Matching for causal effects via multimarginal optimal transport

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Abstract

Matching on covariates is a well-established framework for estimating causal effects in observational studies. The principal challenge in these settings stems from the often high-dimensional structure of the problem. Many methods have been introduced to deal with this challenge, with different advantages and drawbacks in computational and statistical performance and interpretability. Moreover, the methodological focus has been on matching two samples in binary treatment scenarios, but a dedicated method that can optimally balance samples across multiple treatments has so far been unavailable. This article introduces a natural optimal matching method based on entropy-regularized multimarginal optimal transport that possesses many useful properties to address these challenges. It provides interpretable weights of matched individuals that converge at the parametric rate to the optimal weights in the population, can be efficiently implemented via the classical iterative proportional fitting procedure, and can even match several treatment arms simultaneously. It also possesses demonstrably excellent finite sample properties.

1 Introduction

Identifying cause and effect is one of the primary goals of scientific research. The leading approaches to uncover causal effects are randomized controlled trials. Unfortunately, such trials are often practically infeasible on ethical grounds, might not be generalizable beyond the experimental setting due to lack of variation in the population, or simply have too few participants to generate robust results due to financial or logistical restrictions. An attractive alternative is to use observational data, which are ubiquitous, often readily available, and comprehensive.

The main challenge in using observational data for causal inference is the fact that assignment into treatment is not perfectly randomized. This implies that individuals assigned to different treatments may possess systematically different observable and unobservable covariates. Comparing the outcomes between individuals in different treatment groups may then yield a systematically biased estimator of the true causal effect. Matching methods are designed to balance the treatment samples in such a way that differences between the observed covariates of the groups are minimized. This allows the researcher to directly compare the balanced treatment groups for estimating the true causal effect under the assumption that the unobservable covariates of individuals are similar if their observed covariates are similar.

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1.1 Existing approaches and persisting challenges

The most widely adopted matching approach in the setting of a binary treatment is matching on the propensity score (Rosenbaum & Rubin 1983). Many adjustments and refinements have been proposed in the literature, see for instance Austin (2008, 2011) and Imbens (2004) for reviews. The idea is to balance the samples of treatment and control groups by comparing individuals with similar propensity scores, i.e. the probability of receiving the treatment conditional on the observable covariates. Under the assumption that the observed covariates capture all the systematic heterogeneity of individuals, the so-called “unconfoundedness assumption” (Imbens 2000, Imbens & Rubin 2015), the researcher can obtain an estimate of the respective causal effect by comparing the outcomes of individuals in treatment and control group with similar propensity scores. The utility of the propensity score derives from dimension reduction: instead of having to match individual covariates in a possibly high-dimensional space, one can match on a one-dimensional score.

However, propensity score matching is no panacea for unbalanced samples. First, as pointed out in Imbens (2000), in multivalued treatment settings comparing individuals across groups with similar propensity scores is not equivalent to comparing individuals with similar covariates. This induces bias in the procedure and makes the propensity score “less well-suited” in a setting with more than two treatment arms (Imbens 2000, Lopez & Gutman 2017). Recent approaches address this issue at the cost of interpretability (Li & Li 2019). Second, even in binary settings propensity score matching has been argued to potentially introduce bias in finite samples (King & Nielsen 2019). The reason lies in the fact that propensity score matching tries to generate a balanced sample that resembles a randomized trial. This does not imply that all corresponding covariates are matched exactly in finite samples, see King & Nielsen (2019) for a detailed analysis. Third, in high-dimensional settings one usually resorts to estimating the propensity score function based on parametric models, which can introduce misspecification bias.

The main alternative to propensity score matching is to match the covariates directly. There are a multitude of matching approaches and refinements, see for instance Abadie et al. (2004), Abadie & Imbens (2011), Hainmueller (2012), Lopez & Gutman (2017), Morucci et al. (2020), Rosenbaum (1989, 2020), Rosenbaum et al. (2007), Zubizarreta (2015) and references therein. Stuart (2010) provides a concise overview of the fundamental ideas. Kallus (2020) recently introduced a general framework for optimal matching that subsumes many approaches and Dunipace (2021) showed that most existing matching approaches can be phrased in the language of optimal transportation. The most widely used idea is to specify a distance, e.g. a weighted Euclidean distance or some discrepancy measure like the Kullback-Leibler divergence, and to proceed via some form of $k$-nearest neighbor matching (Abadie et al. 2004, Rubin 1973, Stuart 2010).

Direct matching comes with computational and statistical challenges. From a computational perspective, matching covariates in high-dimensional settings is more complex than matching on a one-dimensional score, see for instance Rosenbaum (1989) for a classical analysis. From a statistical perspective, most optimal matching approaches, and especially $k$-nearest neighbors matching approaches or variants thereof, are non-smooth approaches due to the strict cut-off at $k$ neighbors. Therefore, they often provide optimal matchings with poor statistical properties. In particular, the obtained estimators for causal effects are often asymptotically biased and need not converge at the parametric rate as shown in Abadie & Imbens (2006) in the case of $k$-nearest neighbor approaches. Abadie & Imbens (2011) introduced a bias correction for these estimators, but it is computationally complex to implement, potentially prohibitively so in many settings. Analogous rigorous statistical results for similar matching algorithms have been absent in the literature, especially in the multiple treatment setting as argued in Lopez & Gutman (2017).

There is hence a need for a direct matching method that can provide interpretable weights.
of the optimal matches across several treatment arms while possessing good computational and statistical properties.

1.2 Outline of the proposed method

![Figure 1: Optimal matching via entropy-regularized optimal transport in the binary setting.](image)

This article introduces a natural matching method based on multimarginal entropy-regularized optimal transport theory. It is an alternative to existing matching approaches in terms of how it weights the matches. It can be regarded as a nearest-neighbor matching approach where the number of neighbors and corresponding weights are chosen endogenously. The basic idea is best illustrated in the binary setting as in Figure 1. The two measures \( \mu_1 \) and \( \mu_0 \) are the distributions of covariates in the treatment (\( T = 1 \)) and control group (\( T = 0 \)), respectively, which for this illustration we assume are univariate and observed. In this example they are absolutely continuous with respect to Lebesgue measure, but the approach works for any type of measures. \( \gamma \) is a coupling of \( \mu_0 \) and \( \mu_1 \), that is, a joint probability measure such that \( \mu_0 \) and \( \mu_1 \) are its marginal measures. This joint coupling is an approximate optimal transport plan as we explain below. In particular, it defines a weighted set \( A_1 \) of control individuals for each draw \( X_1 \) from the distribution of the treatment group \( \mu_1 \). These weights are defined via the conditional measure \( \gamma(A_1|x_1) \) where \( A_1 \) is the set of control individuals for the given treated individual with covariate \( X_1 = x_1 \).

This weighting is what sets the proposed method apart from other matching approaches. Consider \( k \)-nearest neighbors matching. There, one chooses a fixed number \( k \) of neighbors and weights them uniformly. This is a non-smooth approach for given data (Abadie & Imbens 2006). By contrast, the proposed method chooses a natural weighting \( \gamma(\cdot|x_1) \) of the matched control individuals that takes into account the cost of matching. One commonly chooses distances on the covariate space as the cost function, for instance the Euclidean distance. Then the proposed method naturally re-weights the matched control units in terms of their distance from the treated unit. Figure 2 illustrates this. This provides a natural and smooth weighting procedure and is the main reason why our method enjoys good statistical performance, as we prove in section 4 below.

The proposed method provides an optimal matching in finite samples by construction in contrast to propensity score approaches. This naturally comes with an increased computational cost compared to propensity score methods due to the dimensionality of the problem. However, as a
direct matching approach, it possesses excellent computational properties. It can be solved via the standard *Iterative Proportion Fitting Procedure* (IPFP) (Deming & Stephan 1940), also called the Sinkhorn algorithm (Sinkhorn 1964). This procedure can straightforwardly be extended to the multiple-treatment setting, which we analyze below. In this sense, the proposed method addresses the challenges outlined in the introduction: it (i) provides finite sample optimal matchings and (ii) interpretable weights based on covariate distance, is (iii) computationally efficient with (iv) good statistical properties, and (v) can even provide a joint optimal matching in multivalued treatment settings. We demonstrate the excellent finite sample properties in a simple simulation exercise in section 5.

We provide the statistical properties of the optimal matching obtained via our procedure in section 4. This result allows for a different number of individuals in different treatment arms, which is crucial in practical settings. This complements the other existing statistical result from Harchaoui et al. (2020) who derive asymptotic results in the binary treatment setting and require that the number of individuals in both treatment arms are the same.

In concurrent work to ours Dunipace (2021) provides a matching estimator that is also based on optimal transportation. Their setting is a prediction problem, which is different from ours. They consider two groups: in a given group $A$, all covariates, outcomes, and treatment assignment are observed. In particular, individuals in $A$ can be exposed to either the treatment or control intervention. The question is then to predict the outcomes and the corresponding treatment effect in a group $B$ where only covariates are observed. They use optimal transport matching to impute the outcomes and the corresponding effects. In contrast, we use optimal transportation to jointly balance and re-weight several samples that only receive one type of treatment. In particular, a main result of this paper is to introduce a balancing of the groups via the conditional measure $\gamma(\cdot|x)$ obtained by the joint coupling $\gamma$. Our proposed method hence redefines the estimation for causal effects in a way that is different from existing approaches.

## 2 Matching via entropy-regularized optimal transport

This section briefly introduces the mathematical background on optimal transport needed for the proposed matching estimator. For further information we refer to Santambrogio (2015) and Villani (2003, 2009) for introductions to general optimal transportation theory and to Peyré & Cuturi (2019) for a review of the entropy-regularized optimal transportation approach we consider.
2.1 Optimal transport: a brief overview

For two given marginal distributions $\mu_0$ and $\mu_1$ of characteristics of groups to be matched, defined on spaces $X$ and $Y$ respectively, the classical Kantorovich problem (Villani 2003, chapter 1) consists in finding an optimal transport plan, i.e. a probabilistic matching between the group whose characteristics are distributed as $\mu_0$ and the group whose characteristics are distributed as $\mu_1$. This is a joint coupling $\gamma$ in the space of all couplings $\Pi(\mu_0, \mu_1)$ of these two marginals in such a way that the average cost of transportation of mass from $X$ to $Y$ is minimized. Formally, the Kantorovich problem takes the form

$$\inf_{\gamma \in \Pi(\mu_0, \mu_1)} \int_{X \times Y} c(x, y) \, d\gamma(x, y),$$

where $\Pi(\mu_0, \mu_1)$ is the set of all (Borel-) probability measures on $X \times Y$ whose marginals are $\mu_0$ and $\mu_1$, respectively, and where $c : X \times Y \to \mathbb{R}$ is a cost function encoding the difficulty of moving mass from $X$ to $Y$. In many cases of interest the cost function is chosen to be a metric on the underlying space, such as the Euclidean distance, i.e.

$$c(x, y) \equiv |x - y|^2.$$

A distance function such as the squared Euclidean distance is the most natural choice for a cost function, but our method applies to any cost function that is infinitely often differentiable. This can be useful in settings where the researchers want to take into account more information on the cost of comparing individuals than only the distance of their covariates.

This binary setting can straightforwardly be extended to the multimarginal setting by searching for a joint coupling over several marginals $\{\mu_j\}_{j=1}^J$ (Gangbo & Święch 1998):

$$\inf_{\gamma \in \Pi(\mu_1, \ldots, \mu_J)} \int_{X} c(x) \, d\gamma(x),$$

(1)

where we denote $X = X_1, \ldots, X_J$ and $x := (x_1, \ldots, x_J)$. Note that in the multimarginal setting we index the measures $\mu_j$ starting from 1, in contrast to the binary setting. This is to signify that in a multimarginal setting one does not necessarily have a true control group.

In many cases in the binary setting, for instance when $\mu_0$ possesses a density with respect to Lebesgue measure and the cost function is strictly convex, $\gamma$ is supported on the graph of a function. In this case one obtains a deterministic matching between individuals in $\mu_0$ and individuals in $\mu_1$ that takes the form of a function, i.e. every individual with characteristic $x \in X$ is mapped to at most one individual with characteristic $Y$. A special case of this is Brenier’s classical theorem on the structure of optimal solutions of the Monge-Kantorovich problem in the case of the squared Euclidean distance as a cost function (Brenier 1991). Similar results have been shown in the multimarginal setting, see Agueh & Carlier (2011), Carlier & Ekeland (2010), Gangbo & Święch (1998), Pass (2015).

2.2 Entropy regularized optimal transport and the Schrödinger bridge problem

Unfortunately, the computational and statistical properties of the optimal transport problem (1) are poor. In particular, in practical settings, when the actual distributions $\mu_0$ and $\mu_1$ are unknown and have to be estimated from the observable characteristics of individuals, estimating the optimal matching $\gamma$ suffers from the curse of dimensionality (Forrow et al. 2019, Gunsilius 2021, Hütter & Rigollet 2021, Manole et al. 2021, Weed & Bach 2019). This curse of dimensionality is also computational (Altschuler & Boix-Adsera 2021).
Furthermore, looking for a single perfect match, as the Kantorovich problem does, is often not even desired in finite samples. If the data possess enough observations that can be used for close matchings, then an average of several close matches can provide more robust results and reduce the variance of the estimator. Of course, using several potential matches leads to more bias in estimating causal effects based on the optimal matching (Abadie & Imbens 2006). However, the weighting scheme of the proposed matching approach chooses the number of matches in finite samples automatically and hence to mitigates some of this bias compared to rigid $k$-nearest neighbor matching approaches as we argue below.

This is why we propose to use **entropy-regularized optimal transportation** for the problem of matching for causal effects. Entropy regularization of the Kantorovich problem was introduced in Galichon & Salanié (2010) in economics and in Cuturi (2013) in the machine learning literature and is one of the main ways to compute approximations to optimal transportation matchings in practice (Peyré & Cuturi 2019). From a statistical perspective it is natural because it can be interpreted as maximum likelihood deconvolution (Rigollet & Weed 2018).

To obtain a multimarginal matching between the distributions $\mu_1, \ldots, \mu_J$ of characteristics, we solve the following entropy regularized optimal transport problem for some $\varepsilon > 0$ and a cost function $c(x)$ which we will assume throughout is smooth, i.e. $c(x) \equiv c(x_1, \ldots, x_J) \in C^\infty(\mathcal{X})$:

$$\inf_{\gamma \in \Pi(\mu_1, \ldots, \mu_J)} \int_{\mathcal{X}} c(x) \, d\gamma(x) + \varepsilon KL(\gamma || \otimes_{j=1}^J \mu_j).$$  \hspace{1cm} (2)

Here, $\otimes_j \mu_j(x) = \mu_1(x_1) \otimes \cdots \otimes \mu_J(x_J)$ denotes the independence coupling of the marginal measures $\mu_1, \ldots, \mu_J$, and

$$KL(\gamma || \otimes_j \mu_j) := \begin{cases} \int_{\mathcal{X}} \ln \frac{d\gamma}{\otimes_j \mu_j}(x) \, d\gamma(x) + (\int_{\mathcal{X}} d\otimes_j \mu_j(x) - \int_{\mathcal{X}} d\gamma(x)) & \text{if } \gamma \ll \otimes_j \mu_j \\ +\infty & \text{otherwise} \end{cases}$$

denotes the Kullback-Leibler divergence (Kullback & Leibler 1951, Kullback 1959). From a mathematical perspective, this problem and its regularity properties have been analyzed thoroughly, see for instance Carlier & Laborde (2020), Carlier (2021), Genevay et al. (2019), di Marino & Gerolin (2020) for recent results and references therein. Note that as $\varepsilon \to 0$ the optimal matching $\gamma^*$ solving (2) approximates the optimal matching obtained via the classical Kantorovich problem (1) under mild regularity assumptions (Nutz & Wiesel 2021).

One can formally rewrite the problem in terms of the following entropy projection problem, which is the static Schrödinger bridge problem (Schrödinger 1931, 1932)

$$\inf_{\gamma \in \Pi(\mu_1, \ldots, \mu_J)} \varepsilon KL \left( \gamma \left|\right|\exp \left( \frac{-c}{\varepsilon} \right) \otimes_{j=1}^J \mu_j \right).$$  \hspace{1cm} (3)
2.3 The Schrödinger system and the IPFP

For computational purposes, it is rather useful to consider the dual problem of the Schrödinger problem (3), which is (Carlier & Laborde 2020, di Marino & Gerolin 2020)

$$\inf_{\varphi := (\varphi_1, \ldots, \varphi_J)} F(\varphi) := -\sum_{j=1}^J \int_{X_j} \varphi_j(x_j) d\mu_j(x_j) + \varepsilon \int_{\mathcal{X}} \exp \left( \frac{\sum_{j=1}^J \varphi_j(x_j) - c(x)}{\varepsilon} \right) d\otimes_{j=1}^J \mu_j(x) - \varepsilon,$$

where the potentials $\varphi := (\varphi_1, \ldots, \varphi_J)$ are only assumed to be bounded, i.e. $\varphi := (\varphi_1, \ldots, \varphi_J) \in \prod_{j=1}^J L^\infty(\mu_j)$.

The reason is that the first-order optimality conditions to (4) form the Schrödinger system of the form

$$\exp \left( \frac{\varphi_j(x_j)}{\varepsilon} \right) \int_{\mathcal{X}_{-j}} \exp \left( \frac{\sum_{i \neq j} \varphi_i(x_i) - c(x)}{\varepsilon} \right) d\otimes_{i \neq j} \mu_i(x_{-j}) = 1,$$

for all $1 \leq j \leq J$. This can be solved via the IPFP (Deming & Stephan 1940), also called the Sinkhorn algorithm (Sinkhorn 1964) by recursively solving for the sequences $\{\varphi^m_j\}_{m \in \mathbb{N} \cup \{0\}}$, $j = 1 \ldots, J$ defined via (Carlier & Laborde 2020, di Marino & Gerolin 2020)

$$\varphi^0_1(x_1) = 1$$
$$\varphi^0_j(x_j) = 1 \quad j = 2, \ldots, J$$
$$\vdots$$

$$\varphi^m_j(x_j) = -\varepsilon \log \left( \int_{\mathcal{X}_{-j}} \exp \left( \frac{\sum_{i < j} \varphi^m_i(x_i) + \sum_{i > j} \varphi^m_{i-1}(x_i) - c(x)}{\varepsilon} \right) d\otimes_{i \neq j} \mu_j(x_{-j}) \right) + \lambda^m_{\varphi_j},$$

where the constant $\lambda^m_{\varphi_j}$ takes the form (Carlier 2021, di Marino & Gerolin 2020)

$$\lambda^m_{\varphi_j} = \varepsilon \log \left( \int_{\mathcal{X}_{-j}} \exp \left( \frac{\sum_{i < j} \varphi^m_i(x_i) + \sum_{i > j} \varphi^m_{i-1}(x_i)}{\varepsilon} \right) d\otimes_{i \neq j} \mu_j(x_{-j}) \right).$$

Recently, di Marino & Gerolin (2020) and Carlier (2021) have proved (linear) convergence of the sequence $\varphi^m_j$ to the optimal $\varphi^* := (\varphi^*_1, \ldots, \varphi^*_J)$ as $m \to \infty$ for different degrees of smoothness of the cost function, extending convergence results from the two-marginal case (Chen et al. 2016, Franklin & Lorenz 1989, Rüschendorf 1995).

This dual approach only computes the optimal potentials $\varphi^*$, and only up to the additive constants $\lambda_{\varphi_j}$, which can be fixed by normalization. One can generate the optimal matching $\gamma^*$ from this via

$$d\gamma^* = \exp \left( \frac{\sum_{j=1}^J \varphi^*_j - c(x)}{\varepsilon} \right) \cdot d\otimes_j \mu_j,$$

i.e. the optimal potentials are used to generate the optimal matching $\gamma$ as an exponential tilting of the independence coupling of the marginals $\mu_j$ (di Marino & Gerolin 2020, Proposition 4.6 (3)). $\gamma^*$ and $\varphi^*_j$ all depend on $\varepsilon$, but we make this dependence implicit for notational convenience.

It is the IPFP that makes solving the entropy regularized problem so convenient. The above procedure (6) is written out for general measures $\mu_j$. In practice, where the measures $\mu_j$ are
unknown and have to be estimated from observations, efficient implementations have been proposed, see Peyré & Cuturi (2019) and references therein. In particular, the IFPF is easily parallelizable. Of particular importance for high-dimensional matching scenarios are mini-batch approaches (Genevay et al. 2018, Damodaran et al. 2018) that break the problem into smaller parts.

The entropy regularized optimal transport approach possesses excellent computational properties. In particular, if the regularization parameter $\varepsilon > 0$ is not too small, then the practical algorithm converges quickly to the optimal value (Altschuler et al. 2017). Moreover, the multimarginal Sinkhorn algorithm only requires a polynomial number of iterations (Lin et al. 2019) and can even be implemented in polynomial time in specific settings (Altschuler & Boix-Adsera 2020). By contrast, when $\varepsilon$ is close to zero, the convergence can be slow and unstable, as the IPFP then provides a close approximation of the classical optimal transport problem whose estimation suffers from a curse of dimensionality. However, recent results (Seguy et al. 2018, Pooladian & Niles-Weed 2021) based on classical Wasserstein geometry (Ambrosio et al. 2008, Theorem 12.4.4) show that one can estimate the optimal transport map (if it exists) via a straightforward barycentric projection. This implies that one does not need to take the limit $\varepsilon \to 0$ in practice, which circumvents stability issues; also see the discussion after Corollary 1 in section 4.

For the multimarginal case introduced above, the optimal probabilistic matching $\gamma^*$ of the participants is jointly over all $J$ treatment arms. In particular, for each individual $n_j$ in treatment arm $j$ it provides the optimally weighted matchings in each other treatment arm $i \neq j$. The additional information obtained from the full multimarginal matching comes with an increase in computational cost. That is, we need to specify (and store in memory) the squared distances between all possible points of all 3 marginal measures. This becomes increasingly costly with dimension, even for the most efficient implementations (Lin et al. 2019). In addition, to obtain a tensor joint distribution that can provide a mapping close to a curve in multi-dimensional space, instead of a more uniformly spread-out mass, one needs to specify an $\varepsilon$ much smaller than in the pairwise setting, which can make the algorithm more difficult to converge and bring stability issues.

Therefore, we recommend a pairwise comparisons approach to reduce the computational burden in very high-dimensional settings with many treatment arms. Still, since the binary setting is a special case of the multimarginal setting we phrase and prove all results in the general multimarginal setting.

### 3 Causal effects via optimal transport matching

This section connects the matching problem to inference on causal effects. We rely on the potential outcome framework (Imbens & Rubin 2015, Rubin 1974). Let $Y(j)$ be the potential outcome under the causal inference framework for treatment $j \in \{1, \ldots, J\}$, $T$ be the treatment assignment, and random variable $D$ supported on $\{\tau \in \{0, 1\}^J : \sum_{j=1}^J \tau_j = 1\}$ be the binary vector of the treatment assignment: $T = j$ if and only if $D(j) = 1$. $X \in \mathbb{R}^d$ is the vector of observed covariates. We make the following set of assumptions, the first three standard in the literature (Abadie & Imbens 2006, Imbens 2000, Imbens & Rubin 2015).

**Assumption 1.** For $j = 1, \ldots, J$,

1. (Weak unconfoundedness) $D(j) \perp \perp Y(j)|X$,
2. (Overlap) $P(D(j) = 1|X)$ is bounded away from 0 and 1,
3. Conditional on $D(j) = 1$, the sample is independently drawn from $(Y, X)|D$, and the marginal $X \sim \mu_j$ given $D(j) = 1$,
Given \( D(j) = 1 \), there exists a bounded continuous function \( f_j \) supported on a convex and compact set \( \mathcal{X}_j \subset \mathbb{R}^d \) such that \( f_j(X) = \mathbb{E}(Y|T = j, X) \). For a more explicit notation, we use \( y(j, X) := f_j(X) \) and \( \varepsilon_i = Y_i - y(T_i, X_i) \) are i.i.d. mean-zero noise terms.

Parts 1 and 2 of Assumption 1 are standard. The weak unconfoundedness assumption formalizes the idea of matching on observables: it guarantees that there are no more systematic differences between the unobservable covariates of the groups once the observable characteristics have been accounted for. The weak unconfoundedness assumption was introduced in Imbens (2000) and is slightly weaker than the strong unconfoundedness assumption introduced in Rosenbaum & Rubin (1983) since it is locally constrained for every realization of the treatment assignment. The overlap assumption guarantees that one can find appropriate matches in each group. If this were not the case, the estimate of the causal effect would be biased. It is a fundamental assumption for any matching approach (Imbens & Rubin 2015). Part 3 of Assumption 1 states that all treatment groups are independently sampled; a similar assumption is made in classical matching approaches (Abadie & Imbens 2006). Part 4 introduces regularity assumptions that are weaker than existing assumptions. In particular, we do not specify any parametric restrictions on the relationship between \( Y \) and \( X \) like linearity or convexity and only require additive separability analogously to Abadie & Imbens (2006).

Under part 3 in Assumption 1, we can denote \( X_j := X|D(j) = 1 \), \( X_j \sim \mu_j \) and \( \gamma \) as the joint coupling over \( \prod_{j=1}^J \mathcal{X}_j \) with the marginal distributions \((\mu_1, \ldots, \mu_J)\) obtained via the proposed matching procedure. The expected counterfactual outcome \( \mathbb{E}(Y(t)) \) for treatment \( T = t \) can then be written as \( \mathbb{E}(Y(t)) = \mathbb{E}_X \{ \mathbb{E}(Y(t)|D(t) = 1, X) \} = \mathbb{E}_X(y(t, X)) \).

In the population one hence knows the counterfactual outcome \( Y(j) \) for any treatment status \( T = j \). This is not the case in realized samples, however, which is the “fundamental problem of causal inference” (Holland 1986): for each individual \( i = 1, \ldots, N \) the researcher only observes one potential outcome \( Y_i(j) \) for the given treatment \( T = j \) that the individual was assigned to. In order to compute the causal effect of a treatment, the researcher should compare \( Y_i(j) \) to \( Y_i(k) \), \( k \neq j \) for each \( i \), which is impossible. The idea of matching on covariates is hence to impute the counterfactual outcomes \( Y_i(k) \) for individual \( i \) by considering the outcomes of other individuals that received a different treatment \( k \). The unconfoundedness assumption implies that individuals with similar observable covariates also possess similar unobservable characteristics, which makes matching on observable covariates a feasible approach. This implies that two individuals with the same observable covariates do not systematically differ in their heterogeneity and that one can consider the observed outcome of one individual as the potential outcome of another. This leads us to the following definition of the potential outcome imputed by our proposed method.

**Definition 1.** For the \( j \)-th treatment and \( t \neq j \) denote \( \gamma_{j|t} \) as the conditional measure of covariates in group \( j \) given the covariates in group \( t \) under the joint distribution \( \gamma \). Then under Assumption 1, the expected potential outcome can be expressed in the sample version as

\[
\mathbb{E}(Y(j)) = \frac{1}{N} \sum_{i=1}^N Y_i I(D_i(j) = 1) + \frac{1}{N} \sum_{t=1}^T \sum_{j \neq t} \sum_{k \neq t} Y_k \hat{\gamma}_{N,j|t}(X_k|X_i) I(D_i(t) = 1),
\]  

where \( N = \sum_{j=1}^J N_j \) is the overall number of sample points over all treatment arms and \( \hat{\gamma}_N \) is the empirical counterpart to the optimal matching estimated via the IPFP (6) by replacing \( \mu_j \) with the empirical measures \( \hat{\mu}_{N,j} \) defined below in (10).

Definition 1 focuses on the expected potential outcome, but the formulation (7) provides a general way to obtain estimators of many different types of causal effects: average treatment effects
can be obtained as a difference of expected potential outcomes; quantile treatment effects or differences in Gini coefficients (Imbens & Rubin 2015, chapter 20) can be obtained by composing \( Y_i \) with different functions. It is also straightforward to obtain conditional causal effects by conditioning on specific covariate values \( X = x \).

For comparison, recall that the \( k \)-nearest neighbors matching estimator for the potential outcome \( Y_i(0) \) in the binary treatment case in Abadie & Imbens (2006) is defined as

\[
\hat{Y}_i(0) = \begin{cases} 
Y_i, & \text{if } T_i = 0, \\
\frac{1}{M} \sum_{j \in J_M(i)} Y_j, & \text{if } T_i = 1 
\end{cases}
\]

(8)

where \( J_M(i) \) is a group of \( M \) matches that are closest to \( i \). This group is determined by the distance between the covariates \( X_j \) and \( X_i \). In analogy to (8) we can write (7) as

\[
\hat{Y}_i(0) = \begin{cases} 
Y_i, & \text{if } T_i = 0, \\
\sum_{k \neq i} Y_k \gamma_{N,0}(X_k|X_i) I(D_i(t) = 1), & \text{if } T_i = t, \; t \neq 0 
\end{cases}
\]

(9)

The estimator of the expected counterfactual outcome proposed in (7) is analogous to the \( k \)-nearest neighbor idea (8), with \( J_M(i) \) being replaced by the support of \( \hat{\gamma}_{N,j} \), and the equal weight \( \frac{1}{M} \) replaced by the probability mass \( \hat{\gamma}_{N,0}(X_k|X_i) \). Moreover, recall that in the binary treatment setting, the propensity score approach uses the Horvitz-Thompson type estimator (Horvitz & Thompson 1952) with the selection probability \( r(t,x) := P(T = t|X = x) \) to estimate the average treatment effect \( E(Y(t)) = E \left( \frac{Y(t)}{r(t,X)} \right) \), or alternatively \( E \{ E(Y(t)|r(t,X)) \} \), which shows the connection of the proposed method (7) to the propensity score approach.

### 4 Asymptotic statistical properties

We have introduced the method and argued that it provides interpretable weights and optimal matchings in finite samples via a computationally efficient procedure. The last thing to show are asymptotic statistical properties of the estimator \( \hat{\gamma}_{N} \) of the optimal matching.

Recently Harchaoui et al. (2020) proved asymptotic linearity of the empirical process of the optimal matching in the binary setting under the assumption that both treatment arms contain the same number of observations. Klatt et al. (2020), also in the binary setting, show asymptotic normality of the optimal matching and validity of the bootstrap in the setting where all distributions are purely discrete. We complement these results in the multimarginal setting by allowing for a different number of observations in each arm.

In practice, researchers observe the empirical measures

\[
\hat{\mu}_{N,j} := \frac{1}{N_j} \sum_{n_{j}=1}^{N_j} \delta_{X_{n,j}} 
\]

(10)

for \( j = 1, \ldots, J \), where \( \delta_{X_{n,j}} \) denotes the Dirac measure at the observation \( X_{n,j} \). This allows for differing sample sizes \( N_j \) in each cohort.

Throughout, we assume that we observe independent and identically distributed draws \( X_{n_{j}} \) from the respect distributions \( \mu_{j} \). For notational convenience we will index estimators of functional relationships \( f \) that depend on all \( j \) elements as \( \hat{f}_{N} \), where it is implicitly understood that \( N \) is the overall number of data points across all groups. We require the following mild assumptions for our statistical analysis.
Assumption 2. For all \( j = 1, \ldots, J \) the observable random variables \( \{X_{n_j}\}_{n_j=1,\ldots,N_j} \) are independent and identically distributed draws from the measure \( \mu_j \).

Assumption 3. For all \( j = 1, \ldots, J \) the supports \( X_j \subset \mathbb{R}^d \) of \( \mu_j \) are convex and compact.

Assumption 4. The samples are asymptotically balanced, i.e. there exist constants \( \rho_1, \rho_2, \ldots, \rho_J > 0 \) such that \( \sum_{n_j \in N_j} \rho_j \to \rho_j \) as \( N_j \to \infty \) for all \( j = 1, \ldots, J \).

To simplify the subsequent statements, we define the operator \( T(\varphi) := (T_1(\varphi), \ldots, T_J(\varphi)) \) with

\[
T_j(\varphi)(x_j) = \int_{X_{-j}} \exp \left( \frac{\sum_j \varphi_j(x_j) - c(x)}{\varepsilon} \right) d\prod_{i \neq j} \mu_i(x_{-j}),
\]

which corresponds to the first-order condition of the dual problem of the Schrödinger bridge problem (5). \( T(\varphi) \) maps the Banach space

\[
G := \left\{ \varphi = (\varphi_1, \ldots, \varphi_J) \in \prod_j L^\infty(\mu_j) : \int_{X_j} \varphi_j \, d\mu_j = 0, \ j = 1, \ldots, J - 1 \right\}
\]

into the positive cone

\[
H_{++} := H \cap \prod_j L^\infty_{++}(\mu_j),
\]

where

\[
H := \left\{ \psi := (\psi_1, \ldots, \psi_J) \in \prod_j L^\infty(\mu_j) : \int_{X_1} \psi_1 \, d\mu_1 = \cdots = \int_{X_J} \psi_J \, d\mu_J \right\}
\]

and \( L^\infty_{++}(\mu_j) \) denotes the equivalence classes of positive functions in \( L^\infty(\mu_j) \) (Carlier & Laborde 2020). We need the normalization for the functions in \( G \) because (4) only admits a unique solution \( \varphi^* \) up to additive translation; that is, the objective function \( F(\varphi) \equiv F(\varphi_1, \ldots, \varphi_J) \) in (4) satisfies

\[
F(\varphi_1, \ldots, \varphi_J) = F(\varphi_1 + \lambda_1, \ldots, \varphi_J + \lambda_J)
\]

for any constants \( (\lambda_1, \ldots, \lambda_J) \) that sum to zero. We also denote \( \hat{T}_N(\varphi) \equiv \left( \hat{T}_{N_1}(\varphi), \ldots, \hat{T}_{N_J}(\varphi) \right) \) with

\[
\hat{T}_{N_j}(\varphi) = \int_{X_{-j}} \exp \left( \frac{\sum_j \varphi_j(x_j) - c(x)}{\varepsilon} \right) d\prod_{i \neq j} \hat{\mu}_{N_j}(x_{-j}).
\]

Based on these definitions we have the following result for the asymptotic distribution of the optimal empirical potentials \( \hat{\varphi}^m_{N_j} \) obtained in the \( m \)-th iteration of the IPFP (6).

Lemma 1. Let Assumptions 2 – 4 hold. Then for every \( (N_1, \ldots, N_J) \) there exists a number of iterations \( m \in \mathbb{N} \) in the IPFP (6) such that

\[
\left( \sqrt{N_1}\left( \hat{\varphi}^m_{N_1} - \varphi_1^* \right), \ldots, \sqrt{N_J}\left( \hat{\varphi}^m_{N_J} - \varphi_J^* \right) \right) \rightsquigarrow - (T'(\varphi^*))^{-1}(Z),
\]

where \( \rightsquigarrow \) denotes weak convergence and \( Z \) is the tight mean-zero Gaussian limit element of the form

\[
\left( \sqrt{N_1}\left( \hat{T}_{N_1}(\varphi^*) - T_1(\varphi^*) \right), \ldots, \sqrt{N_J}\left( \hat{T}_{N_J}(\varphi^*) - T_J(\varphi^*) \right) \right).
\]
in $\ell^\infty \left( B_1 \left( \prod_j C^\infty_c (\mathcal{X}_j) \right) \right)$, the space of all bounded functions on the unit ball of all smooth functions $v \equiv (v_1, \ldots, v_J)$ compactly supported $\prod_j \mathcal{X}_j$. The bounded linear operator $T'(\varphi)(u) := (T'_1(\varphi)(u), \ldots, T'_J(\varphi)(u))$ with

$$T'_j(\varphi)(u) = \frac{1}{\varepsilon} \int_{\mathcal{X}_{-j}} \exp \left( \sum_{j=1}^J \frac{\varphi_j - c}{\varepsilon} \right) \sum_{j=1}^J u_j \, d \bigotimes_{i \neq j} \mu_i$$

is the Fréchet-derivative and $(T'(\varphi))^{-1}(u)$ is its inverse.

The number of iterations $m$ needs to be chosen such that

$$\hat{T}_{N_j}(\hat{\varphi}_N^m) = o_P(N^{-\frac{1}{2}}),$$

where $o_P$ is the standard Landau symbol and we always understand statements about probabilities in terms of outer probability (van der Vaart & Wellner 1996, Section 1.2). Lemma 1 shows that the potential functions obtained via the IPFP possess excellent statistical properties. In particular, the proof of Lemma 1 also shows that a standard bootstrap procedure, i.e. a resampling procedure of the observable data with replacement, provides correct results in the sense that the bootstrapped estimator $\tilde{\varphi}_N^{m_N}$ satisfies

$$\left( \sqrt{N_1} \left( \tilde{\varphi}_N^{m_N} - \varphi_1^* \right), \ldots, \sqrt{N_J} \left( \tilde{\varphi}_N^{m_N} - \varphi_J^* \right) \right)$$

weakly converges to a tight limit process conditional on the observed data like the standard empirical process

$$\left( \sqrt{N_1} (\hat{\varphi}_{N_1} - \varphi_1^*), \ldots, \sqrt{N_J} (\hat{\varphi}_{N_J} - \varphi_J^*) \right).$$

This follows from Theorem 13.4 in Kosorok (2008). We refer to Kosorok (2008) and chapter 3.6 in van der Vaart & Wellner (1996) for a detailed analysis of statistical properties of different bootstrap procedures.

Lemma 1 is the main step in deriving the asymptotic distribution of the optimal matching $\gamma^*$ that solves the Schrödinger bridge problem (3). Recall that the optimal matching $\gamma^*$ can be derived from the potentials $\varphi^*$ via (di Marino & Gerolin 2020, Proposition 4.6)

$$\gamma^*(A) = \int_A \exp \left( \sum_{j=1}^J \frac{\varphi^*_j(x_j) - c(x)}{\varepsilon} \right) d \bigotimes \mu_j(x)$$

for any measurable set $A$, i.e.

$$K^*(x) := \exp \left( \sum_{j=1}^J \frac{\varphi^*_j(x_j) - c(x)}{\varepsilon} \right)$$

is the Radon-Nikodym derivative of $\gamma^*$ with respect to $\bigotimes_j \mu_j$. The asymptotic behavior of the Radon-Nikodym derivative is straightforward to obtain via the delta method (van der Vaart & Wellner 1996, chapter 3.9) as in the following lemma.

**Lemma 2.** Let Assumptions 2 – 4 hold. Then for every $(N_1, \ldots, N_J)$ with $N_j = \rho_j N$ there exists
a number of iterations \( m \in \mathbb{N} \) in the IPFP (6) such that

\[
\sqrt{N} \left( \exp \left( \frac{\sum_{j=1}^{J} \hat{\varphi}_{N_j}^m - c}{\varepsilon} \right) - \exp \left( \frac{\sum_{j=1}^{J} \varphi_j^* - c}{\varepsilon} \right) \right) \rightsquigarrow - \exp \left( \frac{\sum_{j} \varphi_j^* - c}{\varepsilon} \right) \sum_{j=1}^{J} P_j^{-1} Z_{\varphi,j}
\]

where

\[
Z_{\varphi} \equiv (Z_{\varphi,1}, \ldots, Z_{\varphi,J}) := - \left( T'(\varphi^*) \right)^{-1} (Z)
\]

and \( Z \) is the mean zero Gaussian limit process from Lemma 1. The limit process is still mean zero Gaussian as it is a linear map of \( Z_{\varphi} \).

Lemma 2 shows that the exponential tilt imposed by \( K^*(x) \) also converges at the parametric rate to a Gaussian process. Hence, if all measures \( \mu_j \) are known, this implies that the optimal coupling converges at the parametric rate to a Gaussian process. Moreover, the Delta method for bootstrapped measures (van der Vaart & Wellner 1996, section 3.9.3) implies that the standard bootstrap procedure works in this case.

Lemma 2 provides the statistical properties of the optimal matching \( \gamma^* \) in the case where \( \mu_j \) are known. In general, this is not the case and we need to take into account the estimation of the measures \( \mu_j \). The following theorem shows that we still have convergence to a Gaussian limit process in this case. Also, the classical bootstrap is still applicable.

**Theorem 1.** Let Assumptions 2 – 4 hold. Denote

\[
K^*(x) := \exp \left( \frac{\sum_{j=1}^{J} \varphi_j^*(x_j) - c(x)}{\varepsilon} \right) \quad \text{and} \quad K_N(x) := \exp \left( \frac{\sum_{j=1}^{J} \hat{\varphi}_{N_j}(x_j) - c(x)}{\varepsilon} \right)
\]

Denote \( d\hat{\gamma}_N(x) := \hat{K}_N(x) d \otimes_{j=1}^{J} \hat{\mu}_N(x) \) and \( d\gamma(x) := K^*(x) d \otimes_{j=1}^{J} \mu_j(x) \). Then for any function \( f \) on \( \prod_j X_j \) in some uniformly bounded Donsker class \( \mathcal{F} \)

\[
\sqrt{N} \left( \int f(x) d\hat{\gamma}_N(x) - \int f(x) d\gamma(x) \right) \rightsquigarrow G
\]

where \( G \) is a mean-zero tight Gaussian process.

Lemma 2 and Theorem 1 show that the optimal balancing possesses excellent statistical properties. Moreover, Theorem 1 implies that the classical bootstrap approach (van der Vaart & Wellner 1996, chapter 3.6) works for deriving confidence regions of the optimal matching. Note that Theorem 1 is focused on functionals of the optimal matching, in contrast to Harchaoui et al. (2020) who focus on the measure-empirical process. The Gaussian limit is achieved for bounded Donsker classes \( \mathcal{F} \), i.e. functional classes that are “small enough” to be estimable with a relatively small number of observations. This is a standard regularity requirement in the theory of empirical processes. Smooth functions, indicator functions and many other functions fall under this category. For a thorough introduction to Donsker classes we refer to van der Vaart & Wellner (1996). Theorem 1 implies the following statistical properties for the induced estimator of the average treatment effect between two groups.

**Corollary 1.**

A. For any \( i, j \in \{1, \ldots, J\}, i \neq j \), denote \( \hat{\gamma}(x_i|x_j) \) as the sample version of the conditional distribution \( \gamma(x_i|x_j) \), then for any function \( f \) in a uniformly bounded Donsker class and for
any $x_j \in X_j$, 
\[ \sqrt{N} \left( \int f(x) \, d\gamma(x|x_j) - \int f(x) \, d\gamma(x|x_j) \right) \sim G_{ij} \]
where $G_{ij}$ is a mean-zero tight Gaussian process.

B. In addition, for the estimator in Definition 1,
\[ \sqrt{N} \left( \tilde{E}_\varepsilon \{Y(j)\} - E(Y(j)) \right) \sim G_j \]

Here, $\tilde{E}_\varepsilon \{Y(j)\}$ is the same as (7) with the subscription $\varepsilon$ to denote the dependence of $\gamma$ on $\varepsilon$.

\[ E\varepsilon Y(j) := E_{T,X} \left\{ \sum_{t \neq j} \int_{X_j} E[Y(j)|T = j, X = x_j] \, d\gamma_{\varepsilon,j|t}(x_j|x_t) \right\} \tag{12} \]

is a biased version of $E(Y(j))$ that depends on $\varepsilon$. $G_j$ is a mean-zero tight Gaussian process.

Corollary 1 shows the connection in terms of statistical properties to the classical $k$-nearest neighbor approach (Abadie & Imbens 2006): in general $E\varepsilon Y(j)$ does not coincide with the sought after expected outcome $E(Y(j))$ in the population, which introduces a bias $E\varepsilon Y(j) - E(Y(j))$. However, our proposed method allows us to remove the induced bias in a simpler manner than the classical nearest neighbor method (Abadie & Imbens 2011). To see this, consider a binary treatment setting, where $T \in \{t, j\}$. We can write

\[ E(Y(j)) = E_{T,X} \{E(Y(j)|T, X) \} \]
\[ = E_{T,X} \{E[Y(j)|T = j, X]I(T = j) + E[Y(j)|T = t, X]I(T = t) \} \]
\[ \approx E_{T,X} \left\{ E[Y|T = j, X]I(T = j) + \int_{X_j} E[Y(j)|T = j, X] \, d\gamma_{\varepsilon,j|t}(x_j|x_t)I(T = t) \right\} \]

Hence the bias term is

\[ \text{Bias} = E_{T,X} \left\{ \left( \int_{X_j} E[Y(j)|T = j, X] \, d\gamma_{\varepsilon,j|t}(x_j|x_t) - E[Y(j)|T = t, X] \right) I(T = t) \right\} \]

Let $f_j(X_t) = E[Y(j)|T = t, X]$ and $f_j(X_j) = E[Y(j)|T = j, X]$. Now if there exists a Monge solution $\gamma_{1-1}$ to the classical optimal transport problem (2) without the penalty term, i.e. a 1-1 mapping from $X_j$ to $X_t$, we know that $\gamma_{\varepsilon} \to \gamma_{1-1}$ as $\varepsilon \to 0$. Suppose that in the Monge solution, the point $X_j = b$ will be mapped to $X_t = a$, then $\int_{X_j} f_j(X_j) \, d\gamma_{\varepsilon,j|t}(x_j|x_t = a) \to f_j(X_t)|X_t = b$ as $\varepsilon \to \infty$. Hence the bias term disappears as $\varepsilon \to 0$ if the Monge solution exists.

This argument shows that the proposed method also has an asymptotic bias, which is not surprising, as our proposed method intuitively is a nearest neighbor approach where the neighbors and weights are chosen endogenously. However, By contrast to the classical nearest neighbor approaches, we can get rid of the bias term by the barycentric projection approach (Seguy et al. 2018, Pooladian & Niles-Weed 2021), which is much easier to implement than de-biasing approaches for nearest neighbor approaches (Abadie & Imbens 2011). In particular, in the most common case where the cost function is chosen to be the squared Euclidean distance, the barycentric projection, and hence the $1-1$-matching, is simply the conditional expectation $\int x_t \, d\gamma_{\varepsilon}(x_t|x_j)$ (Ambrosio et al. 2008, Appendix 12). Therefore, one can obtain an unbiased estimator by a simple regression,
without the need to let $\varepsilon \to 0$. That said, in finite samples, it is often preferred to trade off some bias for a smaller variance of the estimator, in which case a positive $\varepsilon$ is actually preferable.

5 Illustration

The excellent statistical finite-sample properties of the proposed method, especially compared to the standard $k$-nearest neighbor approach (Abadie et al. 2004), can already be appreciated in simple two-dimensional simulation studies. We propose two simulations, one with Gaussian distributions and one with a simple mixture of two Gaussians. To compare the method to the existing nearest neighbor approach, we focus on pairwise matchings.

For the first simulation, we sample 3 groups of covariates, denoted as $X_0, X_1, X_2$, and match both $X_1$ and $X_2$ to $X_0$. The 3 groups of covariates are sampled from bivariate normal distributions as follows.

$$X_0 \sim N\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right), \quad X_1 \sim N\left(\begin{pmatrix} 0.5 \\ -0.2 \end{pmatrix}, \begin{pmatrix} 1 & 0.1 \\ 0.1 & 1 \end{pmatrix}\right), \quad X_2 \sim N\left(\begin{pmatrix} 0.7 \\ -0.2 \end{pmatrix}, \begin{pmatrix} 0.5 & 0.1 \\ 0.1 & 0.5 \end{pmatrix}\right)$$

For the second simulation, the 3 groups of covariates are denoted by $Z_0, Z_1$ and $Z_2$ respectively. Each of them follows a mixture distribution of 2 Gaussians, where $Z_0 \sim 0.7X_0 + 0.3X_1$, $Z_1 \sim 0.5X_1 + 0.5X_3$, and $Z_2 \sim 0.6X_2 + 0.4X_3$. In Figures 3, 3a and 3b we plot the 95% elliptic contour of the bivariate normal distributions for each group before and after matching, based on the mean and covariate matrix estimated from each sample, whereas 3c and 3d give the scatter plots.

In both simulations, we sample $N_0 = 70, N_1 = 60, N_2 = 80$ points from each group respectively. The simulation is performed using the POT python package (Flamary et al. 2021). Figure 3e and 3f show the scatter plots for each group of mixture distributions before and after matching.

For comparison, Figure 4 is the results for the K-means matching with $k = 3$ for samples generated from $X_0$ and $X_1$. The superior performance of our proposed method can already be appreciated in this simple setting by comparing Figures 3d and 4d as well as 3b and 4b: our proposed method seems to obtain closer matches on average. Moreover, in areas where the overlap is somewhat worse the 3-nearest neighbor approach does not provide matches at all, which is the case for instance in the north-east corner of Figure 4d. By contrast, our proposed method provides good matchings for these individuals. The reason is that our proposed method matches all existing individuals without dropping observations. One can straightforwardly change this by considering unbalanced- or partial optimal transport approaches (Peyré & Cuturi 2019), which seamlessly fit into our proposed framework.

6 Conclusion

We have proposed a matching approach for causal inference in observational studies that is based on entropy regularized multimarginal optimal transportation. It can be understood as a nearest neighbor matching method where the number of neighbors and optimal weights are endogenously chosen: the user has to specify a penalty term $\varepsilon > 0$ instead. This proposed method possesses desirable properties. We prove that for positive $\varepsilon$ the optimal matching converges at the parametric rate to the true optimal matching; moreover, the classical bootstrap method can be used to
Figure 3: Covariates plot before and after matching. 95% quantile ellipses are computed based on estimated mean vector and covariance matrix on each sample.
Figure 4: Covariates plot before and after $k$-nearest neighbors matching, $k = 3$. 95% quantile ellipses are computed based on estimated mean vector and covariance matrix on each sample.
obtain confidence regions. Furthermore, in many cases, and in contrast to other nearest neighbor approaches (Abadie & Imbens 2006), one can obtain an unbiased estimator of average treatment effects by a simple barycentric projection (Ambrosio et al. 2008, Seguy et al. 2018, Pooladian & Niles-Weed 2021). In the standard setting, where the cost function is the Euclidean distance as a cost function, the barycentric projection involves estimating a conditional expectation, which is more efficient than other de-biasing approaches for nearest neighbor methods (Abadie & Imbens 2011). Finally, the method possesses excellent computational properties with a strong foundation in computational optimal transport theory (Peyré & Cuturi 2019). In particular, the IFPF is easily parallelizable. This allows the applied researcher to leverage the latest advances in these areas for matching in very high-dimensional spaces. An example of this are mini-batch approaches (Genevay et al. 2018, Damodaran et al. 2018). A simple simulation exercise demonstrates the method’s excellent finite sample properties in comparison to classical $k$-nearest neighbor approaches. Our method matches all individuals, but one can leverage the theory of unbalanced optimal transport (Peyré & Cuturi 2019) to relax this if needed. Finally, the proposed method allows researchers to estimate a joint matching over several treatment arms which could be interesting in answering general non-linear causal questions in this setting.

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## A Proofs

### A.1 Proof of Lemma 1

For the sake of notation we drop the iteration $m$ in the definition of the estimated potentials, i.e. we write $\hat{\varphi}_N$ instead of $\hat{\varphi}_N^m$, unless we need to specify $m$ explicitly.

We split the proof into two lemmas and the main proof. The first lemma describes properties of the optimal solution $\varphi^*$ when applying the Sinkhorn iterations/IPFP. The second lemma provides
the consistency of the empirical analogues of the potential functions $\hat{\phi}_N$ in the space $\prod_j C^{\infty}(\mathcal{X}_j)$. We say that $f_j \in C^{\infty}(\mathcal{X}_j)$ if $f_j \in C^k(\mathcal{X}_j)$ for every multi-index $k := (k_1, \ldots, k_d) \in \mathbb{N}_0^d$, i.e. if

$$
\left\| f_j^{(k)} \right\|_\infty := \sup_{x_j \in \mathcal{X}_j} \left| f_j^{(k)}(x_j) \right| < +\infty \quad \text{for all } k \in \mathbb{N}_0^d
$$

where the expression $f_j^{(k)}$ is shorthand for the $k$-th partial derivative of $f_j$:

$$
f_j^{(k)}(x_j) = \frac{\partial^{|k|}}{\partial x_1^{k_1} \cdots \partial x_d^{k_d}} f_j(x_{j1}, \ldots, x_{jd})
$$

and $|k| = \sum_{i=1}^d k_i$. $\mathbb{N}_0$ denotes the natural numbers including zero. We write

$$
\left\| \varphi \right\|_{C^k} := \sum_{j=1}^J \sum_{0 \leq k \leq |k|} \left\| \varphi_j^{(k)} \right\|_\infty
$$

for the $C^k$-norm of $\varphi \equiv (\varphi_1, \ldots, \varphi_J)$. We also define $\left\| \cdot \right\|_{L^\infty(\mu_j)}$ as the standard essential supremum norm with respect to the measure $\mu_j$ and denote for any $\varphi := (\varphi_1, \ldots, \varphi_J)$

$$
\left\| \varphi \right\|_{L^\infty} := \sum_{j=1}^J \left\| \varphi_j \right\|_{L^\infty(\mu_j)}.
$$

The following lemma is essentially identical to a result in Proposition 1 in Genevay et al. (2019), but for the multimarginal setting. For the sake of completeness we include a proof.

**Lemma 3.** Let Assumptions 2 and 3 hold. Then for any smooth cost function $c \in \prod_{j=1}^J C^{\infty}(\mathcal{X}_j)$ and given measures $\{\mu_j\}_{j=1, \ldots, J}$ the optimal $\varphi^*$ when computed via the IPFP/Sinkhorn algorithm (6) is smooth, i.e. $\varphi^*_j \in C^{\infty}(\mathcal{X}_j)$ for all $j$. Furthermore, all derivatives are bounded:

$$
\left\| \varphi_j^{(k)} \right\|_\infty = O \left( 1 + \varepsilon^{1-k} \right).
$$

**Proof.** Just as in the proof of Proposition 1 in Genevay et al. (2019) we consider the univariate setting, i.e. where each $x_j \in \mathbb{R}$. The extension to the multivariate setting is straightforward. By rearranging terms in (5), we get

$$
\exp \left( -\frac{\varphi_j(x_j)}{\varepsilon} \right) = \int_{\mathcal{X}_{-j}} \exp \left( \sum_{i \neq j} \varphi_i(x_i) - c(x_1, \ldots, x_j) \right) \frac{\varepsilon}{\varepsilon} d \bigotimes_{i \neq j} \mu_i(x_{-j})
$$

After taking the first derivative on both sides and rearranging,

$$
\varphi'_j(x_j) = \int_{\mathcal{X}_{-j}} \exp \left( \sum_{i \neq j} \varphi_i(x_i) - c(x_1, \ldots, x_j) \right) \frac{\partial c(x_1, \ldots, x_j)}{\partial x_j} \frac{\varepsilon}{\varepsilon} d \bigotimes_{i \neq j} \mu_i(x_{-j})
$$

Denote $K_\varepsilon(x) := \exp \left( \sum_{i} \varphi_i(x_i) - \frac{c(x_1, \ldots, x_j)}{\varepsilon} \right)$, and $c'_j(x) = \frac{\partial c(x)}{\partial x_j}$. Note that

$$
\frac{\partial}{\partial x_j} K_\varepsilon(x) = K_\varepsilon(x) \frac{\varphi'_j(x_j) - c'_j(x)}{\varepsilon}.
$$
The \( n \)-th order derivative of the potentials can be obtained by recurrence,

\[
\varphi_j^{(n)}(x_j) = \int_{X-j} K_\varepsilon(x) g_n(x) \, \text{d} \bigotimes_{i \neq j} \mu_i(x_{-j})
\]

\[
g_{n+1}(x) = g_n'(x) + \frac{\varphi_j'(x_j) - c_j'(x)}{\varepsilon} g_n(x)
\]

where \( g_1(x) = c_j'(x) \). \( g(x) \) differs when \( j = 1, \ldots, J \), but for clarity the subscript \( j \) is omitted in \( g(x) \).

Next we prove the following claim by induction on \( n \):

\((P_n)\) For \( i = 0, \ldots, k, \; k = 0, \ldots, n - 2 \), \( \|g_{n-k}^{(i)}\|_\infty \) is bounded by a polynomial in \( \frac{1}{\varepsilon} \) of order \( n - k + i - 1 \).

When \( n = 2 \), \( (i = 0, k = 0) \),

\[
g_2(x) = g_1'(x) + \frac{\varphi_j'(x_j) - c_j'(x)}{\varepsilon} g_1(x)
\]

\[
\|g_2(x)\|_\infty \leq \|g_1'(x)\|_\infty + \|\frac{\varphi_j'(x_j) - c_j'(x)}{\varepsilon} g_1(x)\|_\infty
\]

Let \( C_j = \max_{i \geq 0} |c_j^{(i)}(x)|_\infty \). Since \( \|\varphi_j\|_\infty < \infty \), let \( C = \max\{C_1, \ldots, C_J, K_\varepsilon\} \). Because \( \mu_1, \ldots, \mu_J \) are probability measures, \( \|\varphi_j^{(n)}\|_\infty \leq C \|g_n(x)\|_\infty \). Hence \( \|g_2(x)\|_\infty \leq a_0 + a_1 \frac{1}{\varepsilon} \) for some constant coefficient \( a_0, a_1 \).

Assume that \((P_n)\) is true for some \( n \geq 2 \), i.e. \( \|g_{n-k}^{(i)}\|_\infty \) is bounded by some polynomial

\[
Q_{n-k+i-1}(\frac{1}{\varepsilon}) := \sum_{i=0}^{n-k+i-1} a_i \left( \frac{1}{\varepsilon} \right)^i
\]

We want to show \((P_{n+1})\) is also true.

Note that the given bound for the triangular array \( \left\{ \|g_{n-k}^{(i)}\|_\infty, i = 0, \ldots, k, k = 0, \ldots, n - 2 \right\} \) in \((P_n)\), we only need to show the additional terms \( \{ \|g_{n-k+1}^{(k)}\|_\infty, k = 0, \ldots, n - 1 \} \) having the claimed bound in \((P_{n+1})\).

When \( k = n - 1 \),

\[
g_2^{(n-1)} = g_1^{(n-1)} + \sum_{p=0}^{n-1} \left( \begin{array}{c} n-1 \\ p \end{array} \right) \frac{\varphi_j^{(p+1)} - c_j^{(p+1)}}{\varepsilon} g_1^{(n-p-1)}
\]

\[
\|g_2^{(n-1)}\|_\infty \leq C + \sum_{p=0}^{n-1} \left( \begin{array}{c} n-1 \\ p \end{array} \right) C \|g_{p+1}\|_\infty + C \frac{1}{\varepsilon} C
\]

\((P_n)\) ensures that \( \|g_{p+1}\|_\infty \leq Q_p\left( \frac{1}{\varepsilon} \right) \), \( p = 0, \ldots, n - 1 \), hence \( \|g_2^{(n-1)}\|_\infty \leq Q_{n}\left( \frac{1}{\varepsilon} \right) \).

When \( k < n - 1 \),

\[
\|g_{n+1-k}^{(k)}\|_\infty \leq \|g_{n-k}^{(k+1)}\|_\infty + \sum_{p=0}^{k} \left( \begin{array}{c} k \\ p \end{array} \right) \frac{\|\varphi_j^{(p+1)}\|_\infty + |c_j^{(p+1)}|_\infty}{\varepsilon} \|g_{n-k}^{(k-p)}\|_\infty
\]

\[
\leq Q_{n}\left( \frac{1}{\varepsilon} \right) + \sum_{p=0}^{k} \left( \begin{array}{c} k \\ p \end{array} \right) \frac{Q_p\left( \frac{1}{\varepsilon} \right) + C}{\varepsilon} Q_{n-p-1}\left( \frac{1}{\varepsilon} \right)
\]

\[
\leq Q_{n}\left( \frac{1}{\varepsilon} \right)
\]
Hence the proof for $(P_n)$ is complete. $(P_n)$ implies that $\|\varphi_j^{(n)}\|_\infty \leq Q_{n-1}(\frac{1}{2})$ for any $n \geq 2$ and $j = 1, \ldots, J$, hence the optimal $\varphi$ is smooth.

The following lemma provides the consistency of the optimal potentials $\hat{\varphi}_N$ and all their derivatives as the empirical measures $\otimes_j \hat{\mu}_{N_j}$ converge weakly to $\otimes_j \mu_j$.

**Lemma 4.** Under Assumptions 2 and 3

$$\|\hat{\varphi}_N - \varphi^*\|_{C^k} = o_P(1)$$

for any multi-index $k \in \mathbb{N}_0^d$.

**Proof.** We start with the case $|k| = 0$ and use the fact that $\hat{\varphi}_{N_j}$ is an $M$-estimator (van der Vaart & Wellner 1996, chapter 3.2). Denote the respective objective functions by

$$\hat{F}_N(\varphi) := -\sum_{j=1}^J \int_{\mathcal{X}_j} \varphi_j(x_j) \, d\hat{\mu}_{N_j}(x_j) + \varepsilon \int_{\mathcal{X}} \exp\left(\frac{\sum_{j=1}^J \varphi_j(x_j) - c(x)}{\varepsilon}\right) \, d\otimes_{j=1}^J \hat{\mu}_{N_j}(x)$$

and

$$F(\varphi) := -\sum_{j=1}^J \int_{\mathcal{X}_j} \varphi_j(x_j) \, d\mu_j(x_j) + \varepsilon \int_{\mathcal{X}} \exp\left(\frac{\sum_{j=1}^J \varphi_j(x_j) - c(x)}{\varepsilon}\right) \, d\otimes_{j=1}^J \mu_j(x),$$

where we set $N := \sum_{j=1}^J N_j$. By Lemma 3 we can restrict the setting to $\varphi$ that are bounded and continuous functions, because we know that the solutions to (4) will always be bounded and continuous (and in fact smooth) functions. By Theorem 3 in Varadarajan (1958) the empirical product measure $\otimes_j \hat{\mu}_j$ converges weakly almost surely to the measure $\otimes_j \mu_j$. Since by Lemma 3 the optimal $\varphi_j^*$ (and by the same reasoning also the optimal $\hat{\varphi}_{N_j}$) are bounded continuous functions, this implies that $\hat{F}_N(\varphi) \to F(\varphi)$ pointwise for any bounded and continuous $\varphi$ almost surely and hence in probability.

The objective functions are strictly convex in $\varphi$. It is also easy to see that $\hat{F}_N$ and $F$ are continuous in $\varphi$ with respect to the $\|\cdot\|_\infty$-norm and that $\limsup_{N \to \infty} F_N(\varphi) < +\infty$ for all $\varphi \in \prod_j L^\infty(\mathcal{X}_j)$. Therefore by Corollary 2.3 in Borwein & Vanderwerff (1996) $\hat{F}_N$ converges uniformly on compact subsets of $\prod_j L^\infty(\mathcal{X}_j)$ to $F$. This is the analogous result to the standard result which shows that convex functions on finite dimensional spaces converge uniformly (Rockafellar 1997, Theorem 10.8) but for Banach spaces. Furthermore, the objective functions $\hat{F}_N$ and $F$ are optimized at a unique and well-separated $\hat{\varphi}_N$ and $\varphi^*$, respectively. Since $\hat{F}_N(\varphi)$ converges uniformly on compact subsets of $\prod_j L^\infty(\mathcal{X}_j)$ to $F$, it also converges on a small ball around the optimal $\varphi^*$. It implies that for sufficiently large $N$ the functions $\hat{F}_N$ have a local minimum in this ball. Since $\hat{F}_n$ are strictly convex in $\varphi$, this is also the global minimum, which implies that the sequence $\hat{\varphi}_n$ is uniformly bounded in the $\prod_j L^\infty(\mathcal{X}_j)$-norm and hence uniformly tight. We can therefore apply Corollary 3.2.3 (ii) in van der Vaart & Wellner (1996) to conclude that $\hat{\varphi}_N \to \varphi^*$ in probability.

Based on this the convergence of the derivatives now follows from the Arzelà-Ascoli theorem. We show this by an induction over the multi-indices $k \in \mathbb{N}_0^d$. We know by Lemma 3 that all derivatives $\hat{\varphi}_{N_j}^{(k)}$ and $(\varphi_j^*)^{(k)}$ are bounded. In particular, all derivatives $\hat{\varphi}_{N_j}^{(k)}$ are uniformly bounded. Let $\{\hat{\varphi}_{N_j}\}_{N \in \mathbb{N}}$ be the sequence that we know converges to $\varphi^*$ in $\prod_j L^\infty(\mathcal{X}_j)$.

Now consider the sequences $\{\hat{\varphi}_{N_j}^{(k)}\}_{N \in \mathbb{N}}$ with multi-indices with $|k| = 1$. By Lemma 3 these sequences are uniformly bounded and equicontinuous. Uniform boundedness follows from the first
bullet point in Proposition 1 or Theorem 2 in Genevay et al. (2019), which shows that the constants on the bound of the norm only depend on the dimension $d$, the size of the supports $X_j$, and the bound $\|c^{(k)}\|_\infty$ on all derivatives of the cost function. Since these bounds are independent of the measures in question this implies that all $\hat{\varphi}_N$ are uniformly bounded. Equicontinuity follows from the fact that all derivatives with multi-indices such that $|k| = 2$ are uniformly bounded and the mean value inequality.

But then by the Arzelà-Ascoli theorem, the sequence $\{\varphi_N^{(k)}\}$ with $|k| = 1$ has a subsequence $\{\varphi_{N_m}^{(k)}\}$ that converges uniformly. Since $\{\varphi_N\}$ converges uniformly to $\varphi^*$, this subsequence converges uniformly to $(\varphi^*)^{(k)}$. Now since the original sequence $\{\varphi_N\}$ converges uniformly, this implies that any subsequence converges uniformly to the same element. So repeating the same argument as above for any subsequence $\{\varphi_{N_{m1}}\}$ shows that any such subsequence has a further subsequence $\{\varphi_{N_{m1}}^{(k)}\}$ such that $\{\varphi_{N_{m1}}^{(k)}\}$ converges uniformly to $(\varphi^*)^{(k)}$ for $|k| = 1$. But this implies that any subsequence $\{\varphi_{N_{m1}}^{(k)}\}$ converges uniformly to $(\varphi^*)^{(k)}$ for the multi-index with $|k| = 1$. This implies that the sequence $\{\varphi_{N_m}^{(k)}\}$ converges uniformly to $(\varphi^*)^{(k)}$ for $|k| = 1$.

Now proceed by induction to finish the proof. We have just shown that the sequence $\{\varphi_{N_k}^{(k)}\}$ converges to $(\varphi^*)^{(k)}$ for $|k| = 1$. We know by Lemma 3 that all $\varphi_{N_k}^{(k)}$ with $|k| = 2$ and $|k| = 3$ are uniformly bounded which also implies that the sequence $\varphi_{N_k}^{(k)}$ with $|k| = 2$ is equicontinuous. Apply the same reasoning as above. Doing this for all multi-indices $k \in \mathbb{N}_0^d$ finishes the proof.

We can now prove Lemma 1.

**Proof of Lemma 1.** We prove the statement using standard results from empirical process theory (van der Vaart & Wellner 1996, Kosorok 2008), in particular results for Z-estimators. We consider the integrated version of the Schrödinger system (5) a Z-estimator in the sense of Theorem 3.3.1 in van der Vaart & Wellner (1996) and Theorem 13.4 in Kosorok (2008). In particular, the first-order equations (5) are derived by requiring that the first variation $\delta F(\varphi^*, v)$ (Zeidler 2013, Definition 40.2) of the objective function (4) in any direction $v \in \prod_{j=1}^J L^1(\mu_j)$ vanishes at the optimal $\varphi^*$, i.e.

$$0 = \delta F(\varphi^*, v) := \int_{X_j} \sum_{j=1}^J v_j \left[ \exp \left( \frac{\sum_{j=1}^J \varphi_j - c}{\varepsilon} \right) - 1 \right] d \otimes \mu_j = \sum_{j=1}^J \int_{X_j} v_j \int_{X_{-j}} \left[ \exp \left( \frac{\sum_{j=1}^J \varphi_j - c}{\varepsilon} \right) - 1 \right] d \otimes \mu_i d \mu_j, \quad (13)$$

where the last line follows from Fubini’s theorem and the boundedness of all integrands. (13) holds if and only if the first order conditions (5) are satisfied. We consider $v \in \prod_{j} L^1(\mu_j)$ because $\sum_{j} v_j$ and the term in brackets in (13) form a natural duality bracket in $\left( \prod_{j} L^1(\mu_j), \prod_{j} L^\infty(\mu_j) \right)$, i.e. the Gâteaux derivative

$$F'(\varphi) := \exp \left( \frac{\sum_{j=1}^J \varphi_j - c}{\varepsilon} \right) - 1 \in \left( \prod_{j} L^1(\mu_j) \right)^* = \prod_{j} L^\infty(\mu_j)$$

satisfies

$$\delta F(\varphi, v) = \left\langle F'(\varphi), \sum_j v_j \right\rangle,$$
see Zeidler (2013, section 40.1). By Fubini’s theorem we can also write the first variation in terms of the Schrödinger equations (5) as
\[ \delta F(\varphi, v) = \sum_{j=1}^{J} \langle T_j(\varphi) - 1, v_j \rangle, \]
where
\[ T_j(\varphi)(x_j) = \int_{X_{-j}} \exp \left( \frac{\sum_{j=1}^{J} \varphi_j(x_j) - c(x)}{\varepsilon} \right) d \otimes i \neq j \mu_i(x_{-j}) \]
and \( \langle \cdot, \cdot \rangle \) is the duality bracket with respect to \( \mu_j \).

We can now focus on proving the lemma. It will be based on Theorem 3.3.1 in van der Vaart & Wellner (1996) and Theorem 13.4 in Kosorok (2008). We need to show the following:

(i) \[ \| \hat{\varphi}_N - \varphi^\ast \|_{L^\infty} = o_P(1) \]

(ii) There exists some \( \delta > 0 \) such that the classes
\[ \tilde{F}_\delta,j := \left\{ v_j \left[ \exp \left( \frac{\sum_{j=1}^{J} \varphi_j - c}{\varepsilon} \right) - 1 \right] : \| \varphi - \varphi^\ast \|_{C^k} < \delta \ \forall k \in \mathbb{N}_0^d, \right. \]
\[ v_j \in B_1 \left( C_c^\infty(X_j) \right), \varphi \in \prod_j C_c^\infty(X_j) \} \]
are \( \otimes_j \mu_j \)-Donsker for all \( j \) (see chapters 2.1 and 2.5 in van der Vaart & Wellner (1996) for a definition of Donsker classes). Here, \( C_c^\infty(X_j) \) is the space of all smooth functions with compact support on \( X_j \) and \( B_1 \left( C_c^\infty(X_j) \right) \) is the unit ball in \( C_c^\infty(X_j) \), i.e. the set of all functions \( v_j \) with \( \| v_j \|_{C^k(X_j)} \leq 1 \) for any multi-index \( k \in \mathbb{N}_0^d \).

(iii) As \( \| \varphi - \varphi^\ast \|_{L^\infty} \to 0 \)
\[ \sup_{v_j \in B \left( C_c^\infty(X_j) \right)} \int_X v_j^2 \left( \exp \left( \frac{\sum_{j=1}^{J} \varphi_j - c}{\varepsilon} \right) - \exp \left( \frac{\sum_{j=1}^{J} \varphi^\ast_j - c}{\varepsilon} \right) \right)^2 d \otimes j \mu_j \to 0, \ \ \ j = 1, \ldots, J \]

(iv) \( T(\varphi) := (T_1(\varphi), \ldots, T_J(\varphi)) \) is Fréchet-differentiable with continuously invertible derivative
\[ T_j'(\varphi)(u) = \frac{1}{\varepsilon} \int_{X_{-j}} \exp \left( \frac{\sum_{j=1}^{J} \varphi_j - c}{\varepsilon} \right) \sum_{j=1}^{J} u_j d \otimes i \neq j \mu_i \]
for all \( u := (u_1, \ldots, u_J) \in \prod_{j=1}^{J} L^\infty(\mu_j) \).

(v) \( \left\| \hat{T}_N(\hat{\varphi}_N) \right\|_{L^\infty} = o_P(N^{-1/2}) \) for \( \hat{\varphi}_N \in F \) and
\[ P \left( \left\| \sqrt{N} \hat{T}_{N_1}(\hat{\varphi}_N), \ldots, \sqrt{N} \hat{T}_{N_J}(\hat{\varphi}_N) \right\|_{L^\infty} > \eta |X_N| \right) = o_P(1), \]
where \( X_N \) denotes the sample drawn and where \( \hat{T}_{N_j}(\hat{\varphi}_N) \) denotes a bootstrapped version of the operator (Kosorok 2008, Theorem 13.4), i.e. where we estimate the measures \( \mu_j \) via some
(multiplier) bootstrap procedure, see van der Vaart & Wellner (1996, section 3.6) for details on the bootstrap.

We prove each requirement one by one before putting everything together.

Requirement (i): This follows from Lemma 4.

Requirement (ii): This requirement is needed to provide the asymptotic equicontinuity of the empirical process map corresponding to the estimation equation

\[
\delta F(\varphi^*, v) = 0 \quad \text{for all } v \in B_1 \left( \prod_j C_c^\infty(X_j) \right),
\]

where \(B_1 \left( \prod_j C_c^\infty(X_j) \right)\) denotes the unit ball of all smooth functions \(v \equiv (v_1, \ldots, v_J)\) with compact support on \(\prod_j X_j\). The space of smooth functions is a Fréchet space, so a general way to consider the unit ball in this Fréchet space is to define a weighted series of the \(C^k\)-norms that makes the “\(C^\infty\)-norm” summable, see Treves (2006) for details. The weak convergence of the empirical process of the first-order condition required for obtaining the asymptotic distribution of the empirical process of the potentials can then be shown by the weak convergence of the empirical process corresponding to the first variation (13) for all \(v\) in a sufficient index set \(S \subset \prod_{j=1}^J L^1(\mu_j)\) by Lemma 3.3.5 in van der Vaart & Wellner (1996). A sufficient condition that also provides the fact that this asymptotic distribution will be a tight mean-zero Gaussian process is exactly requirement (ii) above for \(S = B_1 \left( \prod_j C_c^\infty(X_j) \right)\) and follows from Theorem 13.4 (C) in Kosorok (2008).

So to show requirement (ii) we hence have to show two things. First, we need to show that we can set \(S = B_1 \left( \prod_j C_c^\infty(X_j) \right)\). Second, we need to show that \(\mathcal{F}_{\delta,j}\) are indeed \(\otimes_j \mu_j\)-Donsker. For the first statement note that

\[
\left| \exp \left( \sum_j \varphi_j - c \over \varepsilon \right) - \exp \left( \sum_j \varphi_j^* - c \over \varepsilon \right) \right| = \left| \exp \left( \sum_j \varphi_j^* - c \over \varepsilon \right) \left[ \exp \left( \sum_j \varphi_j - \varphi_j^* \over \varepsilon \right) - 1 \right] \right|
\]

\[
\leq \exp \left( \sum_j \| \varphi_j \|_{L^\infty(\mu_j)} - c \over \varepsilon \right) \left| \exp \left( \sum_j \varphi_j - \varphi_j^* \over \varepsilon \right) - 1 \right|
\]

\[
\leq \exp \left( \sum_j \| \varphi_j^* \|_{L^\infty(\mu_j)} - c \over \varepsilon \right) \left| \exp \left( \sum_j \varphi_j - \varphi_j^* \over \varepsilon \right) - 1 \right|
\]

which shows that this term is continuous in some \(\prod_j L^\infty(\mu_j)\)-neighborhood of \(\varphi^*\). Taking the
supremum over \( \prod_{j=1}^{j} X_{j} \) on both sides of the inequality while noting that \( c(x_{1}, \ldots, x_{J}) \geq 0 \) implies

\[
\left\| \exp \left( \sum_{j} \frac{\varphi_{j} - c}{\varepsilon} \right) - \exp \left( \sum_{j} \frac{\varphi_{j}^{*} - c}{\varepsilon} \right) \right\|_{L^{\infty}} \\
\leq \exp \left( \sum_{j} \frac{\| \varphi_{j} - \varphi_{j}^{*} \|_{L^{\infty}(\mu_{j})}}{\varepsilon} \right) \left\| \exp \left( \sum_{j} \frac{\| \varphi_{j} - \varphi_{j}^{*} \|_{L^{\infty}(\mu_{j})}}{\varepsilon} \right) - 1 \right|,
\]

which vanishes as \( \sum_{j} \| \varphi_{j} - \varphi_{j}^{*} \|_{L^{\infty}(\mu_{j})} \to 0 \). Therefore, the Gâteaux derivative obtained via the first variation (13) coincides with the Fréchet-derivative (Zeidler 2013, p. 192). Now Fréchet differentiability in particular implies that the convergence of the linear approximation to the derivative at \( \varphi^{*} \) from any direction \( v \in \prod_{j} L^{1}(\mu_{j}) \) is of the same rate. This further implies that we can infer the derivative in any direction \( v \in \prod_{j} L^{1}(\mu_{j}) \) by only considering directions in a dense subset of \( \prod_{j} L^{1}(\mu_{j}) \). In particular, the equality (13) only has to hold for all \( v \) in a dense subset of the unit ball of \( \prod_{j=1}^{J} L^{1}(\mu_{j}) \). But \( \prod_{j=1}^{J} C_{c}^{\infty}(X_{j}) \) is dense in \( \prod_{j=1}^{J} L^{1}(\mu_{j}) \) (Folland 1999, Proposition 8.17), so that we can focus on the unit ball in \( \prod_{j} C_{c}^{\infty}(X_{j}) \).

So now we need to show that there exists some \( \delta > 0 \) such that \( F_{\delta,j} \) is \( \otimes j \mu_{j} \)-Donsker for all \( j \). For this, we use the concept of bracketing entropy and bracketing numbers (van der Vaart & Wellner 1996, chapter 2.7). Since \( \prod_{j} L^{\infty}(\mu_{j}) \) is a Banach lattice under the standard ordering \( f \preceq g \iff f_{j}(x_{j}) \leq g_{j}(x_{j}) \) for \( \mu_{j} \)-almost all \( x_{j} \) and all \( j \), we can define, for any two functions \( f_{t}, f_{u} \in \prod_{j} L^{\infty}(\mu_{j}) \) the bracket \( [f_{t}, f_{u}] \) as the set of all functions \( f \) such that \( f_{t} \preceq f \preceq f_{u} \). A \( \eta \)-bracket is a bracket \( [f_{t}, f_{u}] \) with \( \| f_{u} - f_{t} \|_{L^{\infty}} < \eta \). For some set \( \mathcal{F} \) of functions the bracketing number \( N_{\eta}(\mathcal{F}, \eta, \| \cdot \|) \) is the minimum number of \( \eta \)-brackets needed to cover \( \mathcal{F} \) in the metric induced by \( \| \cdot \| \) (van der Vaart & Wellner 1996, p. 83).

To show that \( F_{\delta} \) is \( \otimes j \mu_{j} \)-Donsker for some \( \delta > 0 \) we want to show that the corresponding bracketing entropy integral is finite, i.e. that

\[
\int_{0}^{\infty} \sqrt{\ln N_{\| \cdot \|}(\eta, F_{\delta, \otimes j \mu_{j}}, L^{2}(\otimes j \mu_{j}))} \, d\eta < +\infty. \tag{15}
\]

The idea is to treat \( v_{j} \) and

\[
g_{\varphi}(x_{1}, \ldots, x_{J}) \equiv g_{\varphi}(x) := \exp \left( \sum_{j=1}^{J} \frac{\varphi_{j}(x_{j}) - c(x)}{\varepsilon} \right) - 1
\]

separately. The reason is that Corollary 2.7.2 in van der Vaart & Wellner (1996) in combination with the fact that \( X_{j} \subset \mathbb{R}^{d} \) is compact implies that \( B_{1}(\prod_{j} C_{c}^{\infty}(X_{j})) \) is \( \otimes j \mu_{j} \)-Donsker for any dimension \( d \). Moreover, it is a uniformly bounded set. If we can show that the set of all functions \( g_{\varphi} \) for some \( \delta > 0 \) is also a uniformly bounded Donsker class for any dimension \( d \), then their product, i.e. \( F_{\delta} \), will be a Donsker class for any dimension by Example 2.10.8 in van der Vaart & Wellner (1996).

Now by Lemma 3 the optimal \( \varphi^{*} \) obtained via the Sinkhorn algorithm is smooth. Since this holds for any set of measures \( \{ \mu_{j} \}_{1 \leq j \leq J} \) it also holds for \( \hat{\varphi}_{n} \). Moreover, by Lemma 4 we know that \( \hat{\varphi}_{N_{j}} \) converges to \( \varphi_{j}^{*} \) in \( C^{\infty}(X_{j}) \). Hence for some small \( \delta > 0 \) we can find a uniform bound for the
\(\hat{\varphi}_{N_j}\) in \(C^\infty(\chi_j)\) by the reverse triangle inequality:

\[
\|\|\hat{\varphi}_{N}\|_{C^k} - \|\varphi^*\|_{C^k}\| \leq \|\hat{\varphi}_{N} - \varphi^*\|_{C^k} < \delta,
\]

for some \(\delta > 0\) and all multi-indices \(k \in \mathbb{N}_0^d\).

We can now show that the classes

\[
\tilde{F}_{\delta,j} := \left\{ v_j \left[ \exp \left( \frac{\sum_{j=1}^J \varphi_j - c}{\varepsilon} \right) - 1 \right] : \|\varphi - \varphi^*\|_{C^k} < \delta \forall k \in \mathbb{N}_0^d, v_j \in B_1 \left( C^\infty(\chi_j) \right) \right\}
\]

are Donsker. In fact, the class

\[
G_{\delta} := \left\{ \left[ \exp \left( \frac{\sum_{j=1}^J \varphi_j - c}{\varepsilon} \right) - 1 \right] : \|\varphi - \varphi^*\|_{C^k} < \delta \forall k \in \mathbb{N}_0^d, \varphi \in \prod_j C^\infty(\chi_j) \right\}
\]

is a bounded subset of \(\prod_j C^\infty(\chi_j)\) for compact and convex \(\chi_j\). Therefore by Corollary 2.7.2 \(G\) is a uniformly bounded Donsker class for any dimension \(d\). This implies by Example 2.10.8 in van der Vaart & Wellner (1996) that \(\tilde{F}_{\delta,j}\) is a \(\bigotimes_j \mu_j\)-Donsker class in any dimension \(d\).

**Requirement (iii):** This follows immediately by the fact that all \(\chi_j\) are compact and an analogous bound to (14).

**Requirement (iv):** This follows from Proposition 1 in Carlier & Laborde (2020), which shows that \(T'(\varphi)\) is an isomorphism between \(G\) and \(H\). In particular, by the inverse function theorem in Banach spaces, \(T'(\varphi)\) is a local \(C^\infty\)-diffeomorphism between \(E\) and \(F\). Moreover \(T(G)\) is open in \(H_{++}\).

**Requirement (v):** This follows from the linear convergence of the IPFP/Sinkhorn iterations as shown in Carlier (2021). In particular, Remark 3.4 in Carlier (2021) implies that there for any \(N\) there exists some \(m \in \mathbb{N}\) such that both criteria are satisfied. As mentioned in the main text this \(m\) can be rather large because of the exponential bound proved in Theorem 3.3 in Carlier (2021).

We can now put everything together by using Theorem 3.3.1 in van der Vaart & Wellner (1996) and Theorem 13.4 in Kosorok (2008). We show that the five requirements above imply the requirements (A) to (F) in Theorem 13.4 in Kosorok (2008). (A) is implied by the fact that the optimum \(\varphi^*\) is well-separated, which in turn follows from the fact that \(T(\varphi)\) is strictly convex in \(\varphi\). (B) is implied by (i). (C) is implied by (ii). (D) is implied by (iii). (E) is implied by (v). Finally, (F) is implied by (iv). Hence Theorem 13.4 in Kosorok (2008) implies that

\[
\left( \sqrt{N_1} \left( \hat{\varphi}_{N_1} - \varphi_1^* \right), \ldots, \sqrt{N_J} \left( \hat{\varphi}_{N_J} - \varphi_J^* \right) \right) \rightsquigarrow - (T'(\varphi^*))^{-1} (Z),
\]

where \(Z\) is the tight mean-zero Gaussian limit process of

\[
\left( \sqrt{N_1} \left( \hat{T}_{N_1}(\varphi^*) - T_1(\varphi^*) \right), \ldots, \sqrt{N_J} \left( \hat{T}_{N_J}(\varphi^*) - T_J(\varphi^*) \right) \right)
\]
in the space $\ell^\infty \left( \prod_j L^\infty(\mu_j) \right)$ of bounded functions on $\prod_j L^\infty(\mu_j)$. Moreover, Theorem 13.4 in Kosorok (2008) directly implies that a standard bootstrap procedure is valid.

Proof of Theorem 1. We want to derive the asymptotic probability measure of the empirical process

$$\sqrt{N} \left( \int f(x) d\hat{\gamma}_N(x) - \int f(x) d\gamma(x) \right)$$

$$= \sqrt{N} \left( \int f(x) \exp \left( \frac{\sum_{j=1}^J \varphi_{Nj} - c}{\varepsilon} \right) d\otimes_j \hat{\mu}_N - \int f(x) \exp \left( \frac{\sum_{j=1}^J \varphi_j^* - c}{\varepsilon} \right) d\otimes_j \mu_j \right),$$

which is an empirical process indexed by estimated functions (Wellner & van der Vaart 2007). For notational convenience we use the empirical process notation

$$P_N f = \int f(x) d\otimes_j \hat{\mu}_N(x), \quad P f = \int f(x) d\otimes_j \mu_j(x), \quad G_N f = \sqrt{N}(P_N f - P f)$$

and write

$$\sqrt{N} \left( P_N f \hat{K}_N - PfK \right) = \underbrace{G_N \left( f \hat{K}_N - fK \right)}_{G_N fK} + \underbrace{\sqrt{N} P \left( f \hat{K}_N - fK \right)}_{\text{term not shown}}.$$

We proceed term by term. We first show that the first term is asymptotically negligible, i.e. $G_N \left( \hat{K}_N f - K f \right) = o_P(1)$. For this we have to verify the conditions in Lemma 19.24 in van der Vaart (2000). Similar to the proof of Lemma 1, we define the following class of functions

$$\tilde{F}_{Kf} := \left\{ \exp \left( \frac{\sum_{j=1}^J \varphi_j - c}{\varepsilon} \right) f : \varphi \in \prod_j C^\infty(\mathcal{X}_j), f \in \mathcal{F} \right\},$$

where $\mathcal{F}$ is some uniformly bounded Donsker class on $\prod_j \mathcal{X}_j$ by assumption. Using the same argument as in Lemma 1, we split this class into

$$\hat{K}_K := \left\{ \exp \left( \frac{\sum_{j=1}^J \varphi_j - c}{\varepsilon} \right) \right\} : \varphi \in \prod_j C^\infty(\mathcal{X}_j) \right\} \quad \text{and} \quad \mathcal{F}.$$

By Lemma 1 the first has a bounded bracketing entropy integral. Due to the compactness of $\mathcal{X}_j$ and smoothness of functions in $\hat{K}_{\delta, K}$ it is also uniformly bounded and hence a uniformly bounded $\mathbb{P}$-Donsker class. Since the product of two uniformly bounded Donsker classes is a Donsker class by Example 2.10.8 in van der Vaart & Wellner (1996), this implies that $\tilde{F}_{\delta, Kf}$ is also $\mathbb{P}$-Donsker. We also need to show that

$$P \left( \hat{K}_N f - K f \right)^2 = o_P(1).$$

This follows from the exact same idea as requirement (iii) in Lemma 1 from the fact that all $\mathcal{X}_j$ are compact and that $\mathcal{F}$ is a uniformly bounded Donsker class. Therefore, by Lemma 19.24 in van der Vaart (2000) or Lemma 3.3.5 in van der Vaart & Wellner (1996) the first term is uniformly asymptotically negligible, i.e.

$$\sup_{f \in \mathcal{F}} \left| G_N \left( \hat{K}_N f - K f \right) \right| = o_{P^*} \left( 1 + \sqrt{N} \| \varphi^*_N - \varphi^* \|_{C^\infty} \right).$$

(16)
Now focus on the second and third term jointly. The second term is a standard empirical process over a Donsker class which converges to a tight mean-zero Gaussian process. The third term also converges to a tight Gaussian process by the Continuous Mapping Theorem (van der Vaart & Wellner 1996, Theorem 1.11.1) and Lemma 2 where we showed weak convergence to a tight mean-zero Gaussian process.

Both weak convergence results are for the marginal distributions, not the joint distribution, however. So in order to conclude that the sum of the last two terms converges to a tight Gaussian process, we need show that their joint distribution converges to a joint tight Gaussian process.

Let us write out both terms explicitly.

\[ G_N f K = \sqrt{N} \int f \exp \left( \sum_{j=1}^{J} \frac{\varphi_j^* - c}{\varepsilon} \right) d \left( \bigotimes_{j} \hat{\mu}_{N_j} - \bigotimes_{j} \mu_j \right) \]

and

\[ \sqrt{N} P \left( f \hat{K}_N - f K \right) = \sqrt{N} \int f \left[ \exp \left( \sum_{j=1}^{J} \frac{\hat{\varphi}_{N_j}^m - c}{\varepsilon} \right) - \exp \left( \sum_{j=1}^{J} \frac{\varphi_j^* - c}{\varepsilon} \right) \right] d \left( \bigotimes_{j} \mu_j \right) \]

We now show that both terms are asymptotically equal, which implies that they jointly converge to a Gaussian limit process. Since \( \varphi^* \) is a \( Z \)-estimator, it holds

\[ \delta F(\varphi^*, v) = 0 \quad \text{and} \quad \delta \hat{F}_N(\varphi_N^m, v) = o_P(N^{-\frac{1}{2}}) \]

for all \( v \in B_1 \left( \prod_j C_{c}^{\infty}(X^j) \right) \), where the latter follows by choosing a large enough \( m \) in the IPFP, which is always possible. By the fundamental theorem of the calculus of variations it holds that

\[ K - 1 \equiv \exp \left( \sum_{j} \frac{\varphi_j^* - c}{\varepsilon} \right) - 1 = 0. \]

Since smooth functions are dense in the space of integrable functions, it also holds that

\[ \delta F(\varphi^*, f) = 0 \quad \text{and} \quad \delta \hat{F}_N(\varphi_N^m, f) = o_P(N^{-\frac{1}{2}}) \]

uniformly over \( f \in \mathcal{F} \). Then

\[ \sqrt{N} \left( \delta F(\varphi_N^m, f) - \delta F(\varphi^*, f) \right) = \sqrt{N} \left( \delta \hat{F}_N(\varphi_N^m, f) - \delta \hat{F}_N(\varphi_N^m, f) \right) + o_P(1). \]

Moreover, by Lemma 3.3.5 in van der Vaart & Wellner (1996) and the above argument, the second term satisfies

\[ \sqrt{N} \left( \delta F(\varphi_N^m, f) - \delta \hat{F}_N(\varphi_N^m, f) \right) \approx -\sqrt{N} \left( \delta \hat{F}_N(\varphi^*, f) - \delta F(\varphi^*, f) \right) + o_P(1 + \sqrt{N} \| \varphi_N^m - \varphi^* \|_{C^\infty}). \]

Putting both together gives

\[ \sqrt{N} \left( \delta F(\varphi_N^m, f) - \delta F(\varphi^*, f) \right) \]

\[ = -\sqrt{N} \left( \delta \hat{F}_N(\varphi^*, f) - \delta F(\varphi^*, f) \right) + o_P(1 + \sqrt{N} \| \varphi_N^m - \varphi^* \|_{C^\infty}) + o_P(1). \]

But recall that

\[ \delta \hat{F}_N(\varphi^*, f) = \int f \left[ \exp \left( \sum_{j} \frac{\varphi_j - c}{\varepsilon} \right) - 1 \right] d \left( \bigotimes_{j} \hat{\mu}_{N_j} \right) \]
and similar for all other terms. Therefore,

\[
\sqrt{N} (\delta F(\hat{\phi}_N^m, f) - \delta F(\varphi^*, f)) = \int f \left[ \exp \left( \sum_j \frac{\hat{\phi}_{Nj}^m - \varphi_j^*}{\varepsilon} \right) - \exp \left( \sum_j \frac{\varphi_j^* - \varepsilon}{\varepsilon} \right) \right] d \bigotimes_j \mu_j
\]

\[= \sqrt{NP} \left( fK_N - fK \right)
\]

Similarly,

\[
\sqrt{N} (\delta \hat{F}_N(\varphi^*, f) - \delta F(\varphi^*, f)) = \int f \left[ \exp \left( \sum_j \frac{\varphi_j^* - \varepsilon}{\varepsilon} \right) - 1 \right] d \bigotimes_j \hat{\mu}_{Nj} - \bigotimes_j \mu_j
\]

\[= G_N fK - G_N f.
\]

Therefore,

\[
G_N fK + \sqrt{NP} \left( fK_N - fK \right) = G_N f + o_P(1 + \sqrt{N}\|\hat{\phi}_N^m - \varphi^*\|_{C^\infty}) + o_P(1).
\]

Putting everything together we have

\[
\sqrt{N} \left( P_N fK_N - PfK \right) = G_N f + o_P(1 + \sqrt{N}\|\hat{\phi}_N^m - \varphi^*\|_{C^\infty}) + o_P(1).
\]

Since \( f \) lies in a bounded Donsker class by our assumption, it follows that the corresponding limit process of \( \sqrt{N} \left( P_N fK_N - PfK \right) \) is a mean zero tight Gaussian process with covariance \( P\left( f_1 f_2 \right) - Pf_1 Pf_2 \). The conclusion of Theorem 3.6.1 in van der Vaart & Wellner (1996) also implies that the standard bootstrap works.

\[\square\]

**Proof of Lemma 2.** The proof relies on the classical delta method (van der Vaart & Wellner 1996, chapter 3.9).

By the result of Lemma 1,

\[
\left( \sqrt{N_1} \left( \hat{\phi}_{N_1}^m - \varphi_1^* \right), \ldots, \sqrt{N_J} \left( \hat{\phi}_{N_J}^m - \varphi_J^* \right) \right) \rightsquigarrow - (T'(\varphi^*))^{-1} (Z),
\]

We denote

\[Z_{\varphi} \equiv (Z_{\varphi,1}, \ldots, Z_{\varphi,J}) := - (T'(\varphi^*))^{-1} (Z)
\]

as the resulting process. First we show that \( Z_{\varphi} \) is a mean-zero tight Gaussian process. By Proposition 3.1 in Carlier & Laborde (2020), \( T'(\varphi^*) (h) \) is an isomorphism from \( G \) to \( H \) (for the definition of \( G \) and \( H \), see the main text below Assumption 4). By definition, \( T_j'(\varphi^*) (h) \) is a continuous linear mapping w.r.t \( h \) and \( T_j'(\varphi^*) (0) = 0 \). By the linearity of \( (T'(\varphi^*))^{-1} (h) \) and Fubini theorem, \( E Z_{\varphi} = E \left[ - (T'(\varphi^*))^{-1} (Z) \right] = - (T'(\varphi^*))^{-1} (0) = 0 \). By Proposition 7.5 in Kosorok (2008), \( Z_{\varphi} \) is a mean-zero Gaussian process. In addition, because \( (T'(\varphi^*))^{-1} (h) \) is a bijection, \( Z \)
being tight implies that $Z_\varphi$ is a tight process. Therefore, $Z_\varphi$ is a mean-zero tight Gaussian process.

Define $\Phi : \prod_{j=1}^J C^\infty(\mathcal{X}_j) \to \prod_{j=1}^J C^\infty(\mathcal{X}_j)$ as

$$\Phi(\varphi_1, \ldots, \varphi_J) := \exp \left( \frac{\sum_{j=1}^J \varphi_j(x_j) - c(x)}{\varepsilon} \right).$$

Then for any function $h := (h_1, \ldots, h_J) \in \prod_{j=1}^J C^\infty(\mathcal{X}_j)$, and any sequences $\prod_{j=1}^J C^\infty(\mathcal{X}_j) \ni h_n \to h$ and $t_n \to 0$,

$$\frac{\Phi(\varphi + t_n h_n) - \Phi(\varphi)}{t_n} = \exp \left( \frac{1}{\varepsilon} \left( \sum_{j=1}^J \varphi_j + t_n h_{j,n} \right) \right) - \exp \left( \frac{1}{\varepsilon} \sum_{j=1}^J \varphi_j \right) \exp \left( -\frac{1}{\varepsilon} c \right)
= \frac{1}{t_n} \left( \sum_{j=1}^J t_n h_{j,n} \frac{1}{\varepsilon} \exp \left( \frac{1}{\varepsilon} \sum_{j} \varphi_j \right) + O(t_n^2) \right) \exp \left( -\frac{1}{\varepsilon} c \right)
\to \sum_{j=1}^J h_j \frac{1}{\varepsilon} \exp \left( \frac{\sum_{j} \varphi_j - c}{\varepsilon} \right).$$

The Hadamard derivative therefore is

$$\delta \Phi_\varphi(h) = \sum_{j=1}^J h_j \varepsilon \exp \left( \frac{\sum_{j} \varphi_j - c}{\varepsilon} \right).$$

Therefore, by a first-order Taylor approximation,

$$\sqrt{N} \left( \exp \left( \frac{\sum_{j=1}^J \varphi_{m,j}^N - c}{\varepsilon} \right) - \exp \left( \frac{\sum_{j=1}^J \varphi_j^* - c}{\varepsilon} \right) \right)
= \sqrt{N} \delta \Phi_\varphi (\varphi_{m,j}^N - \varphi^*) + o_P (\|\varphi_{m,j}^N - \varphi^*\|_{C^\infty})
= \delta \Phi_\varphi^* (\rho_1^{-\frac{1}{2}} \sqrt{N} (\varphi_{m,j}^{N,1} - \varphi_1^*), \ldots, \rho_J^{-\frac{1}{2}} \sqrt{N} (\varphi_{m,j}^{N,J} - \varphi_J^*)) + o_P (\|\varphi_{m,j}^N - \varphi^*\|_{C^\infty})
\sim \delta \Phi_\varphi^* (\rho^{-\frac{1}{2}})^T Z_\varphi
= \exp \left( \frac{\sum_{j} \varphi_j^* - c}{\varepsilon} \right) \sum_{j=1}^J \rho_j^{-\frac{1}{2}} Z_{\varphi,j},$$

where the weak convergence in line 4 follows from the consistency of the potentials in Lemma 4. The limit expression is also a mean-zero tight Gaussian process since it is a linear map of $Z_\varphi$. $\square$
**Proof of Corollary 1.** We first prove part A. Let $I := \{i, j\}$, and $I^c := \{1, \ldots, J\} \setminus I$.

\[
d\gamma(x_{[j]}) = K(x_{1}, \ldots, x_{J}) \prod_{j=1}^{J} \mu_j(x_j)
\]

\[
= \exp \left\{ \frac{1}{\varepsilon} \left( \sum_{j=1}^{J} \varphi_j(x_j) - c(x_{1}, \ldots, x_{J}) \right) \right\} \prod_{j=1}^{J} \mu_j(x_j)
\]

\[
d\gamma(x_I) = \exp \left\{ \frac{1}{\varepsilon} \sum_{j \in I} \varphi_j(x_j) \right\} \int_{\mathcal{X}_{I^c}} \exp \left\{ \frac{1}{\varepsilon} \left( \sum_{j \in I^c} \varphi_j(x_j) - c(x_{1}, \ldots, x_{J}) \right) \right\} \prod_{j \in I^c} \mu_j(x_j) \prod_{j \in I} \mu_j(x_j)
\]

\[
= \exp \left\{ \frac{1}{\varepsilon} \sum_{j \in I} \varphi_j(x_j) \right\} h(x_I) \prod_{j \in I} \mu_j(x_j)
\]

where $h(x_I) := \int_{\mathcal{X}_{I^c}} \exp \left\{ \frac{1}{\varepsilon} \left( \sum_{j \in I^c} \varphi_j(x_j) - c(x_{1}, \ldots, x_{J}) \right) \right\} \prod_{j \in I^c} \mu_j(x_j)$.

For any $f \in \mathcal{F}$, define $g$ on $\mathcal{X}_j$ as

\[
g(x_j) := \int_{\mathcal{X}_j} f(x_i) \exp \left\{ \frac{1}{\varepsilon} \sum_{j \in I} \varphi_j(x_j) \right\} h(x_I) \, \mu_i(x_i)
\]

For any $B \in \mathcal{B}(\mathcal{X}_j)$, using Fubini theorem,

\[
\mathbb{E}(g(X_j)I_B(X_j)) = \int_{\mathcal{X}_j} g(x_j)I_B(x_j) \, \mu_j(x_j)
\]

\[
= \int_{\mathcal{X}_j} \int_{\mathcal{X}_i} f(x_i)I_B(x_j) \exp \left\{ \frac{1}{\varepsilon} \sum_{j \in I} \varphi_j(x_j) \right\} h(x_I) \, \mu_i(x_i) \, \mu_j(x_j)
\]

\[
= \mathbb{E}(f(X_i)I_B(X_j))
\]

Hence $g(x_j) = \mathbb{E}(f(X_i)|X_j = x_j)$. Now denote

\[
\hat{g}_N(x_j) := \int_{\mathcal{X}_i} f(x_i) \exp \left\{ \frac{1}{\varepsilon} \sum_{j \in I} \varphi_{N,j}(x_j) \right\} \hat{h}(x_I) \, \hat{\mu}_i(x_i),
\]

to show $\sqrt{N}(\mathbb{E}(f(X_i)|X_j = x_j) - \mathbb{E}(f(X_i)|X_j = x_j)) \sim G_{ij}$, we only need to show

\[
\sqrt{N}(\hat{g}_N(x_j) - g(x_j)) \sim G_{ij}
\]
Expanding $g(x_j)$,

\[
g(x_j) = \int_{X_{[-j]}} f(x_i) \exp \left\{ \frac{1}{\varepsilon} \left( \sum_{j=1}^{J} \varphi_j(x_j) - c(x_1, \ldots, x_J) \right) \right\} \, \mathcal{d} \mathcal{\mu}_j(x_j)
\]

\[
= \int_{X_{[-j]}} f(x_i) K(x_1, \ldots, x_J) \, \mathcal{d} \mathcal{\mu}_j(x_j)
\]

\[
\hat{g}_N(x_j) = \int_{X_{[-j]}} f(x_i) \hat{K}_N(x_1, \ldots, x_J) \, \mathcal{d} \mathcal{\mu}_j(x_j)
\]

The rest of the proof for part A follows the same way as in Theorem 1.

For part B, denote $y(j, X) = f_j(X) = \mathbb{E}\{Y(j)|X\}$

\[
\mathbb{E}Y(j) = \int_{X_j} f_j(x_j) \, \mathcal{d}\mu_j(x_j)
\]

In addition, for any $t \neq j$,

\[
\mathbb{E}X_t\{\mathbb{E}_X\{y(j, X_j)|X_t\}\} = \mathbb{E}_X\{y(j, X_t)\} = \mathbb{E}_X\{\mathbb{E}(Y(j)|X_t)\} = \mathbb{E}(Y(j))
\]

Now we can write the sample version in Definition 1 as

\[
\hat{\mathbb{E}}Y(j)I(D(j) = 1) + \hat{\mathbb{E}} \sum_{t \neq j} \int_{X_j} Y(j, x) \, \mathcal{d} \hat{\gamma}_{\varepsilon,j,t}(x|X)I(D(t) = 1)
\]

(17)

Note that $\hat{\mathbb{E}}$ assigns equal weight $\frac{1}{N}$ to each triplet $(Y_i, X_i, T_i)$. From part A, we know the weak convergence of $\int_{X_j} y(j, x) \, \mathcal{d} \hat{\gamma}_{\varepsilon,j,t}(x|X)$ given $X$. Denote $g_j^{(e)}(y, x, t) := \int_{X_j} y(j, s) \, \mathcal{d} \gamma_{\varepsilon,j,t}(s|x)I(T = t)$.

Now we can write a more general version of (17) as $\hat{\mathbb{E}}g_j^{(e)}(Y, X, T)$.

The weak convergence of Definition 1 now becomes

\[
\sqrt{N} \left\{ \mathbb{E}g_j^{(e)} - \mathbb{E}g_j^{(e)}_N \right\} \Rightarrow G_j.
\]

The rest of the proof follows the same method as the proof of Theorem 1.