Statistical matching and subclassification with a continuous dose: characterization, algorithms, and inference

Bo Zhang\(^1\), Emily J. Mackay\(^2\), Mike Baiocchi\(^3\)

\(^1\)Department of Statistics, The Wharton School, University of Pennsylvania, Philadelphia, Pennsylvania, USA  Correspondence: bozhan@wharton.upenn.edu
\(^2\)Department of Anesthesiology and Critical Care, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania, USA
\(^3\)Stanford Prevention Research Center, Stanford University, Palo Alto, California, USA

Abstract: Subclassification and matching are often used to adjust for observed covariates in observational studies; however, they are largely restricted to relatively simple study designs with a binary treatment. One important exception is Lu et al. (2001), who considered optimal pair matching with a continuous treatment dose. In this article, we propose two criteria for optimal subclassification/full matching based on subclass homogeneity with a continuous treatment dose, and propose an efficient polynomial-time algorithm that is guaranteed to find an optimal subclassification with respect to one criterion and serves as a 2-approximation algorithm for the other criterion. We discuss how to incorporate treatment dose and use appropriate penalties to control the number of subclasses in the design. Via extensive simulations, we systematically examine the performance of our proposed method, and demonstrate that combining our proposed subclassification scheme with regression adjustment helps reduce model dependence for parametric causal inference with a continuous treatment dose. We illustrate the new design and how to conduct randomization-based statistical inference under the new design using Medicare and Medicaid claims data to study the effect of transesophageal echocardiography (TEE) during CABG surgery on patients’ 30-day mortality rate.

Keywords: Approximation algorithm; Continuous dose; Edge cover; Full match; Subclassification

1 Bipartite versus non-bipartite matching

1.1 Statistical matching with a binary treatment

In an observational study of a treatment’s effect on the outcome, units involved in the study may differ systematically in their observed pretreatment covariates, thus invalidating a naive comparison between the treated and control groups. Statistical matching and subclassification are commonly used nonparametric strategies to adjust for covariates. For a binary treatment, the ultimate goal
of statistical matching is to embed observational data into an approximate randomized experiment by designing a treated group and a control (or comparison) group that are comparable in their observed covariates in order to reduce bias in the outcome analysis. In his seminal work, Rosenbaum (1989) first formulated the statistical matching problem with a binary treatment as a combinatorial optimization problem of finding a minimum cost flow in a bipartite graph, for which efficient polynomial-time algorithms exist. Many other important developments ensued. Rosenbaum (1991) characterized an optimal design in an observational study with a binary treatment, known as the “full matching”. In a full matching design, matched sets consist of either one treated unit and multiple control units, or one control unit and multiple treated units. Hansen (2004) applied full matching to a study of coaching for the SAT and Hansen and Klopfer (2006) developed efficient network-flow-based algorithms for full matching. Rosenbaum et al. (2007) proposed “fine balance,” a statistical matching tool that exactly balances a few nominal variables. Yang et al. (2012) showed how to obtain “near-fine balance” when fine balance is not attainable, and Pimentel et al. (2015) proposed “refined covariate balance,” in which a sequence of nested, ever more refined, nominal covariates is balanced as closely as possible. More recently, Yu et al. (2020) made network-flow-based matching algorithms even more efficient and scalable by first sparsifying the network and made it feasible to match data from large administrative datasets. Other widely used statistical matching techniques and algorithms include coarsened exact matching (Iacus et al., 2011), integer-programming-based algorithms (Li et al., 2001; Zubizarreta, 2012), and the genetic matching algorithm (Diamond and Sekhon, 2013). R packages optmatch (Hansen, 2007), Matching (Sekhon, 2008), and MatchIt (Stuart et al., 2011) implement most of the aforementioned statistical matching techniques. For more comprehensive reviews on statistical matching, see Ho et al. (2007), Stuart (2010), and Rosenbaum (2002, 2010, 2020). We diverge from these methods quite a bit in this article by considering matching in the context of continuous doses.

1.2 Statistical matching with a continuous dose: optimal non-bipartite pair matching

While statistical matching techniques for a binary treatment abound, they are less developed for a categorical or continuous treatment dose, with a few exceptions (Lu et al. 2001, 2011; Karmakar et al. 2019; Sävje et al. 2020; Nattino et al. 2020). One important development is Lu et al. (2001), who studied “optimal non-bipartite pair matching,” an algorithm that divides \( N = 2I \) units into \( I \) non-overlapping pairs in an optimal way such that the total within-matched-pair distance after matching is minimized. Figure 1 gives a graphical representation of the difference between the
bipartite and non-bipartite setting. In the non-bipartite setting, there is no pre-defined treated or control group, and in principle any unit can be matched to any other unit. Lu et al. (2001)’s optimal non-bipartite pair matching is an analogue of Rosenbaum (1989)’s optimal pair matching when having a continuous treatment dose. R package `nbpmatching` (Lu et al., 2011) implements optimal non-bipartite pair matching using Derig’s efficient polynomial-time algorithm (Derigs, 1988), with a complexity of $O(N^3)$. More recently, optimal non-bipartite pair matching techniques have been successfully applied to instrumental variable studies with a continuous instrumental variable (or encouragement dose); such methods are often referred to as the “near-far” matching in the literature (Baiocchi et al., 2010, 2012) and implemented in the R package `nearfar` (Rigdon et al., 2018).

Figure 1: Left panel: a pair match in a bipartite setting with a binary treatment. Right panel: a pair match in a non-bipartite setting with a many-leveled or continuous treatment dose.

1.3 Pair matching with a continuous or many-leveled dose is not optimal

With a binary treatment, Rosenbaum (1991) found that “there may be no pair matching and no matching with multiple controls that is an optimal subclassification,” and that “a best pair match may be arbitrarily poor compared with the optimal full matching”. These statements remain true in the non-bipartite setting with a continuous dose. To see this, it suffices to consider the following...
simple example with 6 units \( \{a, b, c, d, e, f\} \) and the associated distance matrix

\[
M = \begin{pmatrix}
a & b & c & d & e & f \\
a & 0 & \epsilon & \omega & \omega & \omega \\
b & \epsilon & 0 & \epsilon & \omega & \omega \\
c & \epsilon & \epsilon & 0 & \omega & \omega \\
d & \omega & \omega & \omega & 0 & \epsilon \\
e & \omega & \omega & \omega & \epsilon & 0 \\
f & \omega & \omega & \omega & \epsilon & 0 \\
\end{pmatrix}
\]

with \( \epsilon \ll \omega \). The \( ij \)th entry of \( M \) represents a measure of distance, e.g., the Mahalanobis distance of observed covariates, between unit \( i \) and \( j \). An optimal pair match produces the following three matched pairs:

\[
\Pi_{\text{pair}} = \{ \{a, c\}, \{b, d\}, \{e, f\} \}.
\]

On the other hand, full matching divides \( N \) units into non-overlapping matched sets (or subclasses) of size at least 2. Consider the following full match:

\[
\Pi_{\text{full}} = \{ \{a, b, c\}, \{d, e, f\} \}.
\]

It is evident that in this case \( \Pi_{\text{full}} \) achieves a better matched-sets homogeneity, which we will carefully define later, compared to the optimal non-bipartite pair match \( \Pi_{\text{pair}} \) when \( \epsilon \ll \omega \). See Figure 2 for a more transparent graphical representation. Moreover, since \( \omega \) can be arbitrarily larger than \( \epsilon \), \( \Pi_{\text{full}} \) can be arbitrarily better than \( \Pi_{\text{pair}} \) according to any reasonable homogeneity measure. In the most extreme case with \( \omega = \infty \), there exists no admissible pair match that uses all six units; however, there does exist a feasible full match, and a pretty good one when \( \epsilon \) is small. Lastly, one minor issue with pair matching is that, when the number of units is odd, say \( N = 5 \), the design necessarily discards one unit in order to produce 2 matched pairs; this is no longer a concern with full matching.
Figure 2: Left panel: a full matching $\Pi_{\text{full}}$ dividing six units into two matched sets of three each. Right panel: a pair matching $\Pi_{\text{pair}}$ dividing six units into three matched pairs. When $\omega \gg \epsilon$, the full matching approach on the left yields matched sets with superior homogeneity than the pair matching approach on the right.

1.4 Outline: a characterization of non-bipartite full matching designs, an algorithm, two simulation studies, and an application

Two subclassification homogeneity measures and optimal subclassification with respect to each measure are defined in Section 2. Section 3 proves a useful relationship between the two homogeneity measures; this relationship suggests that any algorithm that finds a subclassification with respect to one homogeneity measure is automatically a 2-approximation algorithm for the other measure. An efficient, polynomial-time algorithm that finds an optimal subclassification with respect to one homogeneity measure and suitable weights is presented in Section 4. Section 5 discusses how to further incorporate the treatment dose in the design stage, and how to probe the middle ground between optimal pair matching and optimal subclassification. Two simulation studies, one examining how combining the proposed subclassification scheme with regression adjustment helps reduce bias of the regression estimator, and the other systematically comparing the proposed subclassification method to optimal pair matching, are presented in Section 6 and 7 respectively. Finally, we apply the proposed design to a study of the effect of transesophageal echocardiography (TEE) during CABG surgery on patients’ 30-day mortality [MacKay et al., 2020; Zhang et al., 2020] in Section 8 and conduct randomized-based inference in Section 9. We conclude with a brief discussion in Section 10.

2 Two measures of subclassification homogeneity

Let $N = \{1, 2, \cdots, N\}$ denote a set of $N$ units and $2^N$ its power set, i.e., the collection of all subsets of $N$. Let $\Pi = \{\Pi_1, \Pi_2, \cdots, \Pi_K\}$ denote a subclassification (or partition) of these $N$ units into $K$ non-overlapping subclasses such that each subclass $\Pi_k$ consists of $|\Pi_k| \geq 2$ units, $\sum_{1 \leq k \leq K} |\Pi_k| = N$, and their union $\bigcup_{1 \leq k \leq K} \Pi_k$ recovers these $N$ units. Finally, let $|\Pi|$ denote the number of subclasses in $\Pi$ and $A$ the set of all possible subclassifications. We first develop notions
of subclass homogeneity.

**Definition 1** (Average pairwise homogeneity). Let $\delta(i, j)$ denote the distance between unit $i$ and $j$. *Average pairwise homogeneity* of subclass $\Pi_k$, denoted as $\nu(\Pi_k)$, refers to the following quantity:

$$
\nu(\Pi_k) = \frac{1}{|\Pi_k| \times (|\Pi_k| - 1)} \sum_{i,j \in \Pi_k, i \neq j} \delta(i, j).
$$

(1)

According to Definition 1, $\nu(\Pi_k)$ is the average distance of all pairwise comparisons among units in subclass $\Pi_k$. Associated with a subclassification $\Pi$ and $\nu(\Pi_k)$ is the following homogeneity measure of $\Pi$:

$$
\nu(\Pi; \mathcal{W}) = \sum_{1 \leq k \leq |\Pi|} w(\Pi_k) \times \nu(\Pi_k),
$$

(2)

where $\mathcal{W} : 2^N \mapsto \mathbb{R} \geq 0$ is a pre-specified weighting scheme that maps each possible subclass $\Pi_k \in 2^N$ to a non-negative real number.

**Definition 2.** A subclassification $\Pi_{\text{opt}}^\nu$ is said to be optimal with respect to the homogeneity measure $\nu(\Pi; \mathcal{W})$ if

$$
\Pi_{\text{opt}}^\nu = \arg \min_{\Pi \in \mathcal{A}} \nu(\Pi; \mathcal{W}).
$$

Definition 2 gives a second sensible criterion that measures subclass homogeneity.

**Definition 3** (Star homogeneity). Let $i^*_k \in \Pi_k$ be a reference unit in subclass $\Pi_k$. *Star homogeneity* refers to the following quantity:

$$
\nu_{\text{star}}(\Pi_k; i^*_k) = \frac{1}{|\Pi_k| - 1} \sum_{j \in \Pi_k, j \neq i^*_k} \delta(i^*_k, j).
$$

(3)

Unlike $\nu(\Pi_k)$ which averages over all pairwise comparisons, $\nu_{\text{star}}(\Pi_k; i^*_k)$ first picks a reference unit, e.g., the one with the highest or lowest dose in the subclass, compares all other units to this reference unit, and then averages over such comparisons. Associated with a subclassification $\Pi$, the star homogeneity, a vector of reference units $i^* = (i^*_1, \ldots, i^*_{|\Pi|})$, $i^*_k \in \Pi_k$, and a weighting scheme $\mathcal{W}$ is a second homogeneity measure of $\Pi$:

$$
\nu_{\text{star}}(\Pi; i^*, \mathcal{W}) = \sum_{1 \leq k \leq |\Pi|} w(\Pi_k) \times \nu_{\text{star}}(\Pi_k; i^*_k).
$$

(4)
Definition 4. A subclassification $\Pi_{\text{opt}}^{\star} = \{\Pi_{\text{opt},1}^{\star}, \ldots, \Pi_{\text{opt},K}^{\star}\}$ with reference units $i_{\text{opt}}^{\star} = (i_{\text{opt},1}^{\star}, \ldots, i_{\text{opt},K}^{\star})$, $i_{\text{opt},k}^{\star} \in \Pi_{\text{opt},k}^{\star}$, is said to be optimal with respect to the homogeneity measure $\nu_{\text{star}}(\Pi; i^{\star}, \mathcal{W})$ if

$$(\Pi_{\text{opt}}^{\star}, i_{\text{opt}}^{\star}) = \arg \min_{\Pi \in A} \arg \min_{i^{\star} \in \Pi_{k}^{\star}, 1 \leq k \leq |\Pi|} \nu_{\text{star}}(\Pi; i^{\star}, \mathcal{W}),$$

where minimization is taken over all subclassifications and possible reference units in each subclass.

Remark 1. In the special case of pair matching, it is easy to check that $\forall i_{k}^{\star} \in \Pi_{k}^{\star}, \nu_{\text{star}}(\Pi_{k}^{\star}; i_{k}^{\star}) = \nu(\Pi_{k})$ for all $\Pi_{k} \in \Pi$, i.e., two measures of subclass homogeneity reduce to the same measure. Moreover, under a weighting scheme that assigns the same weight to all matched pairs, we have $\Pi_{\text{opt}}^{\star} = \Pi_{\text{opt}}^{\nu}$ and this optimal solution is precisely returned by an optimal non-bipartite pair matching algorithm described in Section 1.2.

3 Relationship between $\Pi_{\text{opt}}^{\star}$ and $\Pi_{\text{opt}}^{\nu}$

A subclassification $\Pi_{\text{opt}}^{\star}$ is optimal with respect to the homogeneity measure $\nu_{\text{star}}(\cdot)$ and a weighting scheme $\mathcal{W}$. A natural question arises as to what can be said about its homogeneity under the other measure $\nu(\cdot)$, and how $\nu(\Pi_{\text{opt}}^{\star}; \mathcal{W})$ compares to the optimal $\nu(\cdot)$ homogeneity under the same weights. This section establishes a revealing relationship between $\nu(\Pi_{\text{opt}}^{\star}; \mathcal{W})$ and $\nu(\Pi_{\text{opt}}^{\nu}; \mathcal{W})$.

Lemma 1. Let $\Pi_{k}$ be a subclass with size $|\Pi_{k}|$ and $\delta(i, j)$ a distance that satisfies the triangle inequality. We have

$$\min_{i_{k}^{\star} \in \Pi_{k}} \nu_{\text{star}}(\Pi_{k}; i_{k}^{\star}) \leq \nu(\Pi_{k}),$$

and

$$\nu(\Pi_{k}) \leq \frac{2(|\Pi_{k}| - 1)}{|\Pi_{k}|} \cdot \nu_{\text{star}}(\Pi_{k}; i_{k}^{\star}), \ \forall i_{k}^{\star} \in \Pi_{k}.$$ 

In particular, when $|\Pi_{k}| = 2$, we have $\nu_{\text{star}}(\Pi_{k}; i_{k}^{\star}) = \nu(\Pi_{k}), \ \forall i_{k}^{\star} \in \Pi_{k}$.

Proof. All proofs in this article are in Supplementary Material A.

Let $\nu_{\text{star}}^{\star}(\Pi_{k}) := \min_{i_{k}^{\star} \in \Pi_{k}} \nu_{\text{star}}(\Pi_{k}; i_{k}^{\star})$ be the minimum $\nu_{\text{star}}(\cdot)$ homogeneity of a subclass $\Pi_{k}$ among all reference units $i_{k}^{\star} \in \Pi_{k}$. Define

$$\nu_{\text{star}}^{\star}(\Pi; \mathcal{W}) = \sum_{1 \leq k \leq |\Pi|} w(\Pi_{k}) \cdot \nu_{\text{star}}^{\star}(\Pi_{k}).$$
Corollary 1. For any subclass \( \Pi_k \), we have
\[
\nu^*_\text{star}(\Pi_k) \leq \nu(\Pi_k) \leq 2(|\Pi_k| - 1) \cdot \nu^*_\text{star}(\Pi_k).
\]
Moreover, for any subclassification \( \Pi \) and weighting scheme \( \mathcal{W} \), we have
\[
\nu^*_\text{star}(\Pi; \mathcal{W}) \leq \nu(\Pi; \mathcal{W}) < 2\nu^*_\text{star}(\Pi; \mathcal{W}).
\]

Corollary 1 establishes a link between two homogeneity measures \( \nu(\Pi; \mathcal{W}) \) and \( \nu^*_\text{star}(\Pi; \mathcal{W}) \): any subclassification \( \Pi \) has its \( \nu(\Pi; \mathcal{W}) \) sandwiched between \( \nu^*_\text{star}(\Pi; \mathcal{W}) \) and \( 2\nu^*_\text{star}(\Pi; \mathcal{W}) \). Proposition 1 is an important consequence of Corollary 1.

Proposition 1. Let \( \Pi^\nu_{\text{opt}} \) be an optimal partition with respect to the homogeneity measure \( \nu(\cdot) \) and weighting scheme \( \mathcal{W} \), and \( \Pi^\nu_{\text{opt}} \) optimal with respect to \( \nu(\cdot) \) and the same weighting scheme. We have
\[
\nu(\Pi^\nu_{\text{opt}}; \mathcal{W}) \leq \nu(\Pi_{\text{opt}}^\nu; \mathcal{W}) < 2\nu(\Pi^\nu_{\text{opt}}; \mathcal{W}).
\]
In words, \( \Pi^\nu_{\text{opt}} \) is optimal under the homogeneity measure \( \nu(\cdot) \), and its homogeneity under the other measure \( \nu(\cdot) \) is no worse than the optimal homogeneity under \( \nu(\cdot) \) by a factor of 2.

In the computer science and operations research literature, an approximation algorithm refers to an algorithm that finds an approximate solution to an optimization problem with a provable guarantee on the distance between the approximate solution and the optimal solution; see Vazirani (2013) and Williamson and Shmoys (2011) for general discussion. A \( \rho \)-approximation algorithm refers to an approximation algorithm that returns an approximate solution \( x^\text{approx} \) whose objective function value \( f^\text{approx} \) is no worse than that of the optimal solution \( f_{\text{opt}} \) by a factor of \( \rho \), i.e.,
\[
f_{\text{opt}} \leq f^\text{approx} \leq \rho \times f_{\text{opt}}.
\]

Corollary 2 is an immediate consequence of Proposition 1.

Corollary 2. Let \( \Pi^\nu_{\text{opt}} \) and \( \Pi^\nu_{\text{opt}}^\text{star} \) be defined as in Definition 2 and Definition 4 with respect to the same weighting scheme \( \mathcal{W} \). If ALG is an algorithm for finding \( \Pi^\nu_{\text{opt}}^\text{star} \), then ALG is also a 2-approximation algorithm for finding \( \Pi^\nu_{\text{opt}} \).

Corollary 2 is important and useful because efficient, polynomial-time algorithms do exist for finding \( \Pi^\nu_{\text{opt}}^\text{star} \) with respect to suitable weights, as we demonstrate in the next section.
4 Efficient, polynomial-time algorithms for finding $\Pi_{\text{opt}}^{\text{star}}$ with respect to suitable weights

4.1 Graph, edge cover, and suitable weights

We introduce some useful terminologies from the graph theory to carry forward the discussion. Let $G = (V, E)$ denote a graph with vertex set $V$ and edge set $E$. We use $e = (i, j)$, $i, j \in V$, to denote an edge connecting vertex $i$ and $j$, in which case we say vertex $i$ (and similarly $j$) is incident to edge $e = (i, j)$. A subset of edges $S \subseteq E$ is said to form a star if $S = \{(i, j_1), (i, j_2), \ldots, (i, j_k)\}$; $i$ is often referred to as the internal node or center of the star, and $\{j_1, j_2, \ldots, j_k\}$ leaves.

An edge cover of graph $G$ is a subset of edges $F \subseteq E$ such that all vertices in $G$ are incident to at least one edge in $F$. Let $F$ denote the class of all edge covers of graph $G$, and each edge $e = (i, j)$ be associated with a nonnegative cost $c(i, j)$. The cost of an edge cover $F$ is defined to be

$$\text{COST}(F) = \sum_{(i, j) \in F} c(i, j).$$

Figure 3 gives two examples of an edge cover in the same graph. The cost of the edge cover in the left panel is $1 + 2 + 1.5 + 3 + 4 = 11.5$, and that in the right panel is $1 + 3 + 2 + 3 + 1 + 4 = 14$.

![Figure 3: Two edge covers (bold lines) of the same graph. The cost of the edge cover in the left panel is 11.5 and that in the right panel is 14.](image)

Lemma 2 states that for a suitable choice of weights, homogeneity measure $\nu_{\text{star}}(\Pi; i^*, W)$ corresponds to the cost of a particular edge cover.
Lemma 2. Let $\Pi = \{\Pi_1, \ldots, \Pi_K\}$ be a partition, and $W^{\text{suit}}$ a weighting scheme that assigns $w(\Pi_k) = |\Pi_k| - 1$ to subclass $\Pi_k$. Then

$$\nu_{\text{star}}(\Pi; i^*, W^{\text{suit}}) = \sum_{1 \leq k \leq K} \sum_{j \in \Pi_k, j \neq i_k^*} \delta(i_k^*, j),$$

and $\nu_{\text{star}}(\Pi; i^*, W^{\text{suit}})$ is equal to the cost of an edge cover with connected components $\{\Pi_1, \ldots, \Pi_K\}$ and each connected component $\Pi_k$ being a star with internal vertex $i_k^*$ and leaves $\{j \in \Pi_k, j \neq i_k^*\}$.

4.2 A minimum cost edge cover induces an optimal subclassification $\Pi_{\text{opt}}^{\text{star}}$ with respect to suitable weights

A minimum cost edge cover, i.e., the edge cover that attains the minimum cost among all edge covers of $G$, can be efficiently found in polynomial time (Schrijver, 2003); in fact, the problem of finding a minimum cost edge cover can be reduced to the problem of finding a minimum cost matching in an expanded non-bipartite graph. Moreover, Proposition 2 states that a minimum cost edge cover induces an optimal subclassification with respect to the homogeneity measure $\nu_{\text{star}}(\Pi; i^*, W^{\text{suit}})$ when the edge cost is nonnegative.

Proposition 2. Let $G = (V,E)$ be a graph and $c : E \mapsto \mathbb{R}^{\geq 0}$ a nonnegative cost function. Then

1. There exists a minimum cost edge cover whose connected components are all stars; call this minimum cost star-tiled edge cover $F_{\text{star}}^*$.

2. Let the cost function $c(\cdot)$ of edge $e = (i,j)$ be the distance $\delta(i,j)$, then

$$\text{COST}(F_{\text{star}}^*) = \min_{\Pi \in A; \ i_k^* \in \Pi_k, 1 \leq k \leq |\Pi|} \nu_{\text{star}}(\Pi; i^*, W^{\text{suit}}).$$

In other words, $F_{\text{star}}^*$ induces an optimal subclassification with respect to the homogeneity measure $\nu_{\text{star}}(\Pi; i^*, W^{\text{suit}})$.

4.3 An efficient algorithm that finds minimum cost edge cover

Algorithm 1 transforms the problem of finding a minimum cost edge cover into an optimal non-bipartite matching problem (Schrijver, 2003), the computation complexity of which is $O(|V|^3)$ in a graph with $|V|$ vertices. Algorithm 1 returns a minimum cost edge cover $F^*$; we may further process $F^*$ as described in the proof of Proposition 2 to obtain $F_{\text{star}}^*$, a minimum cost edge cover.
consisting of all stars. It is evident that the complexity of finding a minimum cost edge cover is
the same as optimal non-bipartite matching. The algorithm is further illustrated in Figure 4. We
will refer to the subclassification scheme induced by $F_{\text{star}}^*$ as a “non-bipartite full match design”.

Algorithm 1. Finding a minimum cost edge cover for a graph $G = (V, E)$

**Input:** A graph $G = (V, E)$

1. Create a copy of $G = (V, E)$ with the same topology and edge cost; denote it as
   $G' = (V', E')$.

2. For each $v \in V$ and its counterpart $v' \in V'$, add an edge $(v, v')$; a total of $|V|$ edges are
   added.

3. Assign a cost equal to $2\mu(v)$ to each edge $(v, v')$, where $\mu(v)$ denotes the minimum cost
   among all edges incident to $v \in V$.

4. Solve an optimal non-bipartite matching problem in the graph $G \cup G'$; let $M^*$ denote this
   optimal matching.

5. Delete from $M^*$ any edge in $E'$; replace any edge of the form $(v, v')$ in $M^*$ with an edge
   $(v, u) \in E$ such that $\delta(v, u) = \mu(v)$; denote by $F^*$ the result;

6. Return the minimum cost edge cover $F^*$.

5 Other design considerations

5.1 Incorporating treatment/encouragement doses

With a binary treatment, there is a distance between each treated unit and each control unit, and
this distance unequivocally measures the closeness of the treated and control units in their observed
covariates. With a continuous or many-leveled treatment/encouragement dose, homogeneity in
observed covariates is still an important aspect; however, distances in this case may further take into
account the treatment/encouragement dose in order to design matched sets that are homogeneous
in observed covariates and well-separated in their treatment/encouragement doses [Lu et al., 2001].

This is in particular relevant in instrumental variable studies with a continuous encouragement
dose (i.e., a continuous instrumental variable). It is widely acknowledged that confidence inter-
vals obtained from weak instruments are often excessively long and non-informative [Imbens and
Rosenbaum, 2005]. On the other hand, a large encouragement dose would typically create stronger
incentives for units to accept the treatment, increase the compliance rate, and eventually render the
statistical inference substantially more powerful [Baiocchi et al., 2010; Heng et al., 2019b; Zhang...
Figure 4: Top left: a graph $G = (V, E)$ representing 5 units to be matched. Right: a mirror copy of $G$ is made; 5 edges connecting $v \in G$ and its counterpart $v' \in G'$ are added, each associated with a cost of $2\mu(v)$; optimal non-bipartite matching $M^*$ on the union graph consists of edges in red. Bottom left: two edges in $M^*$ and also in $E'$ are removed; an edge connecting $v \in G$ and $v' \in G'$ is rewired to the corresponding vertex in $G$; the final minimum cost edge cover $F^*$ consists of edges in red.

et al., 2020). For instance, Heng et al. (2019b) derived the asymptotic relative efficiency (ARE) of some commonly-used test statistics when testing the same proportional treatment effect model (Small and Rosenbaum, 2008) with two instrumental variables of different strengths. They found that for a weaker IV with compliance rate $\iota_1$ to achieve the same efficiency as a stronger IV with compliance rate $\iota_2$ ($\iota_2 \geq \iota_1$), the weaker IV needs to have a sample size $(\iota_2/\iota_1)^2$ times larger than that of a stronger IV. Analytic results of this kind provide incentives to separate treatment/encouragement doses in the design stage of an observational study.

How to pursue this design aspect in a non-bipartite full match? Let $\delta(i, j)$ measure the distance between observed covariates, and $Z_i$ and $Z_j$ the encouragement doses of unit $i$ and $j$, respectively. One straightforward way to incorporate the encouragement dose is to define a new distance $\delta'(i, j) = \delta(i, j) + C \times 1\{|Z_i - Z_j| \leq \tau_0\}$, where $C$ is a large penalty applied when the doses of $i$ and $j$ differ by less than or equal to $\tau_0$. Hence, a large $C$ would facilitate an edge cover connecting unit $i$ and
j whose encouragement doses differ by more than $\tau_0$. To illustrate this, we simulated a dataset with $d = 3$ covariates and $n = 1000$ units (see Supplementary Material A.1 for detailed data generating process). For each $\tau_0 \in \{0, 0.1, 0.2, 0.3, 0.4, 0.5\}$, we run Algorithm 1 with $\delta(i,j)$ being the Mahalanobis distance and $C = 100,000$ a large penalty, and report two competing quality measures of a subclassification $\Pi$: $\nu(\Pi_k)$, the average pairwise homogeneity (see Definition 1) of all matched sets $\Pi_k \in \Pi$ (see the left panel of Figure 5), and $\mu(\Pi_k)$, the average absolute “internal-node-minus-leaf” difference in the encouragement dose (for instance, if $\Pi_k$ has 3 units with doses 0.8 (internal node), 0.5 (leaf), and 0.2 (leaf), then $\mu(\Pi_k) = 0.5 \times |0.8 - 0.5| + 0.5 \times |0.8 - 0.2| = 0.45$) of all matched sets $\Pi_k \in \Pi$ (see the right panel of Figure 5). We see a clear pattern of trade-off between $\nu(\Pi_k)$ and $\mu(\Pi_k)$: as $\tau_0$ grows larger, units in the same matched set tend to become increasingly heterogeneous in the encouragement dose, and less homogeneous in the observed covariates. Homogeneity in matched sets reduces bias in statistical inference (Rubin, 1979), while larger difference in the encouragement dose tends to increase compliance and hence efficiency (Heng et al., 2019b). In this way, the trade-off here can be viewed as a classical “bias-variance” trade-off.

![Figure 5: Left panel: boxplots of average pairwise homogeneity $\nu(\Pi_k)$ of all matched sets in each match with different $\tau_0$. Right panel: boxplots of average “internal-node-minus-leaf” difference $\mu(\Pi_k)$ in the treatment/encouragement dose of all matched sets in each match with different $\tau_0$. The number of matched sets is: 448, 445, 428, 406, 368, and 314.](image)

### 5.2 Incorporating matched-sets-cardinality penalty

In a bipartite full matching, there are two parameters controlling for the maximum number of treated and control units in each matched set, respectively. Options `max.controls` and `min.controls` of function `fullmatch` in the R package `optmatch` (Hansen and Klopfer, 2006; Hansen, 2007) serve...
this purpose. For example, setting \texttt{min.controls} = 0.25 would restrict the matched set to have at most 4 treated subjects for one control, and \texttt{max.controls} = 4 at most 4 controls for one treated; together, they restrict the cardinality of matched sets to be at most 5.

In the context of non-bipartite matching with a continuous dose, we may also want to have some control over the size of subclasses and hence how many subclasses in a subclassification. To this end, we consider adding to a homogeneity measure a proper penalty on the cardinality of subclasses. Let the homogeneity measure be \( \nu_{\text{star}} \), and consider the following modified homogeneity measure:

\[
\nu_{\lambda}^{\text{star}}(\Pi; i^*, W) = \nu_{\text{star}}(\Pi; i^*, W) + \lambda \times \left\{ \sum_{\Pi_k \in \Pi} |\Pi_k| - 2 \right\}.
\]

**Definition 5.** A subclassification \( \Pi_{\text{star}}^{\text{opt, } \lambda} = \{\Pi_{\text{star}}^{\text{opt, } \lambda, 1}, \ldots, \Pi_{\text{star}}^{\text{opt, } \lambda, K}\} \) with reference units \( i_{\text{opt, } \lambda} = (i_{\text{opt, } \lambda, 1}, \ldots, i_{\text{opt, } \lambda, K}) \), \( i_{\text{opt, } \lambda, k} \in \Pi_{\text{opt, } \lambda, k}^{\text{star}} \), is said to be optimal with respect to the homogeneity measure \( \nu_{\lambda}^{\text{star}}(\Pi; i^*, W) \) if

\[
(\Pi_{\text{opt, } \lambda}^{\text{star}}, i_{\text{opt, } \lambda}) = \arg \min_{\Pi \in A} \arg \min_{\Pi_k \in \Pi, 1 \leq k \leq |\Pi|} \nu_{\lambda}^{\text{star}}(\Pi; i^*, W)
\]

\[
= \arg \min_{\Pi \in A} \arg \min_{\Pi_k \in \Pi, 1 \leq k \leq |\Pi|} \left\{ \nu_{\text{star}}(\Pi; i^*, W) + \lambda \times \left\{ \sum_{\Pi_k \in \Pi} |\Pi_k| - 2 \right\} \right\}.
\]

Observe that when \( \lambda = 0 \), this definition reduces to Definition 4, when \( \lambda = \infty \), \( \Pi_{\text{opt, } \lambda}^{\text{star}} \) reduces to the solution to optimal non-bipartite pair matching because \( |\Pi_k| - 2 = 0 \) for matched pairs. As \( \lambda \) increases from 0 to \( \infty \), we are effectively exploring the middle ground between a subclassification that is optimal with respect to \( \nu_{\text{star}}(\Pi; i^*, W) \) and an optimal non-bipartite pair matching.

With suitable weights \( W^{\text{suit}} \), we can find \( \Pi_{\text{opt, } \lambda}^{\text{star}} \) efficiently via a slightly modified version of Algorithm 1; in fact, it suffices to modify Step 3 in Algorithm 1 as follows:

3*. Assign a cost equal to \( 2 \mu(v) + 2 \lambda \) to each edge \((v, v')\), where \( \mu(v) \) denotes the minimum cost among all edges incident to \( v \in V \).

Let \( F^{\ast}_{\lambda} \) denote the output from the modified Algorithm 1. Following a similar argument in the proof of Proposition 2, we may further process \( F^{\ast}_{\lambda} \) to obtain \( F^{\ast}_{\text{star, } \lambda} \), an edge cover consisting of all stars. In Supplementary Material A.5, we prove a result analogous to Proposition 2 which states that \( F^{\ast}_{\text{star, } \lambda} \) induces a subclassification that is optimal with respect to \( \nu_{\text{star}}^{\lambda}(\Pi; i^*, W^{\text{suit}}) \).

We end this section with an illustration. The data generating process is the same as in Section
5.1 with $d = 3$ and $n = 1000$. We run the modified Algorithm 1 with $\lambda = 0.01, 0.1, 1, 10, \text{ and } 100$. Figure 6 summarizes the average pairwise homogeneity $\nu(\Pi_k)$, average absolute “internal-node-minus-leaf” dose difference $\mu(\Pi_k)$, and the number of matched sets $|\Pi|$ of the subclassification under each $\lambda$. We use the same distance as in Section 5.1 with $C = 100,000$ and $\tau_0 = 0.3$ for all $\lambda$. As $\lambda$ increases from 0.01 to 100, we see the number of matched sets increases from 369 to 500 (maximum); the measure for matched-sets homogeneity $\nu(\Pi_k)$ and dose heterogeneity $\mu(\Pi_k)$ are very similar when $\lambda = 0.01, 0.1, \text{ and } 1$, and both deteriorate when $\lambda = 10$ (slightly) and $\lambda = 100$ (significantly). Other things equal (e.g., $\nu(\Pi_k)$ and $\mu(\Pi_k)$), one may prefer a design with more matched sets, as the inference is likely to be more efficient.

Figure 6: Top left panel: boxplots of average pairwise homogeneity $\nu(\Pi_k)$ of all matched sets in each match under different $\lambda$. Top right panel: boxplots of average “internal-node-minus-leaf” difference $\mu(\Pi_k)$ in the dose of all matched sets in each match under different $\lambda$. Bottom panel: number of matched sets against different $\log(\lambda)$. 
6 Simulation studies I: non-bipartite matching as a preprocessing step to remove bias in parametric causal inference with a continuous treatment dose

6.1 Goal and structure

It is widely acknowledged that in a binary treatment setting, combining statistical matching with regression adjustment renders analysis more robust to model misspecification and helps remove bias in treatment effect estimation (Rubin, 1973, 1979); hence, many authors advocate using statistical matching as a nonparametric preprocessing step before parametric causal inference (Ho et al., 2007; Stuart, 2010). The primary goal of this section is to assess if combining the non-bipartite full matching developed in this article and regression adjustment helps reduce model dependence and remove bias in the continuous treatment setting.

Our simulation studies in this section can be compactly represented as a $2 \times 2 \times 2 \times 3 \times 2 \times 4$ factorial study with the following factors:

**Factor 1:** treatment effect estimator: $\hat{\beta}_{reg}$ and $\hat{\beta}_{reg, \text{match}}$.

**Factor 2:** dimension of covariates, $d$: 5 and 10.

**Factor 3:** sample size, $n$: 500 and 2000.

**Factor 4:** treatment dose model: a multi-level treatment $Z \sim \text{Uniform}\{-2, -1, 0, 1, 2\}$; two continuous treatments $Z \sim \text{Uniform}[1 - \sqrt{3}, 1 + \sqrt{3}]$ and $Z \sim \text{Exponential}(1)$ so that the continuous treatment $Z$ has mean 1 and variance 1.

**Factor 5:** observed covariates distribution: $X \sim \text{Multivariate Normal}(\mu, \Sigma)$, with $\mu = (cZ, 0, \cdots, 0)^T$ and $\Sigma = \left( \begin{array}{cc} 2^2 & 0 \\ 0 & I_{d-1} \end{array} \right)$ with $c = -2$ and 2.

**Factor 6:** response model: $Y | X, Z \sim \text{Normal}\left( \mathbb{1} \{ \exp\{aX_1 + bX_2\} \leq 100\} + \beta Z + 1, 1 \right)$ with $(a, b) = (-0.5, 0.5), (0.5, -0.5), (0.5, 0.5)$, and $(-0.5, -0.5)$, and $\beta = 1$.

Factor 1 defines the procedures, and Factor 2 through 6 define the data generating processes. Two treatment effect estimators being considered here are $\hat{\beta}_{reg}$, the naive regression adjustment estimator, and $\hat{\beta}_{reg, \text{match}}$, the regression adjustment estimator with a fixed effect for each matched set after non-bipartite full matching. We calculate the bias, standard error, and mean squared error of both estimators under each of the 96 data generating processes defined by Factor 2 through 6.
6.2 Simulation results

Table 1 and 2 summarize the bias and mean squared error of $\hat{\beta}_{\text{reg}}$ and $\hat{\beta}_{\text{reg, match}}$ under each data generating process, respectively. Using non-bipartite matching as a preprocessing step followed by regression adjustment seems to help reduce the bias and the mean squared error in $92/96$ circumstances; the only exceptions are when $Z \sim \text{Uniform}[1 - \sqrt{3}, 1 + \sqrt{3}]$, $d = 10$, and $n = 500$. We also observe that for a fixed $d$, the gain from using statistical matching as a nonparametric preprocessing step seems to increase dramatically as $n$ increases, which is as expected because with a larger $n/d$ ratio, matched sets formed by non-bipartite matching tend to be more homogeneous; on the other hand, when the model is misspecified, a larger sample size does not seem to help remove bias of a naive regression estimator. For instance, when $d = 5$, $Z \sim \text{Exponential}(1)$, $c = 2$, and $(a, b) = (0.5, -0.5)$, $\hat{\beta}_{\text{reg}}$ has a bias of 1.515 when $n = 500$ and a bias of 1.451 when $n = 2000$, while $\hat{\beta}_{\text{reg, match}}$ has a bias of 0.837 when $n = 500$ and the bias reduces to 0.386 when $n = 2000$. Similar qualitative results are observed in all circumstances.

Consistent with the binary treatment case studied in Rubin (1973, 1979) and discussed in Ho et al. (2007), our simulation results seem to suggest that using non-bipartite matching as a nonparametric preprocessing step before regression analysis with a continuous treatment dose helps reduce model dependence and remove some bias.

7 Simulation studies II: non-bipartite full matching versus non-bipartite pair matching

7.1 Goal and structure

In this section, we systematically compare non-bipartite full matching with non-bipartite pair matching. We consider a continuous treatment/encouragement dose $Z \sim \text{Uniform}[0, 1]$, $d = 5$, and the following factors that define a data generating process:

**Factor 1:** sample size, $n$: 500 and 2000.

**Factor 2:** observed covariates distribution: $X \sim \text{Multivariate Normal} (\mu, \Sigma)$, with $\mu = (cZ, 0, \cdots, 0)^T$ and $\Sigma = (\begin{pmatrix} 2^2 & 0 \\ 0 & I_{d-1} \end{pmatrix})$ with $c = -2, -1, 1, \text{and} 2$.

We compare the non-bipartite full matching procedure as in Algorithm 1 and the optimal non-bipartite pair matching procedure in Lu et al. (2001, 2011). This is the third factor:

**Factor 3:** matching procedure: non-bipartite full matching $\mathcal{M}_{\text{nbp, full}}$ and optimal non-bipartite pair matching $\mathcal{M}_{\text{nbp, pair}}$. 

Table 1: Bias of estimators $\hat{\beta}_{\text{reg}}$ and $\hat{\beta}_{\text{reg, match}}$ for each combination of $d$, $n$, $c$, $a$, $b$, and the treatment dose model. Each cell is averaged over 1000 simulations. True $\beta$ is equal to 1.

| $Z \sim \text{Uniform}\{-2, -1, 0, 1, 2\}$ | $d = 5, n = 500$ | $d = 5, n = 2000$ | $d = 10, n = 500$ | $d = 10, n = 2000$ |
|------------------------------------------|-----------------|-----------------|-----------------|-----------------|
| $\hat{\beta}_{\text{reg}}$            | $\hat{\beta}_{\text{reg, match}}$ | $\hat{\beta}_{\text{reg}}$ | $\hat{\beta}_{\text{reg, match}}$ | $\hat{\beta}_{\text{reg}}$ | $\hat{\beta}_{\text{reg, match}}$ |
| $c = -2, (a, b) = (-0.5, -0.5)$        | 0.712            | 0.324            | 0.702            | 0.177            | 0.696            | 0.526            | 0.690            | 0.427            |
| $c = -2, (a, b) = (-0.5, 0.5)$         | 0.707            | 0.327            | 0.694            | 0.178            | 0.708            | 0.538            | 0.704            | 0.435            |
| $c = -2, (a, b) = (0.5, -0.5)$         | 0.697            | 0.323            | 0.700            | 0.176            | 0.696            | 0.542            | 0.686            | 0.423            |
| $c = -2, (a, b) = (0.5, 0.5)$          | 0.702            | 0.337            | 0.700            | 0.176            | 0.696            | 0.533            | 0.696            | 0.430            |
| $c = 2, (a, b) = (-0.5, -0.5)$         | 0.703            | 0.329            | 0.693            | 0.175            | 0.692            | 0.520            | 0.699            | 0.424            |
| $c = 2, (a, b) = (-0.5, 0.5)$          | 0.700            | 0.321            | 0.688            | 0.173            | 0.696            | 0.542            | 0.705            | 0.426            |
| $c = 2, (a, b) = (0.5, -0.5)$          | 0.724            | 0.322            | 0.700            | 0.178            | 0.718            | 0.542            | 0.697            | 0.428            |
| $c = 2, (a, b) = (0.5, 0.5)$           | 0.700            | 0.323            | 0.698            | 0.180            | 0.690            | 0.520            | 0.700            | 0.432            |

$Z \sim \text{Uniform}[1 - \sqrt{3}, 1 + \sqrt{3}]$:

| $c = -2, (a, b) = (-0.5, -0.5)$        | 0.408            | 0.336            | 0.318            | 0.141            | 0.409            | 0.452            | 0.321            | 0.239            |
| $c = -2, (a, b) = (-0.5, 0.5)$         | 0.416            | 0.330            | 0.318            | 0.142            | 0.415            | 0.454            | 0.308            | 0.228            |
| $c = -2, (a, b) = (0.5, -0.5)$         | 0.173            | 0.120            | 0.167            | 0.065            | 0.172            | 0.148            | 0.165            | 0.106            |
| $c = -2, (a, b) = (0.5, 0.5)$          | 0.166            | 0.119            | 0.163            | 0.062            | 0.164            | 0.145            | 0.164            | 0.101            |
| $c = 2, (a, b) = (-0.5, -0.5)$         | 0.415            | 0.322            | 0.313            | 0.146            | 0.406            | 0.457            | 0.317            | 0.235            |
| $c = 2, (a, b) = (0.5, -0.5)$          | 0.421            | 0.342            | 0.309            | 0.144            | 0.394            | 0.448            | 0.317            | 0.237            |

$Z \sim \text{Exponential}(1)$:

| $c = -2, (a, b) = (-0.5, -0.5)$        | 1.574            | 0.838            | 1.447            | 0.391            | 1.537            | 1.094            | 1.470            | 0.724            |
| $c = -2, (a, b) = (-0.5, 0.5)$         | 1.513            | 0.824            | 1.450            | 0.384            | 1.549            | 1.102            | 1.414            | 0.703            |
| $c = -2, (a, b) = (0.5, -0.5)$         | 0.456            | 0.147            | 0.465            | 0.094            | 0.463            | 0.239            | 0.464            | 0.191            |
| $c = -2, (a, b) = (0.5, 0.5)$          | 0.471            | 0.154            | 0.466            | 0.093            | 0.459            | 0.240            | 0.465            | 0.190            |
| $c = 2, (a, b) = (-0.5, -0.5)$         | 0.461            | 0.150            | 0.463            | 0.092            | 0.453            | 0.235            | 0.462            | 0.190            |
| $c = 2, (a, b) = (0.5, -0.5)$          | 1.515            | 0.837            | 1.451            | 0.386            | 1.506            | 1.092            | 1.451            | 0.705            |
| $c = 2, (a, b) = (0.5, 0.5)$           | 1.498            | 0.802            | 1.483            | 0.397            | 1.573            | 1.126            | 1.486            | 0.695            |

For both matching procedures, we consider the following distance:

$$\delta(i, j) = \text{Mahalanobis distance}(i, j) + C \times 1\{|Z_i - Z_j| \leq \tau_0\}.$$ 

As discussed in Section 5.1, $\delta(i, j)$ may incorporate the treatment/encouragement dose $Z$ by adjusting $\tau_0$ and letting $C$ be a large penalty. Throughout the simulations, we let $C = 100,000$ and $\tau_0$ be the fourth factor:

**Factor 4:** minimum distance, $\tau_0$: 0, 0.1, 0.2, 0.3, and 0.4.

To conclude, Factor 1 and 2 define the $2 \times 4 = 8$ data generating processes and Factor 3 and 4 define the $2 \times 5 = 10$ procedures to be studied.
Table 2: Mean squared error (MSE) of estimators $\hat{\beta}_{\text{reg}}$ and $\hat{\beta}_{\text{reg, match}}$ for each combination of $d$, $n$, $c$, $a$, $b$, and the treatment dose model. Each cell is averaged over 1000 simulations. True $\beta$ is equal to 1.

| $Z \sim \text{Uniform}\{-2,-1,0,1,2\}$ | $d = 5$, $n = 500$ | $d = 5$, $n = 2000$ | $d = 10$, $n = 500$ | $d = 10$, $n = 2000$ |
|------------------------------------------|---------------------|---------------------|---------------------|---------------------|
| $c = -2$, $(a, b) = (-0.5, -0.5)$      | 0.617               | 0.166               | 0.519               | 0.042               |
| $c = -2$, $(a, b) = (-0.5, 0.5)$       | 0.618               | 0.164               | 0.509               | 0.044               |
| $c = -2$, $(a, b) = (0.5, -0.5)$       | 0.590               | 0.159               | 0.519               | 0.042               |
| $c = -2$, $(a, b) = (0.5, 0.5)$        | 0.596               | 0.173               | 0.515               | 0.042               |
| $c = 2$, $(a, b) = (-0.5, -0.5)$       | 0.608               | 0.168               | 0.508               | 0.042               |
| $c = 2$, $(a, b) = (-0.5, 0.5)$        | 0.592               | 0.154               | 0.490               | 0.041               |
| $c = 2$, $(a, b) = (0.5, -0.5)$        | 0.631               | 0.160               | 0.517               | 0.043               |
| $c = 2$, $(a, b) = (0.5, 0.5)$         | 0.604               | 0.158               | 0.515               | 0.043               |

| $Z \sim \text{Uniform}\{1 - \sqrt{3},1 + \sqrt{3}\}$ |
|-----------------------------------------------------------|
| $c = -2$, $(a, b) = (-0.5, -0.5)$                         | 0.268               | 0.183               | 0.137               | 0.032               |
| $c = -2$, $(a, b) = (-0.5, 0.5)$                         | 0.274               | 0.174               | 0.138               | 0.032               |
| $c = -2$, $(a, b) = (0.5, -0.5)$                         | 0.042               | 0.022               | 0.031               | 0.006               |
| $c = -2$, $(a, b) = (0.5, 0.5)$                          | 0.046               | 0.024               | 0.032               | 0.006               |
| $c = -2$, $(a, b) = (-0.5, -0.5)$                         | 0.046               | 0.023               | 0.031               | 0.006               |
| $c = -2$, $(a, b) = (-0.5, 0.5)$                         | 0.042               | 0.023               | 0.032               | 0.006               |
| $c = -2$, $(a, b) = (0.5, -0.5)$                         | 0.271               | 0.162               | 0.135               | 0.034               |
| $c = -2$, $(a, b) = (0.5, 0.5)$                          | 0.285               | 0.187               | 0.130               | 0.033               |

| $Z \sim \text{Exponential}(1)$ |
|---------------------------------|
| $c = -2$, $(a, b) = (-0.5, -0.5)$ | 3.244               | 1.109               | 2.325               | 0.237               |
| $c = -2$, $(a, b) = (-0.5, 0.5)$ | 3.030               | 1.075               | 2.330               | 0.228               |
| $c = -2$, $(a, b) = (0.5, -0.5)$ | 0.225               | 0.032               | 0.221               | 0.012               |
| $c = -2$, $(a, b) = (0.5, 0.5)$ | 0.242               | 0.035               | 0.222               | 0.012               |
| $c = -2$, $(a, b) = (-0.5, -0.5)$ | 0.230               | 0.036               | 0.220               | 0.011               |
| $c = -2$, $(a, b) = (-0.5, 0.5)$ | 0.230               | 0.034               | 0.219               | 0.011               |
| $c = 2$, $(a, b) = (0.5, 0.5)$ | 3.038               | 1.101               | 2.324               | 0.232               |
| $c = 2$, $(a, b) = (-0.5, 0.5)$ | 2.990               | 1.022               | 2.429               | 0.247               |

### 7.2 Measurements of success

For a subclassification $\Pi = \{\Pi_1, \cdots, \Pi_K\}$, we compute $\nu(\Pi_k)$, the average Mahalanobis distance among all $(1/2) \times |\Pi_k| \times (|\Pi_k| - 1)$ pairwise comparisons in each subclass $\Pi_k$, and then report the 25th, 50th (median), 75th, and 90th empirical quantiles of $\{\nu(\Pi_k), k = 1, \cdots, K\}$. We also report two weighted averages of $\{\nu(\Pi_k), k = 1, \cdots, K\}$. The weighting scheme $W^{\text{const}}$ assigns an equal weight to each matched set, regardless of its size, which corresponds to letting $w(\Pi_k) \propto 1$ in Definition 2; denote by HM1 this first measure. The second weighting scheme $W^{\text{suit}}$ assigns $w(\Pi_k) \propto |\Pi_k| - 1$ as described in Lemma 2. Denote by HM2 this second measure.

Next, for each subclass, we compute $\nu^*_{\text{star}}(\Pi_k)$, the minimum $\nu(\Pi_k; i_k^*)$ (based on the Mahalanobis distance) among all $i_k^* \in \Pi_k$ as defined in Definition 4. We also report two weighted averages
of \( \nu_{\text{star}}(\Pi_k) \), \( k = 1, \cdots, K \): one with the weighting scheme \( W^{\text{const}} \) and the other \( W^{\text{suit}} \). Denote by HM3 and HM4 these two measures. Smaller values of HM1 through HM4 indicate better matched-sets homogeneity. Note that all four measures reduce to the same average within-matched-pair distance when the subclassification \( \Pi \) consists of only matched pairs.

We also consider a measurement of overall balance. In each subclass \( \Pi_k \), let \( \bar{X}_{i,k,\text{high}} \) denote the average value of the \( i \)th observed covariate \( X_i \) of units with treatment dose greater than or equal to the median treatment dose, and \( \bar{X}_{i,k,\text{low}} \) that of units with treatment dose below the median. For instance, if the subclass consists of 5 units, each with the first observed covariate \( X_i \) \{1.5, 2, 1, 1.5, 2\} and treatment dose \{0.1, 0.2, 0.3, 0.4, 0.5\}, then \( \bar{X}_{i,k,\text{high}} = (1 + 1.5 + 2)/3 = 1.5 \) and \( \bar{X}_{i,k,\text{low}} = (1.5 + 2)/2 = 1.75 \) for this subclass. Let \( d_i = \sum_{\Pi_k \in \Pi} \bar{X}_{i,k,\text{high}} - \sum_{\Pi_k \in \Pi} \bar{X}_{i,k,\text{low}} \) denote the difference in means of the \( i \)th covariate, and define \( SS = \sum_{i=1}^{d} d_i^2 \) to be the sum of the squared differences over all \( d = 5 \) or 10 observed covariates. In an ideal randomization experiment where treatment dose assignment is indeed randomized, distributions of observed covariates in the high and low dose groups are identical, and \( SS \) is small. Hence, smaller \( SS \) values signal better overall balance.

For each subclass \( \Pi_k \), we further calculate \( \mu(\Pi_k) \), the average absolute “internal-node-minus-leaf” difference in \( Z \) as defined in Section 5.1. We report the minimum, 25th, 50th (median), and 75th empirical quantiles of \( \{\mu(\Pi_k), k = 1, \cdots, K\} \). Finally, we report the number of matched set \( |\Pi| \), and the average pairwise Mahalanobis distance and balance measure \( SS \) before matching.

### 7.3 Simulation results

Table 3 and 4 summarize the simulation results when \( d = 5, n = 500 \) and 2000, and \( c = -2 \). Simulation results for the other 6 data generating processes are similar and can be found in Supplementary Material B.2.

We observe three consistent trends. First, when \( \tau_0 = 0 \) and the only goal of statistical matching is homogeneity in covariates \( X \), non-bipartite full matching and non-bipartite pair matching produce similar matched sets and have very similar performance with respect to all measures. Second, we observe that the number of matched sets \( |\Pi| \) decreases in non-bipartite full matching as \( \tau_0 \) increases; this makes sense because more and more matched pairs within which two units have similar doses are no longer deemed preferable by the algorithm because of the large penalty \( C \) attached to the dose. Third, for both non-bipartite full matching and non-bipartite pair matching, all four homogeneity measures HM1 to HM4 deteriorate as \( \tau_0 \) increases and the matching algo-
rithm prefers more separation in the treatment/encouragement doses; however, non-bipartite full matching is capable of striking a much better balance between homogeneity in $X$ and heterogeneity in treatment/encouragement doses compared to non-bipartite pair matching. In fact, when $d = 5$, $n = 2000$, $c = -2$, and $\tau_0 \geq 0.2$, non-bipartite full matching outperforms non-bipartite pair matching simultaneously in all 8 measurements of matched-sets homogeneity (4 quantiles of $\nu(\Pi_k)$ and HM1 through HM4), 4 measurements of heterogeneity in treatment/encouragement doses (4 quantiles of $\mu(\Pi_k)$), and one measurement of overall balance SS. For example, when $\tau_0 = 0.4$, the median within-matched-sets Mahalanobis distance (i.e., 50th of $\nu(\Pi_k)$) is equal to 0.898 for pair matching and 0.756 for full matching, and the overall balance measurement SS is 0.389 for pair matching and as small as 0.105 for full matching.

Finally, Figure 7 helps visualize the difference between an optimal non-bipartite pair match structure and an optimal non-bipartite full match structure using a small simulated dataset with $d = 3$, $n = 50$, and $c = -2$. To facilitate data visualization, we do a principle component analysis (PCA) and plot each unit’s dose against its first principle component (PC1). Top left panel and top right panel depict the match structure of the optimal non-bipartite pair match and optimal non-bipartite full match, both with $\tau_0 = 0.3$. Two bottom panels eliminate matched pairs that are identical in two matches and focus on the match structure that are different in two matches. It is evident that the full match (corresponding to the bottom right panel) tends to connect units that are more different in the dose (i.e., larger difference in the y-axis) but similar in the first PC (i.e., small difference in the x-axis), compare to the pair match (corresponding to the bottom left panel).

Table 3: Simulation results when $d = 5$, $n = 500$, and $c = -2$. Average pairwise Mahalanobis distance before matching is 10 and SS before matching is 1.066.
Figure 7: Visualizing the difference between a non-bipartite pair match and a non-bipartite full match. We generated a small dataset with $d = 3$, $n = 50$, and $c = -2$. Top left panel: optimal non-bipartite pair match with $\tau_0 = 0.3$. Top right panel: optimal non-bipartite full match with $\tau_0 = 0.3$. Two bottom panels eliminate matched pairs that are identical in two matches and focus on the match structure that differ in two matches.
Table 4: Simulation results when \( d = 5, n = 2000, \) and \( c = -2. \) Average pairwise Mahalanobis distance before matching is 10 and \( SS \) before matching is 1.010.

| \( \nu(\Pi_k) \)       | \( \mu(\Pi_k) \)       | \( \Pi \) | Min.  | 25th | 50th | 75th | 90th |
|------------------------|------------------------|----------|-------|------|------|------|------|
|                        |                        |          | 25th  | 50th | 75th | 90th | SS   | (II) |
| Non-Bipartite Pair Match |
| \( \tau_0 = 0 \)       | 0.240 | 0.394 | 0.668 | 1.126 | 0.553 | 0.553 | 0.553 | 0.553 | 0.000 | 0.126 | 0.276 | 0.477 | 0.002 | 1000 |
| \( \tau_0 = 0.1 \)     | 0.266 | 0.440 | 0.747 | 1.255 | 0.614 | 0.614 | 0.614 | 0.614 | 0.100 | 0.207 | 0.340 | 0.520 | 0.006 | 1000 |
| \( \tau_0 = 0.2 \)     | 0.304 | 0.507 | 0.863 | 1.433 | 0.700 | 0.700 | 0.700 | 0.700 | 0.200 | 0.283 | 0.392 | 0.548 | 0.023 | 1000 |
| \( \tau_0 = 0.3 \)     | 0.372 | 0.625 | 1.055 | 1.701 | 0.840 | 0.840 | 0.840 | 0.840 | 0.300 | 0.355 | 0.431 | 0.549 | 0.094 | 1000 |
| \( \tau_0 = 0.4 \)     | 0.541 | 0.898 | 1.448 | 2.205 | 1.131 | 1.131 | 1.131 | 1.131 | 0.400 | 0.428 | 0.467 | 0.531 | 0.389 | 1000 |

| Non-Bipartite Full Match |
| \( \tau_0 = 0 \)       | 0.243 | 0.394 | 0.665 | 1.121 | 0.553 | 0.551 | 0.543 | 0.532 | 0.000 | 0.130 | 0.278 | 0.472 | 0.002 | 969  |
| \( \tau_0 = 0.1 \)     | 0.270 | 0.438 | 0.740 | 1.242 | 0.611 | 0.608 | 0.600 | 0.587 | 0.100 | 0.211 | 0.342 | 0.517 | 0.006 | 964  |
| \( \tau_0 = 0.2 \)     | 0.307 | 0.500 | 0.844 | 1.402 | 0.690 | 0.687 | 0.675 | 0.657 | 0.200 | 0.287 | 0.396 | 0.548 | 0.018 | 951  |
| \( \tau_0 = 0.3 \)     | 0.365 | 0.594 | 0.997 | 1.618 | 0.803 | 0.804 | 0.776 | 0.749 | 0.300 | 0.363 | 0.443 | 0.558 | 0.048 | 918  |
| \( \tau_0 = 0.4 \)     | 0.467 | 0.756 | 1.244 | 1.947 | 0.986 | 1.006 | 0.924 | 0.877 | 0.400 | 0.444 | 0.496 | 0.570 | 0.105 | 842  |

8 Effect of TEE monitoring during CABG surgery on 30-day mortality: study design

8.1 Data and study design

Transesophageal echocardiography (henceforth TEE) is an ultrasound-based, cardiac imaging modality often used in cardiac surgeries to monitor patients’ hemodynamics. Coronary artery bypass graft (henceforth CABG) surgery is the most widely performed surgeries in the U.S. ([The Society of Thoracic Surgeons, 2016](https://www.sts.org)). Evidence supporting the use of TEE during isolated CABG surgeries is equivocal: it is classified by AHA/ACC guidelines as a Class IIb recommendation, meaning its “usefulness/efficacy is less well established by evidence/opinion” ([Hillis et al., 2011](https://jama.ama-assn.org/doi/full/10.1001/jama.2011.7051)). In this section, we apply the proposed non-bipartite full match design to retrospective administrative data from Centers for Medicare and Medicaid Services (CMS) and study the effect of TEE during CABG surgery on patients’ 30-day mortality.

We consider a cluster-level, instrumental variable analysis ([Zhang et al., 2020](https://doi.org/10.1093/epiob/ebv092)) where each hospital defines a natural cluster and each hospital’s preference for TEE usage (defined as the fraction of CABG surgeries using TEE monitoring) is considered a valid instrumental variable after controlling for patients’ composition including average age, percentage of male patients, percentage of white patients, percentage of elective CABG surgeries, and percentage of patients having each of the following important comorbid conditions: arrhythmia, diabetes, congestive heart failure (CHF), hypertension, obesity, pulmonary diseases, and renal diseases, and hospital’s characteristics including total hospitals beds, teaching status, presence of any cardiac intensive care unit, total number of full-time registered nurses, and annual cardiac surgical volume.
Hospitals’ preference is a continuous IV (or encouragement dose). Our goal in the design stage is to divide 1,217 hospitals into subclasses with good subclass homogeneity, overall balance, and good amount of separation in their encouragement doses.

8.2 Matched samples

The first 4 columns of Table 5 summarize the patient composition and hospital characteristics of hospitals whose preference for using TEE during CABG surgery is above the median preference and those below the median preference. We observe a systematic difference between the “above median” and “below median” groups before matching: many standardized differences (defined as the difference in means divided by the standard deviation) are above 0.1 and two-sample Kolmogorov-Smirnov tests suggest that the distribution of 6 covariates, including annual cardiac surgical volume, hospital beds, etc, are statistically different at 0.01 level.

We then applied the developed non-bipartite full matching algorithm to the data using a dose-incorporating distance $\delta'(i, j) = \delta(i, j) + C \times 1\{|Z_i - Z_j| \leq \tau_0\}$ with $\delta(i, j)$ being the Mahalanobis distance between 16 observed pretreatment covariates, $C = 100,000$ a large penalty, $\lambda = 0$, and various choices of $\tau_0$. We followed the advice in Rubin (2007) and conducted the design without access to the outcome data in order to assure the objectivity of the design.

In particular, non-bipartite full matching with $\tau_0 = 0.15$ divides these 1,217 hospitals into 543 matched pairs, 39 matched sets of size 3, 1 of size 4, and 2 of size 5. To get a sense of the balance after matching, we collect hospitals with higher doses in each matched set (including the one with median dose in a matched set with odd cardinality) and refer to them as the “high dose” group. The “high dose” group thus consists of $1 \times 543 + 2 \times 39 + 2 \times 1 + 3 \times 1 = 629$ hospitals. Similarly, we define the other hospitals as “low dose” hospitals. In an ideal (yet unattainable) randomized controlled trial where the dose assignment within each matched set is indeed randomized, the “high dose” and “low dose” groups would have similar distributions of patient composition and hospital characteristics. Non-bipartite full matching seems to replicate this ideal experimental benchmark, as seen from the last 4 columns in Table 5, the “high dose” and “low dose” groups have similar covariate distributions and in fact no Kolmogorov-Smirnov test is significant at 0.1 level. Moreover, before matching, the median Mahalanobis distance among all 1,217 hospitals is 14.14, while the median “average pairwise Mahalanobis distance” is as small as 1.54 after matching. Matched sets also have a good separation in their encouragement doses: the average internal-node-minus-leaf difference in the encouragement dose is 0.46 among all matched sets. In Supplementary Material
C, we further report the covariate balance of non-bipartite full matching under other choices of $\tau_0$. We conduct inference with matched samples under $\tau_0 = 0.15$ because among all matches satisfying the stringent balance requirements (all standardized differences less than 0.1 and no K-S tests significant at 0.1 level), it produces the best separation in the encouragement doses.

Table 5: Covariate balance before and after non-bipartite full matching with a dose-incorporating Mahalanobis distance and $\tau_0 = 0.15$. 1, 217 hospitals are divided into 543 matched pairs, 39 matched sets of size 3, 1 of size 4, and 2 of size 5. After matching, no two-sample Kolmogorov-Smirnov test comparing the covariate distributions in the “high-dose” and “low-dose” groups is significant at 0.1 level.

| Patient Composition            | Before Matching | After Matching |
|-------------------------------|-----------------|----------------|
|                               | Below Median    | Above Median   | Std. Diff. | K-S Test | P-Value | Low Dose Median | Std. Diff. | K-S Test | P-Value | High Dose Median | Std. Diff. | K-S Test | P-Value |
| Mean age, yrs                 | 75.29 (n = 608) | 75.10 (n = 609) | 0.11       | < 0.01   |         | 75.21 (n = 588) | 0.02       | 0.18   |         | 75.18 (n = 629) | 0.06       | 0.20   |         |
| Male, %                       | 0.69            | 0.67           | 0.15       | 0.02     | 0.06     | 0.68            | 0.06       | 0.92   |         | 0.68            | 0.06       | 0.92   |         |
| White, %                      | 0.85            | 0.85           | -0.01      | 0.05     | 0.47     | 0.85            | -0.01      | 0.20   |         | 0.85            | -0.01      | 0.76   |         |
| Elective, %                   | 0.47            | 0.46           | 0.05       | 0.32     | 0.47     | 0.47            | 0.00       | 0.76   |         | 0.47            | 0.00       | 0.76   |         |
| Diabetes, %                   | 0.17            | 0.17           | 0.02       | 0.42     | 0.17     | 0.17            | -0.01      | 0.93   |         | 0.17            | -0.01      | 0.93   |         |
| Renal diseases, %             | 0.09            | 0.09           | 0.07       | 0.07     | 0.09     | 0.09            | 0.01       | 0.69   |         | 0.09            | 0.01       | 0.69   |         |
| Arrhythmia, %                 | 0.12            | 0.11           | 0.10       | < 0.01   | 0.11     | 0.11            | 0.02       | 0.08   |         | 0.11            | 0.02       | 0.08   |         |
| CHF, %                        | 0.12            | 0.11           | 0.09       | 0.12     | 0.12     | 0.12            | 0.01       | 0.27   |         | 0.12            | 0.01       | 0.27   |         |
| Hypertension, %               | 0.30            | 0.29           | 0.05       | 0.32     | 0.29     | 0.30            | -0.04      | 0.96   |         | 0.30            | -0.04      | 0.96   |         |
| Obesity, %                    | 0.06            | 0.06           | 0.06       | 0.03     | 0.06     | 0.06            | 0.03       | 0.36   |         | 0.06            | 0.03       | 0.36   |         |
| Pulmonary diseases, %         | 0.02            | 0.02           | 0.12       | < 0.01   | 0.02     | 0.02            | 0.05       | 0.43   |         | 0.02            | 0.05       | 0.43   |         |

| Hospital Characteristics      | Before Matching | After Matching |
|-------------------------------|-----------------|----------------|
| Cardiac surgical volume       | 571             | 456            | 0.21       | < 0.001  | 537         | 0.09   | 0.09   |
| Teaching hospital, yes/no     | 0.20            | 0.15           | 0.13       | 0.47     | 0.18        | 0.18   | -0.01  | 0.99   |
| Hospital beds                 | 419             | 336            | 0.33       | < 0.001  | 386         | 0.06   | 0.12   |
| Full-time registered nurses   | 722             | 534            | 0.33       | < 0.001  | 646         | 0.06   | 0.14   |
| Cardiac ICU, yes/no           | 0.72            | 0.70           | 0.04       | 0.99     | 0.71        | 0.71   | -0.02  | 0.99   |

9 Effect of TEE monitoring during CABG surgery on 30-day mortality: statistical inference

9.1 Set-up, potential outcomes, and a cluster-level sharp null hypothesis

Does using TEE during CABG surgery reduce patients’ 30-day mortality? In this section, we first generalize the cluster-level, non-bipartite pair match set-up considered in Zhang et al. (2020) to the current full match setting, and discuss how to test Fisher’s sharp null hypothesis of no treatment effect under the new design.

Suppose we have formed $K$ matched sets, indexed by $k = 1, \cdots, K$, each with $n_k$ hospitals, indexed by $j = 1, \cdots, n_k$, so that index $kj$ uniquely identifies one hospital and there are a total of $N = \sum_{k=1}^{K} n_k$ hospitals in total. Each hospital is associated with hospital-level covariates $x_{kj}$ and a hospital-level continuous instrumental variable (or encouragement dose) $z_{kj}^{\text{obs}}$. There are $N_{kj}$
patients in each hospital $kj$, indexed by $i = 1, \ldots, N_{kj}$, so that index $kji$ uniquely identifies one patient. Each patient is associated with a treatment indicator $D_{kji}^{obs}$, outcome of interest $R_{kji}^{obs}$, and individual-level covariates $x_{kji}$. In our application, we have formed 585 matched sets so $K = 585$; $n_k$ is the number of hospitals in each matched set so $n_i = 2, 3, 4, \text{ or } 5$ in our design; hospital-level instrumental variable $Z_{kj} \in [0, 1]$ is hospital’s preference for TEE during CABG surgery; $N_{kj}$ is the number of patients undergoing CABG surgery in hospital $kj$; $D_{kj}$ is a binary indicator equal to 1 if patient $kji$ receives TEE monitoring and 0 otherwise; $R_{kji}$ is patient $kji$’s 30-day mortality status; finally, $x_{kj}$ describes hospital $kj$’s characteristics and $x_{kji}$ patient $kji$’s characteristics. Following Zhang et al. (2020), we assume that after controlling for patient composition and hospital characteristics, preference for TEE usage is a valid cluster-level instrumental variable.

Let $D_{kj}(Z_{kj} = z_{kj})$ denote the potential treatment received of patient $kji$ when the hospital-level IV $Z_{kj}$ is set to $z_{kj}$, and $D_{kj}(Z_{kj})$ is a shorthand for $(D_{kj1}(Z_{kj}), \cdots, D_{kn_{kj}}(Z_{kj}))$. Let $R_{kji}(Z_{kj} = z_{kj}, D_{kj}(Z_{kj}) = d_{kj})$ denote unit $kji$’s potential outcome under $Z_{kj} = z_{kj}$ and $D_{kj}(Z_{kj}) = d_{kj}$. Under exclusion restriction, we have $R_{kji}(Z_{kj}, D_{kj}(Z_{kj})) = R_{kji}(D_{kj}(Z_{kj}))$. Finally, let $Z_{k}^{obs} = \{Z_{k1}^{obs}, \cdots, Z_{kn_{kj}}^{obs}\}$ denote the collection of IV doses in matched set $k$.

A cluster-level Fisher’s sharp null hypothesis states that

$$H_{0,\text{sharp}} : N_{kj}^{-1} \left\{ \sum_{i=1}^{N_{kj}} R_{kji}(D_{kj}(Z_{kj} = z) \right\} = N_{kj}^{-1} \left\{ \sum_{i=1}^{N_{kj}} R_{kji}(D_{kj}(Z_{kj} = z')) \right\}, \forall k, j, \forall z, z' \in Z_{k}^{obs}. \quad (6)$$

The null hypothesis $H_{0,\text{sharp}}$ states that the hospital-aggregate potential outcomes when comparing any pair of two IV doses $z, z' \in Z_{k}^{obs}$ are the same. Setting $N_{kj} = 1, \forall k, j$ reduces the problem to a non-clustered setting.

### 9.2 Randomization-based inference

There are three key ingredients to perform a Fisher-style randomization-based test: a sharp null hypothesis, a randomized treatment assignment scheme, and a test statistic (Rosenbaum, 2002, 2010; Ding et al., 2016).

1. **Sharp null hypothesis:** $H_{0,\text{sharp}}$ is sharp null hypothesis that allows us to impute the potential aggregate-outcome of cluster $kj$ under any IV doses $z \in Z_{k}^{obs}$.

2. **Randomized treatment dose assignment:** In a typical matched-pair design with $I$ matched pairs, there are a total of $2^I$ possible randomization configurations. In a full match...
design, within each matched set of $n_k$ hospitals, there are $n_k!$ many IV dose assignments, each with equal probability; therefore, there are a total of $\prod_{k=1}^K n_k!$ randomizations induced by a full match design. Let $\mathcal{Z}$ denote this collection of all randomizations and $z \in \mathcal{Z}$ one realization.

3. **Test statistic:** With a binary treatment, a commonly-used test statistic for full match design is the rank-sum test; see Rosenbaum (2002, 2004); Heng et al. (2019a). We modify the rank-sum test statistic to reflect the continuous dose. Let $\mathcal{Z} = \{Z_{11}^{obs}, \ldots, Z_{K_{nk}}^{obs}\}$, $R_{kj}^{obs} = N_{kj}^{-1} \left\{ \sum_{i=1}^{N_{kj}} R_{kji}^{obs} \right\}$, and $R = \{R_{11}^{obs}, \ldots, R_{K_{nk}}^{obs}\}$. Consider the double rank sum statistic:

$$T_{double \; rank} = \frac{1}{N^2} \sum_{k=1}^K \sum_{j=1}^{n_k} q_1(Z_{kj}^{obs} \mid Z) \times q_2(R_{kj}^{obs} \mid R),$$

where $q_1(Z_{kj}^{obs} \mid Z)$ the rank of $Z_{kj}^{obs}$ among all doses $Z$, and $q_2(R_{kj}^{obs})$ the rank of $R_{kj}^{obs}$ among all the responses.

Researchers first impute all missing potential outcomes under $H_{0,sharp}$ and then enumerate all $|\mathcal{Z}| = \prod_{k=1}^K n_k!$ possible dose assignments. For each enumerated $Z' = z \in \mathcal{Z}$, calculate the corresponding $R'$ under $Z'$ and the test statistic $T'_{double \; rank}$. The distribution of $T'_{double \; rank}$ is then the exact null distribution of the test statistic $T_{double \; rank}$ under $H_{0,sharp}$ and conditional on the matched samples. By comparing $T_{double \; rank}$ to this exact null distribution, the exact p-value is obtained. In practice, instead of enumerating all $|\mathcal{Z}| = \prod_{k=1}^K n_k!$ possible randomizations, researchers may sample with replacement from $\mathcal{Z}$ and this strategy is sometimes referred to as a “modified randomization test” in the literature (Dwass, 1957; Pagano and Tritchler, 1983) and known to still preserve the level of the test.

9.3 **Results**

For 585 matched sets we formed in the design stage, we generated the reference distribution using 1,000,000 samples from all possible $2^{543} \times 3^{39} \times 4^1 \times 5^2$ randomizations; see Figure 8. We calculated $T_{double \; rank} = 294.27$; hence, one-sided p-value is 0.020 and the null hypothesis $H_{0,sharp}$ is rejected in favor of the alternative hypothesis $\beta < 0$, i.e., using TEE during CABG surgery lowers patients’ 30-day mortality rate, at 0.05 level.
10 Discussion

In this paper we have systematically studied statistical matching and subclassification with a many-leveled and continuous treatment dose. We propose two optimality criteria for subclassification, each based on a natural subclass homogeneity measure. We characterize the relationship between these two criteria and leverage this relationship to develop an efficient polynomial-time algorithm that finds a subclassification that is guaranteed to be optimal with respect to one criterion and near-optimal with respect to the other criterion. Our extensive simulations suggest that non-bipartite matching combined with regression adjustment helps remove bias in parametric causal inference; thus, we would recommend routinely using non-bipartite matching as a pre-processing step, as advocated by many researchers (Rubin, 1973, 1979; Ho et al., 2007; Stuart, 2010) in a binary treatment setting. Moreover, we found non-bipartite full match is advantageous over non-bipartite pair match in separating the treatment/encouragement doses and maintaining good subclass homogeneity and overall balance; therefore, the new design may be particularly useful in instrumental variable studies where separation of the IVs (or encouragement doses) would render outcome analysis much more efficient (Baiocchi et al., 2010).
Supplementary Materials

Supplementary Material A.1-A.4 contains proofs of Lemma 1, Corollary 1, and Proposition 1-2. Supplementary Material A.5 proves that the output from the modified Algorithm 1 $F_{\text{star},\lambda}^*$ induces a subclassification that is optimal with respect to $\nu_{\text{star}}(\Pi; i^*, W_{\text{suit}})$. Supplementary Material B.1 summarizes the data generating process underlying the illustrative examples in Section 5. Supplementary Material B.2 provides additional simulation results. Supplementary Material C provides further details on statistical matching in the application with different choices of the tuning parameter $\tau_0$.

References

Baiocchi, M., Small, D. S., Lorch, S., and Rosenbaum, P. R. (2010). Building a stronger instrument in an observational study of perinatal care for premature infants. *Journal of the American Statistical Association*, 105(492):1285–1296.

Baiocchi, M., Small, D. S., Yang, L., Polsky, D., and Groeneveld, P. W. (2012). Near/far matching: a study design approach to instrumental variables. *Health Services and Outcomes Research Methodology*, 12(4):237–253.

Derigs, U. (1988). Solving non-bipartite matching problems via shortest path techniques. *Annals of Operations Research*, 13(1):225–261.

Diamond, A. and Sekhon, J. S. (2013). Genetic matching for estimating causal effects: A general multivariate matching method for achieving balance in observational studies. *Review of Economics and Statistics*, 95(3):932–945.

Ding, P., Feller, A., and Miratrix, L. (2016). Randomization inference for treatment effect variation. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 78(3):655–671.

Dwass, M. (1957). Modified randomization tests for nonparametric hypotheses. *The Annals of Mathematical Statistics*, pages 181–187.

Hansen, B. B. (2004). Full matching in an observational study of coaching for the sat. *Journal of the American Statistical Association*, 99(467):609–618.

Hansen, B. B. (2007). Optmatch: Flexible, optimal matching for observational studies. *R News*, 7(2):18–24.
Hansen, B. B. and Klopfer, S. O. (2006). Optimal full matching and related designs via network flows. *Journal of Computational and Graphical Statistics*, 15(3):609–627.

Heng, S., Kang, H., Small, D. S., and Fogarty, C. B. (2019a). Increasing power for observational studies of aberrant response: An adaptive approach. *arXiv preprint arXiv:1907.06770*.

Heng, S., Zhang, B., Han, X., Lorch, S. A., and Small, D. S. (2019b). Instrumental variables: to strengthen or not to strengthen? *arXiv preprint arXiv:1911.09171*.

Hillis, L. D., Smith, P. K., Anderson, J. L., Bittl, J. A., Bridges, C. R., Byrne, J. G., Cigarroa, J. E., DiSesa, V. J., Hiratzka, L. F., Hutter, A. M., et al. (2011). 2011 accf/aha guideline for coronary artery bypass graft surgery: a report of the american college of cardiology foundation/american heart association task force on practice guidelines developed in collaboration with the american association for thoracic surgery, society of cardiovascular anesthesiologists, and society of thoracic surgeons. *Journal of the American College of Cardiology*, 58(24):e123–e210.

Ho, D. E., Imai, K., King, G., and Stuart, E. A. (2007). Matching as nonparametric preprocessing for reducing model dependence in parametric causal inference. *Political Analysis*, 15(3):199–236.

Iacus, S. M., King, G., and Porro, G. (2011). Multivariate matching methods that are monotonic imbalance bounding. *Journal of the American Statistical Association*, 106(493):345–361.

Imbens, G. W. and Rosenbaum, P. R. (2005). Robust, accurate confidence intervals with a weak instrument: quarter of birth and education. *Journal of the Royal Statistical Society: Series A (Statistics in Society)*, 168(1):109–126.

Karmakar, B., Small, D. S., and Rosenbaum, P. R. (2019). Using approximation algorithms to build evidence factors and related designs for observational studies. *Journal of Computational and Graphical Statistics*, 28(3):698–709.

Li, Y. P., Propert, K. J., and Rosenbaum, P. R. (2001). Balanced risk set matching. *Journal of the American Statistical Association*, 96(455):870–882.

Lu, B., Greevy, R., Xu, X., and Beck, C. (2011). Optimal nonbipartite matching and its statistical applications. *The American Statistician*, 65(1):21–30.
Lu, B., Zanutto, E., Hornik, R., and Rosenbaum, P. R. (2001). Matching with doses in an observational study of a media campaign against drug abuse. *Journal of the American Statistical Association*, 96(456):1245–1253.

MacKay, E. J., Zhang, B., Heng, S., and Ye, T. (2020). Protocol for a retrospective, comparative effectiveness study of the association between transesophageal echocardiography (TEE) monitoring used in coronary artery bypass graft (CABG) surgery and clinical outcomes. *medRxiv*.

Nattino, G., Lu, B., Shi, J., Lemeshow, S., and Xiang, H. (2020). Triplet matching for estimating causal effects with three treatment arms: A comparative study of mortality by trauma center level. *Journal of the American Statistical Association*, pages 1–10.

Pagano, M. and Trichler, D. (1983). On obtaining permutation distributions in polynomial time. *Journal of the American Statistical Association*, 78(382):435–440.

Pimentel, S. D., Kelz, R. R., Silber, J. H., and Rosenbaum, P. R. (2015). Large, sparse optimal matching with refined covariate balance in an observational study of the health outcomes produced by new surgeons. *Journal of the American Statistical Association*, 110(510):515–527.

Rigdon, J., Baiocchi, M., and Basu, S. (2018). Near-far matching in R: the nearfar package. *Journal of Statistical Software*, 86(CS-5).

Rosenbaum, P. R. (1989). Optimal matching for observational studies. *Journal of the American Statistical Association*, 84(408):1024–1032.

Rosenbaum, P. R. (1991). A characterization of optimal designs for observational studies. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 53(3):597–610.

Rosenbaum, P. R. (2002). *Observational Studies*. Springer.

Rosenbaum, P. R. (2004). Design sensitivity in observational studies. *Biometrika*, 91(1):153–164.

Rosenbaum, P. R. (2010). *Design of observational studies*. Springer.

Rosenbaum, P. R. (2020). Modern algorithms for matching in observational studies. *Annual Review of Statistics and Its Application*, 7:143–176.

Rosenbaum, P. R., Ross, R. N., and Silber, J. H. (2007). Minimum distance matched sampling with fine balance in an observational study of treatment for ovarian cancer. *Journal of the American Statistical Association*, 102(477):75–83.
Rubin, D. B. (1973). Matching to remove bias in observational studies. *Biometrics*, pages 159–183.

Rubin, D. B. (1979). Using multivariate matched sampling and regression adjustment to control bias in observational studies. *Journal of the American Statistical Association*, 74(366a):318–328.

Rubin, D. B. (2007). The design versus the analysis of observational studies for causal effects: parallels with the design of randomized trials. *Statistics in Medicine*, 26(1):20–36.

Sävje, F., Higgins, M. J., and Sekhon, J. S. (2020). Generalized full matching. *Political Analysis*.

Schrijver, A. (2003). *Combinatorial optimization: polyhedra and efficiency*. Springer Science & Business Media.

Sekhon, J. S. (2008). Multivariate and propensity score matching software with automated balance optimization: the matching package for R. *Journal of Statistical Software*.

Small, D. S. and Rosenbaum, P. R. (2008). War and wages: the strength of instrumental variables and their sensitivity to unobserved biases. *Journal of the American Statistical Association*, 103(483):924–933.

Stuart, E. A. (2010). Matching methods for causal inference: A review and a look forward. *Statistical Science*, 25(1):1–21.

Stuart, E. A., King, G., Imai, K., and Ho, D. (2011). Matchit: nonparametric preprocessing for parametric causal inference. *Journal of Statistical Software*.

The Society of Thoracic Surgeons (2016). The STS Adult Cardiac Surgery Database (ACSD).

Vazirani, V. V. (2013). *Approximation algorithms*. Springer Science & Business Media.

Williamson, D. P. and Shmoys, D. B. (2011). *The design of approximation algorithms*. Cambridge university press.

Yang, D., Small, D. S., Silber, J. H., and Rosenbaum, P. R. (2012). Optimal matching with minimal deviation from fine balance in a study of obesity and surgical outcomes. *Biometrics*, 68(2):628–636.

Yu, R., Silber, J. H., Rosenbaum, P. R., et al. (2020). Matching methods for observational studies derived from large administrative databases. *Statistical Science*, 35(3):338–355.
Zhang, B., Heng, S., MacKay, E. J., and Ye, T. (2020). Bridging preference-based instrumental variable studies and cluster-randomized encouragement experiments: study design, noncompliance, and average cluster effect ratio. *arXiv preprint arXiv:2007.06772*.

Zubizarreta, J. R. (2012). Using mixed integer programming for matching in an observational study of kidney failure after surgery. *Journal of the American Statistical Association*, 107(500):1360–1371.
Supplementary Materials for “Statistical matching and subclassification with a continuous dose: characterization, algorithms, and inference”

Abstract

Supplementary Material A.1-A.4 contains proofs of Lemma 1, Corollary 1, and Proposition 1-2. Supplementary Material A.5 proves that the output from the modified Algorithm 1 $F_{\text{star},\lambda}$ induces a subclassification that is optimal with respect to $\nu_{\text{star}}^\lambda(\Pi;1^*, W^{\text{suit}})$. Supplementary Material B.1 summarizes the data generating process underlying the illustrative examples in Section 5. Supplementary Material B.2 provides additional simulation results. Supplementary Material C provides further details on statistical matching in the application with different choices of the tuning parameter $\tau_0$.

Supplementary Material A: Proofs

A.1: Proof of Lemma 1

Proof. Consider the first inequality. Observe that the following identity holds

$$\sum_{i_k^* \in \Pi_k} (|\Pi_k| - 1) \times \nu_{\text{star}}(\Pi_k; i_k^*) = \sum_{i,j \in \Pi_k, i \neq j} \delta(i, j) = (|\Pi_k| - 1) \times |\Pi_k| \times \nu(\Pi_k),$$

which implies that $\nu(\Pi_k) = \frac{1}{|\Pi_k|} \times \sum_{i^*_k \in \Pi_k} \nu_{\text{star}}(\Pi_k; i^*_k) = \nu_{\text{star}}(\Pi_k; i^*_k)$; hence, we have

$$\min_{i^*_k \in \Pi_k} \nu_{\text{star}}(\Pi_k; i^*_k) \leq \nu_{\text{star}}(\Pi_k; i^*_k) = \nu(\Pi_k),$$

as desired. Next, consider the other inequality. Fix $i^*_k \in \Pi_k$. Divide $(|\Pi_k| - 1) \times |\Pi_k|$ pairwise comparisons into two mutually exclusive index sets $\Lambda_1$ and $\Lambda_2$. Let $\Lambda_1 = \{(i, j) \mid i \neq j, i = i^*_k \text{ or } j = i^*_k\}$, and $\Lambda_2 = \{(i, j) \mid i \neq j, i \neq i^*_k \text{ and } j \neq i^*_k\}$. Note that $|\Lambda_1| = 2(|\Pi_k| - 1), |\Lambda_2| = (|\Pi_k| - 2)(|\Pi_k| - 1)$, and $|\Lambda_1| + |\Lambda_2| = (|\Pi_k| - 1) \times |\Pi_k|$. Write

$$|\Pi_k| \times (|\Pi_k| - 1) \times \nu(\Pi_k) = \sum_{i,j \in \Pi_k, i \neq j} \delta(i, j) = \sum_{(i,j) \in \Lambda_1} \delta(i, j) + \sum_{(i,j) \in \Lambda_2} \delta(i, j).$$

The first term $\sum_{(i,j) \in \Lambda_1} \delta(i, j) = \sum_{j \neq i^*_k, j \in \Pi_k} \delta(i_k^*, j) + \sum_{i \neq i_k^*, i \in \Pi_k} \delta(i, i_k^*) = 2 \cdot (|\Pi_k| - 1) \cdot \nu_{\text{star}}(\Pi_k; i_k^*).$

By the triangle inequality, the second term $\sum_{(i,j) \in \Lambda_2} \delta(i, j)$ satisfies

$$\sum_{(i,j) \in \Lambda_2} \delta(i, j) \leq \sum_{(i,j) \in \Lambda_2} \delta(i, i_k^*) + \delta(i_k^*, j) = 2 \cdot (|\Pi_k| - 2) \times \sum_{j \in \Pi_k, j \neq i_k^*} \delta(i_k^*, j)$$

$$= 2 \cdot (|\Pi_k| - 2) \cdot (|\Pi_k| - 1) \cdot \nu_{\text{star}}(\Pi_k; i_k^*).$$
Add up the two terms and we have

$$|\Pi_k| \times (|\Pi_k| - 1) \times \nu(\Pi_k) \leq 2 \times (|\Pi_k| - 1) \times \nu_{\text{star}}(\Pi_k; i_k^*) + 2 \times (|\Pi_k| - 2) \times (|\Pi_k| - 1) \times \nu_{\text{star}}(\Pi_k; i_k^*)$$

$$= 2 \times (|\Pi_k| - 1)^2 \times \nu_{\text{star}}(\Pi_k; i_k^*).$$

Divide both sides by $|\Pi_k| \times (|\Pi_k| - 1)$ and the desired result follows.

\[\square\]

A.2: Proof of Corollary 1

Proof. The first part of the statement is a direct consequence of Lemma 1. To prove the second part, observe that

$$\nu^*_{\text{star}}(\Pi; W) = \sum_{1 \leq k \leq |\Pi|} w(\Pi_k) \cdot \nu^*_{\text{star}}(\Pi_k) \leq \sum_{1 \leq k \leq |\Pi|} w(\Pi_k) \cdot \nu(\Pi_k)$$

$$\leq \sum_{1 \leq k \leq |\Pi|} w(\Pi_k) \cdot \frac{2(|\Pi_k| - 1)}{|\Pi_k|} \cdot \nu^*_{\text{star}}(\Pi_k) < 2 \sum_{1 \leq k \leq |\Pi|} w(\Pi_k) \cdot \nu^*_{\text{star}}(\Pi_k) = 2 \nu^*_{\text{star}}(\Pi; W).$$

\[\square\]

A.3: Proof of Proposition 1

Proof. First, $\nu(\Pi_{\text{opt}}^\nu; W) \leq \nu(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W)$ follows from the definition of $\Pi_{\text{opt}}^\nu$. To prove the other inequality, apply Corollary 1 to $\Pi_{\text{opt}}^{\nu_{\text{star}}}$ and $\Pi_{\text{opt}}^\nu$ and obtain:

$$\nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) \leq \nu(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) < 2 \nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W),$$

$$\nu^*_{\text{star}}(\Pi_{\text{opt}}^\nu; W) \leq \nu(\Pi_{\text{opt}}^\nu; W) < 2 \nu^*_{\text{star}}(\Pi_{\text{opt}}^\nu; W). \quad (8)$$

We then have

$$\nu(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) - \nu(\Pi_{\text{opt}}^\nu; W) \leq 2 \nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) - \nu^*_{\text{star}}(\Pi_{\text{opt}}^\nu; W)$$

$$= \nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) + (\nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) - \nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W))$$

$$\leq \nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) \leq \nu(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) \leq \nu(\Pi_{\text{opt}}^{\nu_{\text{star}}}; W) \leq \nu(\Pi_{\text{opt}}^\nu; W),$$

where (I) follows from (8), (II) and (III) follow from the fact that $\nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}) = \nu_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}})$ has the minimum homogeneity among all subclassifications and hence $\nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}) - \nu^*_{\text{star}}(\Pi_{\text{opt}}^{\nu_{\text{star}}}) \leq 0$, and (IV) follows again from (8).

\[\square\]
A.4: Proof of Proposition 2

Proof. We first prove the first part of the claim. Let $F^*$ be a minimum cost edge cover. Suppose there exists a connected component in $F^*$ that is not a star, then there exists a length-3 path of the form $i - i' - j - j'$. Break it into two pieces $i - i'$ and $j - j'$; the result is another edge cover with non-increasing cost. Repeat the process until there is no length-3 path and hence all connected components are stars. Call this final edge cover $F^*_\text{star}$. $F^*_\text{star}$ has its cost at most equal to that of $F^*$ and hence a minimum cost edge cover. Next we prove the second part. By Lemma 2, for each $\Pi$ and a set of reference units $i^* = (i^*_1, \cdots, i^*_{|\Pi|})$, its homogeneity measure $\nu_{\text{star}}(\Pi; i^*, W^\text{suit})$ corresponds to the cost of an edge cover. Since $F^*_\text{star}$ attains the minimum cost among all edge covers, we necessarily have

$$\text{COST}(F^*_\text{star}) \leq \min_{\Pi \in \mathcal{A}; i^*_k \in \Pi_k, 1 \leq k \leq |\Pi|} \nu_{\text{star}}(\Pi; i^*, W^\text{suit}).$$

(9)

On the other hand, the edge cover $F^*_\text{star}$ has all its connected components stars by the first part of the claim. Let $\Pi^*_\text{star}$ be a partition such that $\Pi^*_k$ is the $k$th connected components of $F^*_\text{star}$ and the reference unit $i^*_k$ the internal node $i^*_{k,\text{star}}$ of the $k$th connected components of $F^*_\text{star}$. Let $i^*_{\text{star}} = (i^*_1, \text{star}, \cdots, i^*_{|\Pi^*_\text{star}|,\text{star}})$. It is evident that $\text{COST}(F^*_\text{star}) = \nu_{\text{star}}(\Pi^*_{\text{star}}; i^*_{\text{star}}, W^\text{suit})$. Hence,

$$\text{COST}(F^*_\text{star}) \geq \min_{\Pi \in \mathcal{A}; i^*_k \in \Pi_k, 1 \leq k \leq |\Pi|} \nu_{\text{star}}(\Pi; i^*, W^\text{suit}).$$

(10)

Combine (10) with (9) and we have established the second part of the claim.

A.5: $F^*_{\text{star},\lambda}$ induces a subclassification that is optimal with respect to $\nu^\lambda_{\text{star}}(\Pi; i^*, W^\text{suit})$

Recall that $F^*_{\text{star},\lambda}$ is the output of the following modified Algorithm 1:

1. Create a copy of $G = (V, E)$ with the same topology and edge cost; denote it as $G' = (V', E')$.
2. For each $v \in V$ and its counterpart $v' \in V'$, add an edge $(v, v')$; a total of $|V|$ edges are added.
3. Assign a cost equal to $2\mu(v) + 2\lambda$ to each edge $(v, v')$, where $\mu(v)$ denotes the minimum cost among all edges incident to $v \in V$.
4. Solve an optimal non-bipartite matching problem in the graph $G \cup G'$; let $M^*$ denote this optimal matching.
5. Delete from $M^*$ any edge in $E'$; replace any edge of the form $(v, v')$ in $M^*$ with an edge $(v, u) \in E$ such that $\delta(v, u) = \mu(v)$; denote by $F^*_\lambda$ the result;

6. Break all length-$3$ paths of the form $i - i' - j - j'$ into two pieces $i - i'$ and $j - j'$ so that $F^*_\lambda$ is reduced to $F^*_{\text{star,} \lambda}$;

7. Return the minimum cost edge cover consisting of all stars $F^*_{\text{star,} \lambda}$.

We prove that $F^*_{\text{star,} \lambda}$ induces a subclassification that is optimal with respect to $\nu^\lambda_{\text{star}}(\Pi; i^*, W^\text{suit})$.

Let $F$ be an edge cover with connected components $\{\Pi_1, \cdots, \Pi_K\}$ and each connected component $\Pi_k$ being a star with internal vertex $i^*_k$ and leaves $\{j \in \Pi_k, j \neq i^*_k\}$. Define its cost

$$\text{COST}_\lambda(F) = \sum_{1 \leq k \leq K} \sum_{j \in \Pi_k, j \neq i^*_k} \delta(i^*_k, j) + \lambda \times \left\{ \sum_{\Pi_k \in \Pi} |\Pi_k| - 2 \right\}. \quad (11)$$

Now consider the subclassification $\Pi = \{\Pi_1, \cdots, \Pi_K\}$. We have

$$\nu^\lambda_{\text{star}}(\Pi; i^*, W^\text{suit}) = \nu_{\text{star}}(\Pi; i^*, W^\text{suit}) + \lambda \times \left\{ \sum_{\Pi_k \in \Pi} |\Pi_k| - 2 \right\}$$
$$= \sum_{1 \leq k \leq K} \sum_{j \in \Pi_k, j \neq i^*_k} \delta(i^*_k, j) + \lambda \times \left\{ \sum_{\Pi_k \in \Pi} |\Pi_k| - 2 \right\} \quad (12)$$
$$= \text{COST}_\lambda(F).$$

Next, we prove the output from the modified Algorithm 1 attains the minimal $\text{COST}_\lambda(\cdot)$ among all edge covers. To this end, let $F^*_{\text{star,} \lambda}$ denote the edge cover returned from the modified Algorithm 1 that consists of all stars. Let $\Pi^*_{\text{star,} 1} = \{\Pi^*_{\text{star,} 1}, \cdots, \Pi^*_{\text{star,} K}\}$ denote the subclassification induced by $F^*_{\text{star,} \lambda}$. Since $F^*_{\text{star,} \lambda}$ consists only of stars, each $\Pi^*_{\text{star,} k}$ has an internal node $i^*_{\text{star,} k}$.

Consider the matching $M^*$ returned by Step 4 of the modified Algorithm 1. Let $(i, j)$ denote an unordered pair so that $(i, j)$ and $(j, i)$ refer to the same edge in a graph. We have

$$\sum_{(i,j) \in M^*} \delta(i, j) = \sum_{(i,j) \in M^* \cap E} \delta(i, j) + \sum_{(i,j) \in M^* \cap E'} \delta(i, j) + \sum_{(i,j) \in M^*, i \in E, j \in E'} \delta(i, j)$$
$$= \sum_{(i,j) \in M^* \cap E} \delta(i, j) + \sum_{(i,j) \in M^* \cap E'} \delta(i, j) + \sum_{(i,j) \in M^*, i \in E, j \in E'} \{2\mu(i) + 2\lambda\}. \quad (13)$$

Consider subclass $\Pi^*_{\text{star,} k}$. By construction, if $\Pi^*_{\text{star,} k}$ satisfies $|\Pi^*_{\text{star,} k}| > 2$, it must have $|\Pi^*_{\text{star,} k}| - 2$
edges connecting \((v, v')\), \(v \in E, v' \in E'\) before being re-wired. Therefore,

\[
\frac{1}{2} \sum_{(i,j) \in M^*} \delta(i,j) = \sum_{1 \leq k \leq K} \sum_{j \in \Pi_{\text{star},k}^*, j \neq i_k^*} \delta(i_k^*, j) + \lambda \times \left\{ \sum_{\Pi_{\text{star},k}^* \in \Pi_{\text{star}}} |\Pi_{\text{star},k}^*| - 2 \right\}
\]

\[= \text{COST}_\lambda(F_{\text{star},*}). \tag{14} \]

Now let \(F'\) be another edge cover with induced subclassification \(\Pi_{\text{star}}' = \{\Pi_{\text{star},1}', \cdots, \Pi_{\text{star},K}'\}\) and each subclass \(\Pi_{\text{star},k}'\) having internal node \(i_k'\). We can reverse the modified Algorithm 1 and recover a matching \(M'\) in the graph \(G \cup G'\). Since \(M^*\) is the minimum cost matching, we immediately have

\[
\text{COST}_\lambda(F_{\text{star},*}) = \frac{1}{2} \sum_{(i,j) \in M^*} \delta(i,j) \leq \frac{1}{2} \sum_{(i,j) \in M'} \delta(i,j) = \text{COST}_\lambda(F'), \ \forall \text{ edge cover } F'.
\]

Combine this result with (12), we immediately have

\[
\text{COST}_\lambda(F_{\text{star},*}) \leq \min_{\Pi \in \mathcal{A} : i_k' \in \Pi_{\text{star}}, 1 \leq k \leq |\Pi|} \nu^\lambda_{\text{star}}(\Pi; \cdot^*, \mathcal{W}^\text{suit}). \tag{15}
\]

Lastly, note that \(\text{COST}_\lambda(F_{\text{star},*})\) is equal to the \(\nu^\lambda_{\text{star}}(\cdot; \cdot, \mathcal{W}^\text{suit})\) homogeneity with respect to the subclassification and internal nodes \(F_{\text{star},*}\) induces; therefore, we have

\[
\text{COST}_\lambda(F_{\text{star},*}) \geq \min_{\Pi \in \mathcal{A} : i_k' \in \Pi_{\text{star}}, 1 \leq k \leq |\Pi|} \nu^\lambda_{\text{star}}(\Pi; i^*, \mathcal{W}^\text{suit}). \tag{16}
\]

Combined (15) and (16) and the desired result follows.

**Supplementary Material B: Additional details on the simulation studies**

**B.1: Data generating process for the illustrative example in Section 5**

The data generating process is similar to those in the simulation section in the main article and is as follows:

\[
Z \sim \text{Uniform}[0,1], \\
X \sim \text{Multivariate Normal}(\mu, \Sigma), \text{ with } \mu = (-2Z, 0, 0)^T, \text{ and } \Sigma = \begin{pmatrix} Z^2 & 0 \\ 0 & I_2 \end{pmatrix}, \\
Y | X, Z \sim \text{Normal}\left(1 \{\exp(0.8X_1 + 0.5X_2) \leq 100\} + Z + 2, 1\right) .
\]
### B.2: Additional simulation results

Table 6: Simulation results when $d = 5$, $n = 500$, and $c = -1$. Average pairwise Mahalanobis distance before matching is 10 and SS before matching is 0.316.

| $\tau_0$ | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
|----------|------|------|------|------|-----|-----|-----|-----|------|------|------|------|---|-----|
| 0        |      |      |      |      |     |     |     |     | 0.955 | 0.955 | 0.955 | 0.955 | 0.002 | 0.134 | 0.289 | 0.494 | 0.007 | 250 |
| 0.1      |      |      |      |      |     |     |     |     | 1.052 | 1.052 | 1.052 | 1.052 | 0.102 | 0.216 | 0.354 | 0.538 | 0.010 | 250 |
| 0.2      |      |      |      |      |     |     |     |     | 1.182 | 1.182 | 1.182 | 1.182 | 0.201 | 0.291 | 0.406 | 0.564 | 0.021 | 250 |
| 0.3      | 0.655 | 1.088 | 1.777 | 2.724 | 1.383 | 1.383 | 1.383 | 1.383 | 0.301 | 0.361 | 0.441 | 0.558 | 0.056 | 250 |
| 0.4      | 0.919 | 1.504 | 2.359 | 3.449 | 1.816 | 1.816 | 1.816 | 1.816 | 0.400 | 0.430 | 0.470 | 0.534 | 0.162 | 250 |

Table 7: Simulation results when $d = 5$, $n = 2000$, and $c = -1$. Average pairwise Mahalanobis distance before matching is 10 and SS before matching is 0.266.

| $\tau_0$ | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
|----------|------|------|------|------|-----|-----|-----|-----|------|------|------|------|---|-----|
| 0        |      |      |      |      |     |     |     |     | 0.955 | 0.955 | 0.955 | 0.955 | 0.002 | 0.139 | 0.292 | 0.489 | 0.007 | 242 |
| 0.1      |      |      |      |      |     |     |     |     | 1.047 | 1.042 | 1.026 | 1.001 | 0.102 | 0.221 | 0.356 | 0.534 | 0.010 | 240 |
| 0.2      |      |      |      |      |     |     |     |     | 1.166 | 1.159 | 1.140 | 1.108 | 0.202 | 0.296 | 0.410 | 0.565 | 0.018 | 238 |
| 0.3      | 0.648 | 1.048 | 1.706 | 2.621 | 1.338 | 1.331 | 1.297 | 1.248 | 0.301 | 0.370 | 0.454 | 0.571 | 0.037 | 231 |
| 0.4      | 0.827 | 1.319 | 2.077 | 3.090 | 1.622 | 1.636 | 1.530 | 1.448 | 0.401 | 0.448 | 0.503 | 0.578 | 0.072 | 215 |

| $\tau_0$ | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
|----------|------|------|------|------|-----|-----|-----|-----|------|------|------|------|---|-----|
| 0        |      |      |      |      |     |     |     |     | 0.955 | 0.955 | 0.955 | 0.955 | 0.002 | 0.140 | 0.293 | 0.490 | 0.007 | 1000 |
| 0.1      |      |      |      |      |     |     |     |     | 1.047 | 1.042 | 1.029 | 1.003 | 0.102 | 0.222 | 0.356 | 0.537 | 0.010 | 1000 |
| 0.2      |      |      |      |      |     |     |     |     | 1.166 | 1.159 | 1.141 | 1.109 | 0.202 | 0.296 | 0.411 | 0.562 | 0.018 | 1000 |
| 0.3      | 0.648 | 1.048 | 1.706 | 2.621 | 1.338 | 1.331 | 1.297 | 1.248 | 0.301 | 0.370 | 0.454 | 0.571 | 0.037 | 231 |
| 0.4      | 0.827 | 1.319 | 2.077 | 3.090 | 1.622 | 1.636 | 1.530 | 1.448 | 0.401 | 0.448 | 0.503 | 0.578 | 0.072 | 215 |

| $\tau_0$ | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
|----------|------|------|------|------|-----|-----|-----|-----|------|------|------|------|---|-----|
| 0        |      |      |      |      |     |     |     |     | 0.955 | 0.955 | 0.955 | 0.955 | 0.002 | 0.139 | 0.293 | 0.490 | 0.007 | 969 |
| 0.1      |      |      |      |      |     |     |     |     | 1.047 | 1.042 | 1.029 | 1.003 | 0.102 | 0.221 | 0.356 | 0.537 | 0.010 | 964 |
| 0.2      |      |      |      |      |     |     |     |     | 1.166 | 1.159 | 1.141 | 1.109 | 0.202 | 0.295 | 0.411 | 0.561 | 0.010 | 955 |
| 0.3      | 0.354 | 0.574 | 0.959 | 1.561 | 0.776 | 0.772 | 0.754 | 0.728 | 0.300 | 0.369 | 0.451 | 0.569 | 0.013 | 931 |
| 0.4      | 0.449 | 0.723 | 1.184 | 1.862 | 0.943 | 0.951 | 0.892 | 0.847 | 0.400 | 0.446 | 0.500 | 0.575 | 0.028 | 868 |
Table 8: Simulation results when $d = 5$, $n = 500$, and $c = 1$. Average pairwise Mahalanobis distance before matching is 10 and SS before matching is 0.303.

| $\tau_0$ | $\nu(\Pi_k)$ | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | $\mu(\Pi_k)$ | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
|----------|----------------|------|------|------|------|-----|-----|-----|-----|----------------|------|------|------|------|-----|-----|
| 0        | Non-Bipartite Pair Match | 0.431 | 0.714 | 1.197 | 1.929 | 0.955 | 0.955 | 0.955 | 0.955 | 0.002 | 0.133 | 0.289 | 0.494 | 0.007 | 250 |
| 0.1      | 0.470 | 0.794 | 1.325 | 2.116 | 1.051 | 1.051 | 1.051 | 1.051 | 0.102 | 0.216 | 0.355 | 0.537 | 0.011 | 250 |
| 0.2      | 0.546 | 0.906 | 1.503 | 2.356 | 1.180 | 1.180 | 1.180 | 1.180 | 0.201 | 0.292 | 0.407 | 0.563 | 0.020 | 250 |
| 0.3      | 0.657 | 1.087 | 1.774 | 2.722 | 1.381 | 1.381 | 1.381 | 1.381 | 0.301 | 0.362 | 0.441 | 0.558 | 0.054 | 250 |
| 0.4      | 0.916 | 1.497 | 2.349 | 3.442 | 1.809 | 1.809 | 1.809 | 1.809 | 0.400 | 0.430 | 0.471 | 0.558 | 0.054 | 250 |
| $\tau_0 = 0.1$ | Non-Bipartite Full Match | 0.479 | 0.794 | 1.325 | 2.116 | 1.051 | 1.051 | 1.051 | 1.051 | 0.102 | 0.216 | 0.355 | 0.537 | 0.011 | 250 |
| 0.1      | 0.485 | 0.791 | 1.310 | 2.093 | 1.046 | 1.040 | 1.025 | 1.000 | 0.102 | 0.221 | 0.357 | 0.534 | 0.010 | 250 |
| 0.2      | 0.550 | 0.894 | 1.471 | 2.310 | 1.165 | 1.157 | 1.139 | 1.107 | 0.202 | 0.297 | 0.411 | 0.563 | 0.018 | 250 |
| 0.3      | 0.649 | 1.049 | 1.702 | 2.613 | 1.337 | 1.329 | 1.297 | 1.248 | 0.301 | 0.371 | 0.454 | 0.571 | 0.036 | 250 |
| 0.4      | 0.829 | 1.320 | 2.075 | 3.082 | 1.621 | 1.632 | 1.531 | 1.450 | 0.401 | 0.448 | 0.502 | 0.578 | 0.070 | 250 |

Table 9: Simulation results when $d = 5$, $n = 2000$, and $c = 1$. Average pairwise Mahalanobis distance before matching is 10 and SS before matching is 0.263.

| $\tau_0$ | $\nu(\Pi_k)$ | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | $\mu(\Pi_k)$ | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
|----------|----------------|------|------|------|------|-----|-----|-----|-----|----------------|------|------|------|------|-----|-----|
| 0        | Non-Bipartite Pair Match | 0.239 | 0.395 | 0.668 | 1.128 | 0.553 | 0.553 | 0.553 | 0.553 | 0.001 | 0.132 | 0.288 | 0.493 | 0.001 | 1000 |
| 0.1      | 0.265 | 0.437 | 0.741 | 1.243 | 0.609 | 0.609 | 0.609 | 0.609 | 0.100 | 0.215 | 0.354 | 0.537 | 0.002 | 1000 |
| 0.2      | 0.299 | 0.496 | 0.840 | 1.393 | 0.683 | 0.683 | 0.683 | 0.683 | 0.200 | 0.290 | 0.405 | 0.562 | 0.006 | 1000 |
| 0.3      | 0.356 | 0.594 | 0.998 | 1.618 | 0.799 | 0.799 | 0.799 | 0.799 | 0.300 | 0.361 | 0.439 | 0.557 | 0.021 | 1000 |
| 0.4      | 0.496 | 0.817 | 1.322 | 2.037 | 1.040 | 1.040 | 1.040 | 1.040 | 0.400 | 0.430 | 0.470 | 0.533 | 0.087 | 1000 |
| $\tau_0 = 0.1$ | Non-Bipartite Full Match | 0.268 | 0.436 | 0.734 | 1.232 | 0.607 | 0.603 | 0.595 | 0.582 | 0.100 | 0.219 | 0.356 | 0.534 | 0.002 | 964 |
| 0.1      | 0.302 | 0.491 | 0.825 | 1.368 | 0.676 | 0.672 | 0.662 | 0.645 | 0.200 | 0.295 | 0.409 | 0.562 | 0.005 | 955 |
| 0.2      | 0.355 | 0.575 | 0.960 | 1.561 | 0.777 | 0.772 | 0.755 | 0.728 | 0.300 | 0.369 | 0.451 | 0.569 | 0.013 | 931 |
| 0.3      | 0.448 | 0.722 | 1.184 | 1.865 | 0.944 | 0.950 | 0.893 | 0.847 | 0.400 | 0.446 | 0.500 | 0.575 | 0.028 | 868 |
Table 10: Simulation results when $d = 5$, $n = 500$, and $c = 2$. Average pairwise Mahalanobis distance before matching is 10 and SS before matching is 1.032.

| $\tau_0$ | $\nu(\Pi_k)$ | $\mu(\Pi_k)$ |
|----------|----------------|----------------|
|          | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
| $0$      | 0.430 | 0.712 | 1.197 | 1.934 | 0.956 | 0.956 | 0.956 | 0.956 | 0.002 | 0.127 | 0.277 | 0.478 | 0.010 | 250 |
| $0.1$    | 0.480 | 0.800 | 1.338 | 2.132 | 1.061 | 1.061 | 1.061 | 1.061 | 0.102 | 0.209 | 0.343 | 0.522 | 0.022 | 250 |
| $0.2$    | 0.554 | 0.924 | 1.535 | 2.408 | 1.205 | 1.205 | 1.205 | 1.205 | 0.201 | 0.285 | 0.395 | 0.551 | 0.059 | 250 |
| $0.3$    | 0.680 | 1.134 | 1.851 | 2.832 | 1.436 | 1.436 | 1.436 | 1.436 | 0.301 | 0.358 | 0.434 | 0.552 | 0.188 | 250 |
| $0.4$    | 0.972 | 1.592 | 2.490 | 3.627 | 1.913 | 1.913 | 1.913 | 1.913 | 0.400 | 0.429 | 0.469 | 0.533 | 0.544 | 250 |

Table 11: Simulation results when $d = 5$, $n = 2000$, and $c = 2$. Average pairwise Mahalanobis distance before matching is 10 and SS before matching is 1.024.

| $\tau_0$ | $\nu(\Pi_k)$ | $\mu(\Pi_k)$ |
|----------|----------------|----------------|
|          | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
| $0$      | 0.239 | 0.394 | 0.669 | 1.127 | 0.553 | 0.553 | 0.553 | 0.553 | 0.000 | 0.126 | 0.276 | 0.476 | 0.002 | 1000 |
| $0.1$    | 0.266 | 0.440 | 0.748 | 1.255 | 0.614 | 0.614 | 0.614 | 0.614 | 0.100 | 0.207 | 0.340 | 0.520 | 0.007 | 1000 |
| $0.2$    | 0.304 | 0.507 | 0.864 | 1.432 | 0.700 | 0.700 | 0.700 | 0.700 | 0.200 | 0.283 | 0.392 | 0.548 | 0.023 | 1000 |
| $0.3$    | 0.372 | 0.626 | 1.056 | 1.703 | 0.840 | 0.840 | 0.840 | 0.840 | 0.300 | 0.355 | 0.431 | 0.549 | 0.095 | 1000 |
| $0.4$    | 0.543 | 0.899 | 1.446 | 2.203 | 1.131 | 1.131 | 1.131 | 1.131 | 0.400 | 0.428 | 0.467 | 0.531 | 0.394 | 1000 |

Non-Bipartite Full Match

| $\tau_0$ | $\nu(\Pi_k)$ | $\mu(\Pi_k)$ |
|----------|----------------|----------------|
|          | 25th | 50th | 75th | 90th | HM1 | HM2 | HM3 | HM4 | Min. | 25th | 50th | 75th | SS | $|\Pi|$ |
| $0$      | 0.243 | 0.394 | 0.665 | 1.121 | 0.553 | 0.551 | 0.543 | 0.532 | 0.001 | 0.130 | 0.278 | 0.471 | 0.002 | 968 |
| $0.1$    | 0.270 | 0.438 | 0.741 | 1.243 | 0.612 | 0.608 | 0.600 | 0.587 | 0.100 | 0.211 | 0.342 | 0.517 | 0.006 | 964 |
| $0.2$    | 0.306 | 0.499 | 0.844 | 1.398 | 0.689 | 0.686 | 0.674 | 0.657 | 0.200 | 0.288 | 0.397 | 0.548 | 0.018 | 951 |
| $0.3$    | 0.364 | 0.594 | 0.996 | 1.616 | 0.803 | 0.804 | 0.775 | 0.748 | 0.300 | 0.364 | 0.442 | 0.558 | 0.049 | 917 |
| $0.4$    | 0.467 | 0.756 | 1.240 | 1.947 | 0.985 | 0.983 | 0.923 | 0.877 | 0.400 | 0.444 | 0.496 | 0.570 | 0.107 | 842 |
Supplementary Material C: Additional details on the application

Tables 12 to 16 summarize the covariate balance after non-bipartite full matching with choices of \( \tau_0 = 0, 0.05, 0.10, 0.20, \) and \( 0.30, \) and complement Table 5 in the main article (\( \tau_0 = 0.15 \)). In practice, practitioners would do a few matches, possibly with different distance specifications and various tuning parameters, all without access to the outcome data, evaluate the balance of each match, and settle down on one match and carry forward the outcome analysis. There are at least two considerations in our application, proximity of units and homogeneity of units’ encouragement doses in matched sets. Matches with \( \tau_0 = 0, 0.05, 0.10, \) and \( 0.15 \) (but not with \( \tau_0 = 0.20 \) or \( 0.30 \)) all met stringent covariate balance criteria: the standardized differences of all 16 covariates in the “high dose” group and the “low dose” group are less than 0.10 and K-S statistics not significant at 0.1 level. Hence, we choose among these 4 matches the one with the most pronounced encouragement dose difference, i.e., \( \tau_0 = 0.15 \).

Table 12: Covariate balance after non-bipartite full matching with \( \tau_0 = 0 \) and \( \lambda = 0 \). Full matching forms 574 matched pairs and 23 matched sets of size 3. The median “average pairwise Mahalanobis distance” is 1.30 after matching. The average internal-node-minus-leaf difference in the encouragement dose is 0.34 among all matched sets

| Patient Composition | Before Matching | Above Median | Below Median | Std. Diff. | K-S Test | Low Dose | High Dose | Std. Diff. | K-S Test | P-Value |
|---------------------|-----------------|--------------|--------------|------------|----------|----------|-----------|------------|----------|---------|
| Mean age, yrs       | 75.29           | 75.10        | 0.11         | < 0.01     | 75.19    | 75.20    | -0.01     | 0.93       |          |
| Male, %             | 0.69            | 0.67         | 0.15         | 0.02       | 0.68     | 0.68     | -0.02     | 0.97       |          |
| White, %            | 0.85            | 0.85         | -0.01        | 0.05       | 0.85     | 0.85     | -0.02     | 0.75       |          |
| Elective, %         | 0.47            | 0.46         | 0.05         | 0.32       | 0.47     | 0.47     | 0.02      | 0.90       |          |
| Diabetes, %         | 0.17            | 0.17         | 0.02         | 0.42       | 0.17     | 0.17     | 0.03      | 0.96       |          |
| Renal diseases, %   | 0.09            | 0.09         | 0.07         | 0.07       | 0.09     | 0.09     | 0.01      | 0.69       |          |
| Arrhythmia, %       | 0.12            | 0.11         | 0.10         | < 0.01     | 0.11     | 0.12     | -0.04     | 0.65       |          |
| CHF, %              | 0.12            | 0.11         | 0.09         | 0.12       | 0.12     | 0.12     | -0.00     | 0.64       |          |
| Hypertension, %     | 0.30            | 0.29         | 0.05         | 0.32       | 0.29     | 0.29     | -0.01     | 0.98       |          |
| Obesity, %          | 0.06            | 0.06         | 0.06         | 0.03       | 0.06     | 0.06     | 0.01      | 0.93       |          |
| Pulmonary diseases, %| 0.02            | 0.02         | 0.12         | < 0.01     | 0.02     | 0.02     | 0.05      | 0.99       |          |
| Hospital Characteristics |              |             |              |            |          |          |          |            |          |
| Cardiac surgical volume | 571        | 456         | 0.21         | < 0.001    | 519      | 509      | 0.02      | 0.57       |          |
| Teaching hospital, yes/no | 0.20      | 0.15        | 0.13         | 0.47       | 0.18     | 0.18     | -0.01     | 1.00       |          |
| Hospital beds       | 419            | 336         | 0.33         | < 0.001    | 382      | 374      | 0.03      | 0.63       |          |
| Full-time registered nurses | 722    | 534         | 0.33         | < 0.001    | 631      | 626      | 0.01      | 0.95       |          |
| Cardiac ICU, yes/no | 0.72           | 0.70         | 0.04         | 0.99       | 0.71     | 0.71     | 0.01      | 1.00       |          |
Table 13: Covariate balance after non-bipartite full matching with $\tau_0 = 0.05$ and $\lambda = 0$. Full matching forms 565 matched pairs and 29 matched sets of size 3. The median “average pairwise Mahalanobis distance” is 1.39 after matching. The average internal-node-minus-leaf difference in the encouragement dose is 0.40 among all matched sets.

| Patient Composition                  | Before Matching | After Matching | K-S Test | Low Dose | High Dose | K-S Test |
|--------------------------------------|-----------------|----------------|----------|----------|-----------|----------|
|                                      | Below Median    | Above Median   | Std. Diff. | P-Value  | Low Dose  | High Dose | Std. Diff. | P-Value  |
| Mean age, yrs                        | 75.29           | 75.10          | 0.11      | < 0.01   | 75.16     | 75.23     | -0.04     | 1.00     |
| Male, %                              | 0.69            | 0.67           | 0.15      | 0.02     | 0.68      | 0.68      | 0.04      | 0.92     |
| White, %                             | 0.85            | 0.85           | -0.01     | 0.05     | 0.85      | 0.85      | -0.02     | 0.15     |
| Elective, %                          | 0.47            | 0.46           | 0.05      | 0.32     | 0.47      | 0.47      | 0.01      | 0.58     |
| Diabetes, %                          | 0.17            | 0.17           | 0.02      | 0.42     | 0.17      | 0.17      | -0.00     | 1.00     |
| Renal diseases, %                    | 0.09            | 0.09           | 0.07      | 0.07     | 0.09      | 0.09      | 0.03      | 0.47     |
| Arrhythmia, %                        | 0.12            | 0.11           | 0.10      | < 0.01   | 0.11      | 0.11      | -0.01     | 0.90     |
| CHF, %                               | 0.12            | 0.11           | 0.09      | 0.12     | 0.12      | 0.12      | 0.01      | 0.50     |
| Hypertension, %                      | 0.30            | 0.29           | 0.05      | 0.32     | 0.29      | 0.29      | -0.02     | 0.66     |
| Obesity, %                           | 0.06            | 0.06           | 0.06      | 0.03     | 0.06      | 0.06      | 0.03      | 0.88     |
| Pulmonary diseases, %                | 0.02            | 0.02           | 0.12      | < 0.01   | 0.02      | 0.02      | 0.07      | 0.63     |

Table 14: Covariate balance after non-bipartite full matching with $\tau_0 = 0.10$ and $\lambda = 0$. Full matching forms 566 matched pairs, 27 matched sets of size 3, and 1 matched set of size 4. The median “average pairwise Mahalanobis distance” is 1.46 after matching. The average internal-node-minus-leaf difference in the encouragement dose is 0.42 among all matched sets.

| Hospital Characteristics              | Before Matching | After Matching | K-S Test | Low Dose | High Dose | K-S Test |
|---------------------------------------|-----------------|----------------|----------|----------|-----------|----------|
|                                      | Below Median    | Above Median   | Std. Diff. | P-Value  | Low Dose  | High Dose | Std. Diff. | P-Value  |
| Cardiac surgical volume               | 571             | 456            | 0.21      | < 0.001  | 527       | 500       | 0.05      | 0.40     |
| Teaching hospital, yes/no             | 0.20            | 0.15           | 0.13      | 0.47     | 0.18      | 0.18      | 0.01      | 1.00     |
| Hospital beds                         | 419             | 336            | 0.33      | < 0.001  | 387       | 369       | 0.07      | 0.28     |
| Full-time registered nurses           | 722             | 534            | 0.33      | < 0.001  | 646       | 610       | 0.06      | 0.32     |
| Cardiac ICU, yes/no                   | 0.72            | 0.70           | 0.04      | 0.99     | 0.71      | 0.71      | 0.01      | 1.00     |
Table 15: Covariate balance after non-bipartite full matching with $\tau_0 = 0.20$ and $\lambda = 0$. Full matching forms 537 matched pairs, 36 matched sets of size 3, 5 matched set of size 4, and 3 matched sets of size 5. The median “average pairwise Mahalanobis distance” is 1.57 after matching. The average internal-node-minus-leaf difference in the encouragement dose is 0.49 among all matched sets.

| Patient Composition | Before Matching | After Matching |
|---------------------|-----------------|----------------|
|                     | Below Median (n = 608) | Above Median (n = 609) | Std. Diff. | K-S Test P-Value | Low Dose Median (n = 589) | High Dose Median (n = 628) | Std. Diff. | K-S Test P-Value |
| Mean age, yrs       | 75.29           | 75.10           | 0.11     | < 0.01       | 75.23               | 75.16               | 0.04     | 0.07             |
| Male, %             | 0.69            | 0.67            | 0.15     | 0.02         | 0.68                | 0.68                | 0.05     | 0.89             |
| White, %            | 0.85            | 0.85            | -0.01    | 0.05         | 0.85                | 0.85                | -0.02    | 0.66             |
| Elective, %         | 0.47            | 0.46            | 0.05     | 0.32         | 0.47                | 0.47                | 0.03     | 0.82             |
| Diabetes, %         | 0.17            | 0.17            | 0.02     | 0.42         | 0.17                | 0.17                | -0.01    | 0.96             |
| Renal diseases, %   | 0.09            | 0.09            | 0.07     | 0.07         | 0.09                | 0.09                | 0.02     | 0.63             |
| Arrhythmia, %       | 0.12            | 0.11            | 0.10     | < 0.01       | 0.12                | 0.11                | 0.04     | 0.07             |
| CHF, %              | 0.12            | 0.11            | 0.09     | 0.12         | 0.12                | 0.11                | 0.02     | 0.31             |
| Hypertension, %     | 0.30            | 0.29            | 0.05     | 0.32         | 0.29                | 0.30                | -0.04    | 0.74             |
| Obesity, %          | 0.06            | 0.06            | 0.06     | 0.03         | 0.06                | 0.06                | 0.02     | 0.38             |
| Pulmonary diseases, %| 0.02            | 0.02            | 0.12     | < 0.01       | 0.02                | 0.02                | 0.06     | 0.50             |

Table 16: Covariate balance after non-bipartite full matching with $\tau_0 = 0.30$ and $\lambda = 0$. Full matching forms 448 matched pairs, 64 matched sets of size 3, 18 matched set of size 4, 9 matched sets of size 5, and 2 matched sets of size 6. The median “average pairwise Mahalanobis distance” is 1.74 after matching. The average internal-node-minus-leaf difference in the encouragement dose is 0.54 among all matched sets.

| Hospital Characteristics | Before Matching | After Matching |
|--------------------------|-----------------|----------------|
|                         | Below Median (n = 608) | Above Median (n = 609) | Std. Diff. | K-S Test P-Value | Low Dose Median (n = 572) | High Dose Median (n = 645) | Std. Diff. | K-S Test P-Value |
| Cardiac surgical volume  | 571             | 456            | 0.21     | < 0.001       | 542                 | 484                 | 0.11     | 0.08             |
| Teaching hospital, yes/no| 0.20            | 0.15           | 0.13     | 0.47         | 0.18                | 0.18                | 0.00     | 1.00             |
| Hospital beds           | 419             | 336            | 0.33     | < 0.001      | 394                 | 362                 | 0.13     | 0.08             |
| Full-time registered nurses| 722            | 534            | 0.33     | < 0.001      | 659                 | 596                 | 0.11     | 0.10             |
| Cardiac ICU, yes/no     | 0.72            | 0.70           | 0.04     | 0.99         | 0.71                | 0.71                | -0.01    | 1.00             |