tau}_{n}(C_{n}) - \mathbb{E}[\hat{\tau}_{n}(C_{n})])^{2}] \leq \frac{\bar{\psi}}{n^{2}} \sum_{k=1}^{K_{n}} n_{k}^{2} + \frac{4(g(\psi_{R}) - \psi_{R}^{2})}{n} + o(1/K_{n})$$

$$= \frac{\bar{\psi}}{n^{2}} \sum_{k=1}^{K_{n}} n_{k}^{2} + \frac{4g(\psi_{R}) - \bar{\psi}}{n} + o(1/K_{n}).$$

Since $4g(\psi_R) - \bar{\psi} = 4(g(\psi_R) - \psi_R^2) \ge 0$ and the first term is lower bounded by $\bar{\psi}/K_n$, we have that

$$\mathbb{E}_{\mu}[(\hat{\tau}_{n}(C_{n}) - \mathbb{E}[\hat{\tau}_{n}(C_{n})])^{2}] \leq \left(\frac{\bar{\psi}}{n^{2}} \sum_{k=1}^{K_{n}} n_{k}^{2} + \frac{4g(\psi_{R}) - \bar{\psi}}{n}\right) (1 + o(1)).$$

Upper bound on MSE We can upper bound the worst-case MSE as

$$\mathbb{E}_{\mu}[(\hat{\tau}_{n}(C_{n}) - \tau_{n,\mu})^{2}] \leq \left(\bar{\phi}_{n}^{2}b_{n}(C_{n})^{2} + \frac{\bar{\psi}}{n^{2}}\sum_{k=1}^{K_{n}}n_{k}^{2} + \frac{4g(\psi_{R}) - \bar{\psi}}{n}\right)(1 + o(1))$$

$$= \left(\mathcal{B}_{n}^{*}(C_{n}, 1) + \frac{4g(\psi_{R}) - \bar{\psi}}{n}\right)(1 + o(1)).$$

Lower Bound on MSE (Upper Bound is achievable) To prove the upper bounds are achievable, it is left to show that the potential outcomes defined in (28) achieves the bound for the variance, because we have already proved that it achieves the worst-case bias in the proof of Lemma 3.1. For this construction, $\mu_i(1) = \psi_R$ and $\mu_i(0) = \psi_R - \bar{\phi}_n$. Plugging them into (43), it is easy to see that the variance is within $(1 + O(\bar{\phi}_n))$ times the upper bound. By Assumption 3, it implies the worst-case variance is achieved by (28).

C.11 Proof of Theorem 6.2

Assume without loss of generality that $|\psi_{Ri}| \ge |\psi_{Li}|$ for all i. Then $\bar{\psi}_i = \psi_{Ri} > 0$.

Worst-case bias Following the proofs of Lemma 3.1, we can prove that

$$\left| \tau_{n,\mu} - \mathbb{E}_{\mu}[\hat{\tau}_n(\mathcal{C}_n)] \right| \leq \bar{\phi}_n b_{n,\alpha}(\mathcal{C}_n),$$

and it can be achieved by the following construction of potential outcomes:

$$\mu_i(1, \mathbf{d}_{-i}) = \mu_i(0, \mathbf{d}_{-i}) = \bar{\psi}_i - \bar{\phi}_n \frac{\alpha_i}{|\mathcal{N}_i|} \sum_{k \in \mathcal{N}_i} (1 - \mathbf{d}_k). \tag{44}$$

Note that the above construction is legitimate because $\bar{\phi}_n \leq \psi_{Ri} - \psi_{Li}$ and $\alpha_i \leq 1$, implying that $\mu_i(\mathbf{d}) \in [\psi_{Li}, \psi_{Ri}]$.

Worst-case variance Following the proof of Lemma C.2, we can recover (36):

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}_{\mu} [\hat{\tau}_n(\mathcal{C}_n)] \right)^2 \right] = \frac{1}{n^2} \sum_{k=1}^{K_n} \left(\sum_{i: c(i)=k} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0})) \right)^2 + o(1/K_n).$$

Since $|\mu_i(1)|, |\mu_i(0)| \leq \bar{\psi}_i$,

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}[\hat{\tau}_n(\mathcal{C}_n)] \right)^2 \right] \leq \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 + o(1/K_n).$$

On the other hand, for the potential outcomes defined in (44), $\mu_i(\mathbf{1}) = \bar{\psi}_i/2$, $\mu_i(\mathbf{0}) = \bar{\psi}_i/2 - \bar{\phi}_n$. In this case,

$$\frac{1}{n^2} \sum_{k=1}^{K_n} \left(\sum_{i:c(i)=k} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0})) \right)^2 = \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i - \bar{\phi}_n \right)^2 \\
= \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 - 2\bar{\phi}_n \sum_{k=1}^{K_n} \frac{n_k}{n^2} \left(\sum_{i \in c_k} \bar{\psi}_i \right) + \bar{\phi}_n^2 \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \\
\ge \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 - \frac{2\bar{\phi}_n}{K_n} \left(\frac{1}{n} \sum_{i=1}^n \bar{\psi}_i \right) + \frac{\bar{\phi}_n^2}{K_n},$$

where the last line applies Assumption 4 for the second term and Cauchy-Schwarz inequality for the third term. Since $(1/n)\sum_{i=1}^{n} \bar{\psi}_i \leq \bar{\psi} = O(1)$ and $\bar{\phi}_n = o(1)$ by Assumption 3,

$$\frac{1}{n^2} \sum_{k=1}^{K_n} \left(\sum_{i:c(i)=k} (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0})) \right)^2 \ge \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 + o(1/K_n)$$

Thus,

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}[\hat{\tau}_n(\mathcal{C}_n)] \right)^2 \right] = \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 + o(1/K_n).$$

By Cauchy-Schwarz inequality,

$$\sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 = \frac{1}{n^2} \sum_{k=1}^{K_n} \left(\sum_{i \in c_k} \bar{\psi}_i \right)^2 \geq \frac{1}{K_n} \left(\frac{1}{n} \sum_{i=1}^n \bar{\psi}_i \right)^2 \geq \frac{\underline{\psi}^2}{K_n}.$$

Thus,

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n(\mathcal{C}_n) - \mathbb{E}[\hat{\tau}_n(\mathcal{C}_n)] \right)^2 \right] = \sum_{k=1}^{K_n} \frac{n_k^2}{n^2} \left(\frac{1}{n_k} \sum_{i \in c_k} \bar{\psi}_i \right)^2 (1 + o(1)).$$

Worst-case MSE Finally, since the worst-case bias and variance are both achieved by (44), the worst-case MSE is the worst-case bias square plus the worst-case variance.

C.12 Proof of Theorem 6.3

We separately provide bounds on the worst-case bias and variance.

Upper bound on the worst-case bias. Let

$$\tau_{n,\mu}^{w} = \frac{1}{\|w\|_{1}} \sum_{i=1}^{n} w_{i}(\mu_{i}(\mathbf{1}) - \mu_{i}(\mathbf{0})),$$

and

$$U_n^*(\mathcal{C}_n, w) = \bar{\phi}_n b_n^w(\mathcal{C}_n) + (\psi_R - \psi_L) \sum_{i=1}^n \left| \frac{w_i}{\|w\|_1} - \frac{1}{n} \right|.$$

Following verbatim the proof of Lemma 3.1, we have

$$\sup_{\mu \in \mathcal{M}} \left| \mathbb{E}_{\mu} [\hat{\tau}_{n}^{w}] - \tau_{n,\mu}^{w} \right| = \sup_{\mu \in \mathcal{M}} \left| \sum_{i=1}^{n} \frac{w_{i}}{\|w\|_{1}} \left(\mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1}) | D_{i} = 1 \right] - \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{0}) | D_{i} = 0 \right] \right) \right|$$

$$\leq \sup_{\mu(1,\cdot) \in \otimes_{i=1}^{n} \mathcal{M}_{1,i}} \left| \sum_{i=1}^{n} \frac{w_{i}}{\|w\|_{1}} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1}) | D_{i} = 1 \right] \right|$$

$$+ \sup_{\mu(0,\cdot) \in \otimes_{i=1}^{n} \mathcal{M}_{0,i}} \left| \sum_{i=1}^{n} \frac{w_{i}}{\|w\|_{1}} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{0}) | D_{i} = 0 \right] \right|$$

$$\leq \bar{\phi}_{n} \sum_{i=1}^{n} \frac{w_{i}}{\|w\|_{1}} \frac{1}{|\mathcal{N}_{i}|} \left| \mathcal{N}_{i} \bigcap \left\{ j : c(i) \neq c(j) \right\} \right|,$$

where the last line follows (27) in the proof of Lemma 3.1. Now we bound $|\tau_{n,\mu}^w - \tau_{n,\mu}|$. By the triangle inequality and Assumption 2 (i),

$$|\tau_{n,\mu}^w - \tau_{n,\mu}| = \Big| \sum_{i=1}^n (\mu_i(\mathbf{1}) - \mu_i(\mathbf{0})) \left(\frac{w_i}{\|w\|_1} - \frac{1}{n} \right) \Big| \le (\psi_R - \psi_L) \sum_{i=1}^n \Big| \frac{w_i}{\|w\|_1} - \frac{1}{n} \Big|.$$

Thus, we have proved that

$$\sup_{\mu \in \mathcal{M}} \left| \mathbb{E}_{\mu} [\hat{\tau}_n^w] - \tau_{n,\mu} \right| \le U_n^*(\mathcal{C}_n, w). \tag{45}$$

Lower bound (achievability) of worst-case bias To prove the achievability, we consider the following constructions of the potential outcomes:

$$\mu_i(1, \mathbf{d}_{-i}) = \mu_i(1) - \bar{\phi}_n \frac{1}{|\mathcal{N}_i|} \sum_{k \in \mathcal{N}_i} (1 - \mathbf{d}_k), \quad \mu_i(0, \mathbf{d}_{-i}) = \mu_i(\mathbf{0}) + \bar{\phi}_n \frac{1}{|\mathcal{N}_i|} \sum_{k \in \mathcal{N}_i} \mathbf{d}_k,$$
 (46)

and

$$(\mu_i(\mathbf{1}), \mu_i(\mathbf{0})) = \begin{cases} (\psi_L + \bar{\phi}_n, \psi_R - \bar{\phi}_n) & (\text{if } w_i / ||w||_1 \ge 1/n) \\ (\psi_R, \psi_L) & (\text{otherwise}) \end{cases}$$

Under Assumption $2, \bar{\phi}_n \leq \psi_R - \psi_L, \mu \in \mathcal{M}$. For this choice of μ , repeating the above steps,

$$\mathbb{E}_{\mu}[\hat{\tau}_{n}^{w}] - \tau_{n,\mu}^{w} = \sum_{i=1}^{n} \frac{w_{i}}{\|w\|_{1}} \left(\mathbb{E}\left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1})|D_{i} = 1\right] - \mathbb{E}\left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{0})|D_{i} = 0\right] \right) \\
= -\bar{\phi}_{n} \sum_{i=1}^{n} \frac{w_{i}}{\|w\|_{1}} \left(\frac{1}{|\mathcal{N}_{i}|} \sum_{k \in \mathcal{N}_{i}} \mathbb{E}[(1 - D_{k}) | D_{i} = 1] + \frac{1}{|\mathcal{N}_{i}|} \sum_{k \in \mathcal{N}_{i}} \mathbb{E}[D_{k} | D_{i} = 0] \right) \\
= -\bar{\phi}_{n} \sum_{i=1}^{n} \frac{w_{i}}{\|w\|_{1}} \frac{1}{|\mathcal{N}_{i}|} |\mathcal{N}_{i} \cap \left\{ j : c(i) \neq c(j) \right\} \right|, \tag{47}$$

and (letting $(\cdot)_+ = \max\{\cdot, 0\}$)

$$\tau_{n,\mu}^{w} - \tau_{n,\mu} = \sum_{i=1}^{n} (\mu_{i}(\mathbf{1}) - \mu_{i}(\mathbf{0})) \left(\frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right)$$

$$= -(\psi_{R} - \psi_{L}) \sum_{i=1}^{n} \left| \frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right| + 2\bar{\phi}_{n} \sum_{i=1}^{n} \left(\frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right)_{+}$$

$$= -(\psi_{R} - \psi_{L} - \bar{\phi}_{n}) \sum_{i=1}^{n} \left| \frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right|,$$

where the last line is due to the fact that because $w_i \geq 0$,

$$\sum_{i=1}^{n} \left(\frac{w_i}{\|w\|_1} - \frac{1}{n} \right) = 0 \Longrightarrow \sum_{i=1}^{n} \left(\frac{w_i}{\|w\|_1} - \frac{1}{n} \right)_+ = \sum_{i=1}^{n} \left(\frac{w_i}{\|w\|_1} - \frac{1}{n} \right)_- = \frac{1}{2} \sum_{i=1}^{n} \left| \frac{w_i}{\|w\|_1} - \frac{1}{n} \right|.$$

Putting two pieces together, for this choice of μ ,

$$|\mathbb{E}_{\mu}[\hat{\tau}_{n}^{w}] - \tau_{n,\mu}| = U_{n}^{*}(\mathcal{C}_{n}, w) - \bar{\phi}_{n} \sum_{i=1}^{n} \left| \frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right|.$$
(48)

By definition,

$$U_n^*(\mathcal{C}_n, w) \ge (\psi_R - \psi_L) \sum_{i=1}^n \left| \frac{w_i}{\|w\|_1} - \frac{1}{n} \right|.$$

Thus, because $\bar{\phi}_n = o(1)$ under Assumption 3, $\bar{\phi}_n \sum_{i=1}^n \left| \frac{w_i}{\|w\|_1} - \frac{1}{n} \right| = o(U_n^*(\mathcal{C}_n, w))$ and

$$|\mathbb{E}_{\mu}[\hat{\tau}_{n}^{w}] - \tau_{n,\mu}| = U_{n}^{*}(\mathcal{C}_{n}, w)(1 + o(1)).$$

Combining (45) and (48), we prove the result for the worst-case bias.

Upper bound on the worst-case variance. Following the proof of Lemma C.2, we obtain that

$$\begin{split} &\mathbb{E}_{\mu}\Big[\Big(\hat{\tau}_{n}^{w}(C_{n}) - \mathbb{E}_{\mu}[\hat{\tau}_{n}^{w}(C_{n})]\Big)^{2}\Big] \\ &= \frac{4}{\|w\|_{1}^{2}} \sum_{i,j} w_{i}w_{j} \operatorname{Cov}\Big(\mu_{i}(D_{i}, \mathbf{D}_{-i})[2D_{i} - 1], \mu_{j}(D_{j}, \mathbf{D}_{-j})[2D_{j} - 1]\Big) \\ &= \frac{4}{\|w\|_{1}^{2}} \sum_{i,j} w_{i}w_{j} \operatorname{Cov}\Big(\mu_{i}(D_{i}, \mathbf{D}_{-i})[2D_{i} - 1], \mu_{j}(D_{j}, \mathbf{D}_{-j})[2D_{j} - 1]\Big) + \\ &\mathcal{O}\left(\frac{\bar{\phi}_{n}}{\|w\|_{1}^{2}} \cdot \sum_{i,j:c(i) \neq c(j)} w_{i}w_{j}I(j \in B_{i} \cup G_{i})\right) \quad \text{(by Lemma C.1 and that } b_{n}(C_{n}) \leq 1) \\ &= \frac{4}{\|w\|_{1}^{2}} \sum_{i,j:c(i) = c(j)} \frac{w_{i}w_{j}}{4} (\mu_{i}(1) + \mu_{i}(\mathbf{0}))(\mu_{j}(1) + \mu_{j}(\mathbf{0})) + \mathcal{O}\left(\frac{\bar{\phi}_{n}}{\|w\|_{1}^{2}} \cdot \sum_{i,j:c(i) = c(j)} w_{i}w_{j}\Big) + \\ &\mathcal{O}\left(\frac{\bar{\phi}_{n}}{\|w\|_{1}^{2}} \cdot \sum_{i,j:c(i) \neq c(j)} w_{i}w_{j}I(j \in B_{i} \cup G_{i})\right) \quad \text{(by Lemma C.2)} \\ &= \frac{4}{\|w\|_{1}^{2}} \sum_{i,j:c(i) = c(j)} \frac{w_{i}w_{j}}{4} (\mu_{i}(1) + \mu_{i}(\mathbf{0}))(\mu_{j}(1) + \mu_{j}(\mathbf{0})) \\ &\mathcal{O}\left(\frac{\bar{\phi}_{n}}{\|w\|_{1}^{2}} \cdot \sum_{i,j} w_{i}w_{j}I(j \in B_{i} \cup G_{i})\right) \quad \text{(because } c(i) = c(j) \Longrightarrow j \in B_{i} \cup G_{i}) \\ &= \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i) = k} w_{i}(\mu_{i}(1) + \mu_{i}(\mathbf{0}))\right)^{2} + \mathcal{O}\left(\frac{\bar{\phi}_{n}}{\|w\|_{1}^{2}} \cdot \sum_{i,j} I(j \in B_{i} \cup G_{i})\right) \quad \text{(because } w_{i} \leq \bar{w} \text{ and } \|w\|_{1} \geq \underline{w}n \\ &= \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i) = k} w_{i}(\mu_{i}(1) + \mu_{i}(\mathbf{0}))\right)^{2} + \mathcal{O}\left(\frac{\bar{\phi}_{n}}{n^{2}} \cdot \sum_{i,j} I(j \in B_{i} \cup G_{i})\right) \quad \text{(because } w_{i} \leq \bar{w} \text{ and } \|w\|_{1} \geq \underline{w}n \end{pmatrix} \\ &= \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i) = k} w_{i}(\mu_{i}(1) + \mu_{i}(\mathbf{0})\right)\right)^{2} + \mathcal{O}\left(\frac{\bar{\phi}_{n}}{n^{2}} \cdot \sum_{i,j} |B_{i} \cup G_{i}|\right). \end{aligned}$$

It has been shown in the proof of Lemma 3.1, that

$$\frac{\bar{\phi}_n}{n^2} \cdot \sum_i |B_i \cup G_i| = o(1/K_n).$$

Thus,

$$\mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} [\hat{\tau}_{n}^{w}(\mathcal{C}_{n})] \right)^{2} \right] = \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} w_{i}(\mu_{i}(\mathbf{1}) + \mu_{i}(\mathbf{0})) \right)^{2} + o(1/K_{n}). \tag{49}$$

By Assumption 2 (i) and the definition (7) of $\bar{\psi}$, we have

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} [\hat{\tau}_{n}^{w}(\mathcal{C}_{n})] \right)^{2} \right] \leq \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i: c(i)=k} w_{i} \right)^{2} \cdot \bar{\psi} + o(1/K_{n}).$$

Lower bound (achievability) of worst-case variance On the other hand, for potential outcomes defined in (28), similar to (37),

$$\mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} [\hat{\tau}_{n}^{w}(\mathcal{C}_{n})] \right)^{2} \right] = \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} w_{i} \right)^{2} \cdot (\bar{\psi}^{1/2} - \bar{\phi}_{n})^{2} + o(1/K_{n})$$

$$= \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} w_{i} \right)^{2} \cdot \bar{\psi}(1+o(1)) + o(1/K_{n}).$$

By Cauchy-Schwarz inequality,

$$\sum_{k=1}^{K_n} \left(\sum_{i:c(i)=k} w_i \right)^2 \ge \frac{1}{K_n} \left(\sum_{k=1}^{K_n} \sum_{i:c(i)=k} w_i \right)^2 = \frac{\|w\|_1^2}{K_n}.$$
 (50)

Therefore, the proof of worst-case variance is completed.

C.13 Proof of Theorem 6.4

We prove the following more general result:

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_n^w(\mathcal{C}_n) - \mathbb{E}_{\mu} [\hat{\tau}_n^w(\mathcal{C}_n)] \right)^2 \right] + \lambda \left(\tau_{n,\mu} - \mathbb{E}_{\mu} [\hat{\tau}_n^w(\mathcal{C}_n)] \right)^2 \quad \in [1/4,1] \cdot \mathcal{B}_n^*(\mathcal{C}_n, w, \lambda) (1 + o(1)).$$

Upper bound The upper bound is a direct consequence of Theorem 6.3.

Lower bound To prove the lower bound, we assume $|\psi_R| \ge |\psi_L|$ without loss of generality; otherwise we replace all $\mu_i(\cdot)$ by $-\mu_i(\cdot)$ and the worst-case MSE does not change. In this case, it must be that $\psi_R \ge \frac{\psi_R + \psi_L}{2} \ge 0$ and $\bar{\psi} = 2\psi_R$. Consider μ that satisfies (46) and

$$(\mu_i(\mathbf{1}), \mu_i(\mathbf{0})) = \begin{cases} (\frac{\psi_R + \psi_L}{2} - \bar{\phi}_n, \psi_R - \bar{\phi}_n) & (\text{if } w_i / ||w||_1 \ge 1/n) \\ (\psi_R, \frac{\psi_R + \psi_L}{2}) & (\text{otherwise}) \end{cases}.$$

In this case, (47) remains to hold and

$$\tau_{n,\mu}^{w} - \tau_{n,\mu} = \sum_{i=1}^{n} (\mu_{i}(\mathbf{1}) - \mu_{i}(\mathbf{0})) \left(\frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right) = -\frac{\psi_{R} - \psi_{L}}{2} \sum_{i=1}^{n} \left| \frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right|.$$

Thus,

$$|\mathbb{E}_{\mu}[\hat{\tau}_{n,\mu}^{w}] - \tau_{n,\mu}| = \bar{\phi}_{n}b_{n}^{w}(\mathcal{C}_{n},\lambda) + \frac{\psi_{R} - \psi_{L}}{2} \sum_{i=1}^{n} \left| \frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right|$$

$$\geq \frac{1}{2} \left(\bar{\phi}_{n}b_{n}^{w}(\mathcal{C}_{n},\lambda) + (\psi_{R} - \psi_{L}) \sum_{i=1}^{n} \left| \frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right| \right).$$
(51)

On the other hand, note that

$$\mu_i(\mathbf{1}) + \mu_i(\mathbf{0}) \ge \psi_R + \frac{\psi_R + \psi_L}{2} - 2\bar{\phi}_n \ge \psi_R - 2\bar{\phi}_n = \bar{\psi}/2 - 2\bar{\phi}_n.$$

By (49),

$$\mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} \left[\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) \right] \right)^{2} \right] \geq \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} w_{i} \right)^{2} \cdot \frac{1}{4} \bar{\psi}(1+o(1)) + o(1/K_{n}).$$

By (50),

$$\mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} \left[\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) \right] \right)^{2} \right] \ge \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} w_{i} \right)^{2} \cdot \frac{1}{4} \bar{\psi}(1+o(1)). \tag{52}$$

Putting together (51) and (52), we conclude that

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu} \left[\left(\hat{\tau}_{n}^{w}(\mathcal{C}_{n}) - \mathbb{E}_{\mu} [\hat{\tau}_{n}^{w}(\mathcal{C}_{n})] \right)^{2} \right] + \lambda \left(\tau_{n,\mu} - \mathbb{E}_{\mu} [\hat{\tau}_{n}^{w}(\mathcal{C}_{n})] \right)^{2}$$

$$\geq \frac{1}{4} \mathcal{B}_{n}^{*}(\mathcal{C}_{n}, w, \lambda) (1 + o(1)).$$

Remark 10. From the above proof, it is not hard to show that the worst-case MSE, up to 1 + o(1) terms, can be formulated as

$$\max_{\mu_{i}(\mathbf{1}),\mu_{i}(\mathbf{0})\in[\psi_{L},\psi_{R}]} \frac{1}{\|w\|_{1}^{2}} \sum_{k=1}^{K_{n}} \left(\sum_{i:c(i)=k} w_{i}(\mu_{i}(\mathbf{1}) + \mu_{i}(\mathbf{0})) \right)^{2} + \lambda \left(\bar{\phi}_{n} b_{n}^{w}(\mathcal{C}_{n}) + \sum_{i=1}^{n} (\mu_{i}(\mathbf{1}) - \mu_{i}(\mathbf{0})) \left(\frac{w_{i}}{\|w\|_{1}} - \frac{1}{n} \right) \right)^{2}$$

C.14 Proof of Theorem 6.5

Upper bound on the worst-case bias. Consider first the worst-case bias. Following the argument in the proof of Lemma 3.1,

$$\sup_{\mu \in \mathcal{M}} \left| \mathbb{E}_{\mu}[\hat{\tau}_{n}] - \tau_{n,\mu} \right| \leq \sup_{\mu(1,\cdot) \in \otimes_{i=1}^{n} \mathcal{M}_{1,i}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1}) | D_{i} = 1 \right] \right| + \sup_{\mu(0,\cdot) \in \otimes_{i=1}^{n} \mathcal{M}_{0,i}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{0}) | D_{i} = 0 \right] \right|.$$

Following verbatim the proof of Lemma 3.1, we can write

$$\sup_{\mu(1,\cdot)\in\otimes_{i=1}^{n}\mathcal{M}_{1,i}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{1}) | D_{i} = 1 \right] \right| = \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \mathbb{E} \left[\sum_{k\in\mathcal{N}_{i}} (1 - D_{k}) | D_{i} = 1 \right]$$

$$\leq \frac{\bar{\phi}_{n}}{2n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \left| j \in \mathcal{N}_{i} : c(i) \neq c(j) \right| + \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \left(|\mathcal{N}_{i}| - \sum_{k\in\mathcal{N}_{i}} \mathbb{E}[D_{k}|D_{i} = 1] \right) 1 \{ c(i) = c(k) \},$$

where the first term of the second line uses the fact that $\mathbb{E}[(1-D_k) \mid D_i = 1] = 1 - (q_1 + q_0)/2 = 1/2$ if $c(k) \neq c(i)$. For c(i) = c(k), we can write

$$\mathbb{E}[D_k|D_i=1] = \frac{P(D_k=1,D_i=1)}{P(D_i=1)} = 2P(D_k=1,D_i=1) = (q_1^2 + q_0^2).$$

Similarly, we can write

$$\sup_{\mu(0,\cdot)\in\otimes_{i=1}^{n}\mathcal{M}_{0,i}} \left| \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[\mu_{i}(D_{i}, \mathbf{D}_{-i}) - \mu_{i}(\mathbf{0}) | D_{i} = 0 \right] \right| \\
\leq \frac{\bar{\phi}_{n}}{2n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \left| j \in \mathcal{N}_{i} : c(i) \neq c(j) \right| + \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} \left(\sum_{k \in \mathcal{N}_{i}} \mathbb{E}[D_{k} | D_{i} = 0] \right) 1\{c(i) = c(k)\}.$$

For c(i) = c(k), we can write

$$\mathbb{E}[D_k|D_i=0] = \frac{P(D_k=1, D_i=0)}{P(D_i=0)} = q_0(1-q_0) + q_1(1-q_1).$$

By collecting terms, we can write (since $q_1 + q_0 = 1$)

$$\sup_{\mu \in \mathcal{M}} \left| \mathbb{E}_{\mu}[\hat{\tau}_{n}] - \tau_{n,\mu} \right| \leq \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} |j \in \mathcal{N}_{i} : c(i) \neq c(j)|$$

$$+ \frac{\bar{\phi}_{n}}{n} \sum_{i=1}^{n} \frac{1}{|\mathcal{N}_{i}|} 2(1 - q_{1}^{2} - q_{0}^{2}) |\mathcal{N}_{i} \bigcap \{j \in \mathcal{N}_{i} : c(i) = c(j)\} |.$$

Since $q_1 + q_0 = 1$, $1 - q_1^2 - q_0^2 = (q_1 + q_0)^2 - q_1^2 - q_0^2 = 2q_1q_0$. Recall the definition (6), we can write the upper bound as

$$\bar{\phi}_n \{b_n(\mathcal{C}_n) + 4q_1q_0(1 - b_n(\mathcal{C}_n))\}.$$

Lower bound (achievability) of worst-case bias Following the proof of lower bound in Lemma 3.1, we can show that the potential outcomes defined in (28) achieves the above upper bound.

Upper bound on the worst-case variance Consider now the variance component. Following verbatim the reasoning of Lemma 3.2, we can write

$$\mathbb{E}\left[\left(\hat{\tau}_n - \mathbb{E}[\hat{\tau}_n]\right)\right] = \frac{4}{n^2} \sum_{i,j:c(i)=c(j)} \operatorname{Cov}\left(D_i, D_j\right) (\mu_i(\mathbf{1}) + \mu_i(\mathbf{0})) (\mu_j(\mathbf{1}) + \mu_j(\mathbf{0})) + o(1/K_n).$$

Thus,

$$\sup_{\mu \in \mathcal{M}} \mathbb{E}\left[\left(\hat{\tau}_n - \mathbb{E}[\hat{\tau}_n]\right)\right] \le \frac{4}{n^2} \sum_{i,j:c(i)=c(j)} \operatorname{Cov}\left(D_i, D_j\right) \bar{\psi} + o(1/K_n).$$

Note that we can write for c(i) = c(j),

$$\mathbb{E}[D_i D_j] - \mathbb{E}[D_i] \mathbb{E}[D_j] = \left[\frac{q_1^2 + q_0^2}{2} - \frac{1}{4} \right] = \frac{1}{4} (2q_1^2 + 2q_0^2 - 1).$$

Since
$$q_1 + q_0 = 1$$
, $2q_1^2 + 2q_0^2 - 1 = 2q_1^2 + 2q_0^2 - (q_1 + q_0)^2 = (q_1 - q_0)^2$.

Lower bound (achievability) of worst-case variance Following the proof of lower bound in Lemma 3.2, we can show that the potential outcomes defined in (28) also achieves the above upper bound.

Worst-case MSE Since (28) achieves both the worst-case bias and variance, the worst-case MSE is simply their sum.

C.15 Proof of Lemma B.1

First, we note that $\tilde{\epsilon}$ does not depend on **d** and

$$\mathbf{C}(\mathbf{d}) \equiv \mathbf{C} \triangleq \operatorname{Cor}((\mathbf{I} - \gamma_n \mathbf{L})^{-1} \epsilon) = \mathbf{D}_n^{-1/2} (\mathbf{I} - \gamma_n \mathbf{L})^{-2} \mathbf{D}_n^{-1/2},$$

where

$$\mathbf{D}_n = \operatorname{diag}((\mathbf{I} - \gamma_n \mathbf{L})^{-2})$$

It is well-known that the unnormalized Laplacian V - A is positive semi-definite (e.g. Von Luxburg, 2007). Thus, $V^{-1/2}AV^{-1/2} \leq I$, implying that

$$\|\mathbf{L}\|_{\mathrm{op}} = \|\mathbf{V}^{-1/2} \cdot \mathbf{V}^{-1/2} \mathbf{A} \mathbf{V}^{-1/2} \cdot \mathbf{V}^{1/2}\|_{\mathrm{op}} \le \|\mathbf{V}^{1/2}\|_{\mathrm{op}} \cdot \|\mathbf{V}^{-1/2}\|_{\mathrm{op}}.$$

Since A is connected, the minimum degree is at least 1. Thus,

$$\|\mathbf{L}\|_{\mathrm{op}} \leq \sqrt{\mathcal{N}_{n,\mathrm{max}}}.$$

Since $\gamma_n \sqrt{N_{n,\text{max}}} = o(1)$, for sufficiently large n,

$$\|\gamma_n \mathbf{L}\|_{\text{op}} < 1/2 \Longrightarrow \|\mathbf{I} - \gamma_n \mathbf{L}\|_{\text{op}} > 1/2.$$

Then

$$\|(\mathbf{I} - \gamma_n \mathbf{L})^{-1} - \mathbf{I}\|_{\mathrm{op}} = \|(\mathbf{I} - \gamma_n \mathbf{L})^{-1} \cdot \gamma_n \mathbf{L}\|_{\mathrm{op}} < 2\|\gamma_n \mathbf{L}\|_{\mathrm{op}} = o(1).$$

As a result,

$$\|(\mathbf{I} - \gamma_n \mathbf{L})^{-2} - \mathbf{I}\|_{\mathrm{op}} = o(1),$$

and

$$\|\mathbf{D}_n - \mathbf{I}\|_{\mathrm{op}} = o(1).$$

Therefore,

$$\|\mathbf{C} - \mathbf{I}\|_{\mathrm{op}} = o(1).$$