
Counterfactual Identifiability via Dynamic Optimal Transport

Fabio De Sousa Ribeiro[†]

Ainkaran Santhirasekaram

Ben Glocker

Imperial College London, UK

Abstract

We address the open question of counterfactual identification for high-dimensional multivariate outcomes from observational data. [Pearl \(2000\)](#) argues that counterfactuals must be identifiable (i.e., recoverable from the observed data distribution) to justify causal claims. A recent line of work on counterfactual inference shows promising results but lacks identification, undermining the causal validity of its estimates. To address this, we establish a foundation for multivariate counterfactual identification using continuous-time flows, including non-Markovian settings under standard criteria. We characterise the conditions under which flow matching yields a unique, monotone, and rank-preserving counterfactual transport map with tools from dynamic optimal transport, ensuring consistent inference. Building on this, we validate the theory in controlled scenarios with counterfactual ground-truth and demonstrate improvements in axiomatic counterfactual soundness on real images.

1 Introduction

It has been argued that shortcomings in today’s deep models reveal an overreliance on statistical associations and a lack of *causal* understanding ([Schölkopf et al., 2021](#); [Bareinboim et al., 2022](#)). This view has sparked interest in causality within machine learning ([Peters et al., 2017](#); [Castro et al., 2020](#); [Schölkopf, 2022](#)). Causal reasoning is the process of drawing conclusions from a causal model, which represents our assumptions about the data-generating process. Thus, causality and generative modelling are inextricably linked. [Pearl \(2009\)](#) formalised causal inference using the Structural Causal Model (SCM) framework, in which variables are generated by functional assignments and dependencies are represented by a graph. This framework (with *do*-calculus ([Pearl, 1995](#))) expresses causal queries and, under stated assumptions, *identifies* causal effects that can be estimated from data.

Why is *identification* essential? Without identification it is impossible to make a precise causal claim: there can exist observationally equivalent models that yield different answers, and providing such guarantees is what causal methods are designed for ([Bareinboim et al., 2022](#); [Hyvärinen et al., 2024](#)). Indeed, *do*-calculus ([Pearl, 1995](#)) is an identification tool that tells us whether a causal effect can be determined from observed data and a set of assumptions encoded in a causal graph. Further, [Pearl \(2000\)](#) insists that any counterfactual query be bound by an identifiability requirement, that is, that there exists a unique mapping from the observed data distribution to the counterfactual of interest.

This work focuses on the identification of high-dimensional counterfactuals from observational data. Counterfactuals are hypothetical scenarios given observed evidence, for example, one may query “What would Y have been, had X been x ”. Counterfactuals have broad scientific utility, supporting the evaluation of interventions ([Kusner et al., 2017](#); [Tsirtsis and Rodriguez, 2023](#)), the characterisation of causal relationships ([Karimi et al., 2020](#); [Budhathoki et al., 2022](#)), and the generation of targeted synthetic data for downstream tasks ([Pitis et al., 2022](#); [Roschewitz et al., 2024](#); [Mehta et al., 2025](#)).

[†]Email: f.de-sousa-ribeiro@imperial.ac.uk

Deep generative models are increasingly being used to parameterise SCMs (Pawlowski et al., 2020; Sanchez and Tsafaris, 2021; Ribeiro et al., 2023; Komanduri et al., 2024; Kumar et al., 2025; Rasal et al., 2025; Xia et al., 2025). While the inferred counterfactuals are promising, the lack of identification precludes warranted causal interpretations of the estimates beyond statistical predictions. We aim to course-correct this practice. Counterfactual identification is arguably the most ambitious goal in causal analysis, as counterfactuals sit at the top of the causal hierarchy and subsume all other causal queries (Bareinboim et al., 2022). Thus, existing identification results are limited, with classical symbolic methods (Tian and Pearl, 2000; Pearl, 2001; Shpitser and Pearl, 2007) not having been developed for high-dimensional variables (Xia et al., 2023; Nasr-Esfahany and Kiciman, 2023).

Nasr-Esfahany et al. (2023) established counterfactual identification of bijective mechanisms, proposing a flow-based estimation method similar to Pawlowski et al. (2020); Khemakhem et al. (2021). However, their identification results only extend to multi-dimensional variables under the Backdoor Criterion (BC) and sufficient *variability* (Hyvärinen et al., 2019), stating that: “it is not clear how to generalise the monotonicity condition to multi-dimensional variables” in Markovian causal structures. This is a well-known issue with close connections to ICA (Hyvärinen and Pajunen, 1999) and disentanglement (Locatello et al., 2019). In this work, we characterise a multivariate generalisation of monotonicity to provably solve this problem, without imposing an arbitrary coordinate order.

We establish a foundation for counterfactual identification of high-dimensional, multivariate outcomes (e.g. images) from observational data, built on continuous-time flows. We characterise the conditions under which flow matching yields a unique, rank-preserving counterfactual transport map using tools from dynamic optimal transport. Our results address causal validity issues in prior work and extend to non-Markovian settings under standard criteria. We validate our theory in controlled scenarios with counterfactual ground-truth, and improve axiomatic counterfactual soundness on real images.

2 Related Work

Pearl’s Causal Hierarchy (PCH) (Pearl and Mackenzie, 2018) defines three levels of causal abstraction: *associational* (\mathcal{L}_1); *interventional* (\mathcal{L}_2), and *counterfactual* (\mathcal{L}_3). The PCH Theorem (Bareinboim et al., 2022) states that cross-layer inference of \mathcal{L}_i quantities using $\mathcal{L}_{<i}$ data is generally not possible without further assumptions. Pearl (1995)’s *do*-calculus is a sound and complete procedure for determining the identifiability of an \mathcal{L}_2 causal quantity from \mathcal{L}_1 data, given a causal graph. Counterfactual identification (\mathcal{L}_3) represents the most ambitious goal in causal analysis as it sits at the top of the PCH and therefore subsumes all other causal queries (Pearl, 2009). Subsequently, known counterfactual identification results are comparatively limited in number and scope to date, and existing constraints needed for \mathcal{L}_3 identification can be broadly categorised as either graphical or functional in nature.

Classical identification techniques involve symbolic methods and assumptions about the causal graph to identify counterfactual queries from both \mathcal{L}_1 and \mathcal{L}_2 data (Tian and Pearl, 2000; Pearl, 2001; Shpitser and Pearl, 2007). Recently, graph-based criteria have been extended to nested counterfactuals and fairness-aware queries (Zhang and Bareinboim, 2018; Correa et al., 2021), whereas functional identification has moved towards neural and nonparametric schemes that approximate or bound counterfactuals (Hartford et al., 2017; Xia et al., 2023; Melnychuk et al., 2023; Geffner et al., 2024; Pan and Bareinboim, 2024; Wu et al., 2025), even in non-identifiable settings (Gresele et al., 2022). Identification results predicated on monotonicity (Lu et al., 2020; Vlontzos et al., 2023; Javaloy et al., 2023) and bijectivity (Nasr-Esfahany et al., 2023) constraints are of primary interest to our work, since they generalise a broad range of model classes with known identifiability results, such as linear and nonlinear additive noise models (Shimizu et al., 2006; Hoyer et al., 2008; Peters et al., 2014), post-nonlinear models (Zhang and Hyvärinen, 2009), and location-scale models (Immer et al., 2023).

Establishing counterfactual identification of high-dimensional Markovian SCMs is a timely contribution, as many recent works rely on such assumptions (Pawlowski et al., 2020; Sanchez and Tsafaris, 2021; Sánchez-Martin et al., 2022; Ribeiro et al., 2023; Chen et al., 2024; Rasal et al., 2025). However, these methods lack an identification strategy and cannot support causal claims, posing operational risk. Of particular relevance to our work is optimal transport (Brenier, 1991; Caffarelli, 1992; Benamou and Brenier, 2000; Villani et al., 2008; Santambrogio, 2015; Peyré et al., 2019), and modern continuous-time flow models (Chen et al., 2018; Lipman et al., 2023; Liu et al., 2023; Albergo and Vanden-Eijnden, 2023; Pooladian et al., 2023; Tong et al., 2024), which in combination form the basis of our theoretical results and practical counterfactual inference model prescription.

3 Preliminaries

3.1 Structural Causal Models

Definition 3.1 (Structural Causal Model (SCM) (Pearl, 2009)). An SCM $\mathfrak{C} = (\mathbf{U}, \mathbf{X}, \mathcal{F})$ is a mathematical tool designed to express and infer causal quantities. It consists of: (i) a set of exogenous variables $\mathbf{U} = \{U_1, \dots, U_n\}$ determined by factors outside of \mathfrak{C} , and distributed according to $P_{\mathbf{U}}$; (ii) a set of endogenous variables $\mathbf{X} = \{X_1, \dots, X_n\}$ determined by other variables in \mathfrak{C} ; and (iii) a set of functions $\mathcal{F} = \{f_1, \dots, f_n\}$ specifying the causal generative process mapping \mathbf{U} to \mathbf{X} :

$$X_i := f_i(\mathbf{PA}_i, U_i), \quad \mathbf{PA}_i \subseteq \mathbf{X} \setminus \{X_i\}, \quad \text{for } i = 1, \dots, n, \quad (1)$$

where \mathbf{PA}_i is the subset of endogenous variables that directly cause X_i , called its *parents*. If the causal generative process is acyclic, an SCM can be represented by a Directed Acyclic Graph (DAG).

Counterfactual Inference. A counterfactual is a claim about what would have happened if some fact were different, all else being equal. SCMs can express and answer counterfactual queries of the form: “Given that we observed $\mathbf{X} = \mathbf{x}$, what would \mathbf{X} have been had X_i been set to x^* ”. An intervention sets chosen variables to specified values, e.g. $do(X_i := x^*)$ or $do(\mathbf{X}_S := \mathbf{x}_S^*)$, where $S \subseteq \{1, \dots, n\}$ indexes the intervened variables in the SCM, and the components of \mathbf{x}_S^* may differ¹. Counterfactual inference proceeds in three steps: (i) **Abduction**: infer the posterior distribution over the exogenous variables $P_{\mathbf{U}|\mathbf{X}=\mathbf{x}}$, given observed evidence $\mathbf{X} = \mathbf{x}$; (ii) **Action**: intervene, e.g., apply $do(X_i := x^*)$, to obtain a modified SCM \mathfrak{C}_{x^*} ; (iii) **Prediction**: use the SCM \mathfrak{C}_{x^*} and the posterior over the exogenous variables $P_{\mathbf{U}|\mathbf{X}=\mathbf{x}}$ to compute the counterfactual distribution $P_{\mathbf{X}}^{\mathfrak{C}_{x^*}|\mathbf{X}=\mathbf{x}}$.

Without loss of generality, in this work, we focus on the counterfactual identification (\mathcal{L}_3) of causal mechanisms f_i of multi-dimensional ($d > 1$) variables $X_i \in \mathbf{X}$, given only observational data (\mathcal{L}_1).

3.2 Optimal Transport: Static & Dynamic

Optimal Transport (OT) (Villani et al., 2008; Santambrogio, 2015; Peyré et al., 2019) is a suite of techniques for learning an optimal map between measures that minimises a transport cost.

Monge and Kantorovich Formulation. Let $\mathcal{P}(\Omega)$ be the set of probability measures on $\Omega \subset \mathbb{R}^d$. The Monge formulation of OT seeks a map $T : \Omega \rightarrow \Omega$ between two distributions $\mu, \nu \in \mathcal{P}(\Omega)$ that pushes μ forward to ν (i.e., $T_{\#}\mu = \nu$) while minimising a transport cost function $c : \Omega \times \Omega \rightarrow \mathbb{R}$:

$$W_c(\mu, \nu) := \inf_{T_{\#}\mu = \nu} \int_{\Omega} c(x, T(x)) d\mu(x), \quad \text{e.g.} \quad c(x, T(x)) = \|x - T(x)\|^2. \quad (2)$$

However, a transport map T may fail to exist, for instance when μ is discrete and ν is continuous. The Kantorovich formulation of OT relaxes the Monge problem and seeks an optimal coupling $\pi \in \Pi(\mu, \nu)$, where $\Pi(\mu, \nu) \subset \mathcal{P}(\Omega \times \Omega)$ denotes the set of couplings with marginals μ and ν ²:

$$\pi^* = \arg \min_{\pi \in \Pi(\mu, \nu)} \int_{\Omega \times \Omega} c(x, y) d\pi(x, y). \quad (3)$$

An optimal π^* always exists, and when a Monge map T also exists, both formulations coincide. Brenier (1991)’s theorem states that, under fairly general conditions, there is a unique and monotone optimal transport map $T = \nabla \phi$, where $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is a convex function. In this work, we show that this result has far-reaching implications for the counterfactual identification of causal mechanisms.

Benamou-Brenier Formulation. Benamou and Brenier (2000) showed that the above formulation, known as *static* OT with quadratic cost, can be equivalently expressed using a *dynamic* formulation. In simplified terms, one seeks a time-dependent velocity field $v : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$, for $t \in [0, 1]$, that transports p_0 to p_1 along a flow defined by an Ordinary Differential Equation (ODE):

$$v^* = \arg \min_{v \in \mathcal{V}} \left\{ \int_0^1 \mathbb{E} [\|v(X_t, t)\|^2] dt : dX_t = v(X_t, t) dt, X_0 \sim p_0, (X_1)_{\#}p_0 = p_1 \right\}, \quad (4)$$

where \mathcal{V} is the set of admissible velocity fields, i.e., fields that are measurable, ensure a well-posed flow with a unique ODE solution, and yield finite kinetic energy while transporting p_0 to p_1 .

¹There are other types of interventions, such as replacing f_i by some new mechanism \tilde{f}_i .

²That is, for any measurable sets $A, B \subset \Omega$, we have that $\pi(A \times \Omega) = \mu(A)$ and $\pi(\Omega \times B) = \nu(B)$.

3.3 Neural ODEs and Flow Matching

Continuous Normalizing Flows (CNFs) (Chen et al., 2018) seek to learn a mapping from a simple base distribution $X_0 \sim p_0$ to the data distribution $X_1 \sim p_{\text{data}}$ using an ODE, whose time-dependent vector field $v : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$ is parameterised by a neural network with parameters θ :

$$\forall t \in [0, 1], \quad dX_t = v_t(X_t; \theta) dt, \quad p_t := (X_t)_\# p_0. \quad (5)$$

Flow Matching (FM) (Lipman et al., 2023; Liu et al., 2023; Albergo and Vanden-Eijnden, 2023) trains CNFs simulation-free by regressing a parameterised vector field onto a known target field:

$$\min_{\theta} \int_0^1 \mathbb{E}_{X_1 \sim p_{\text{data}}, X_t \sim p_t} \left[\|v_t(X_t; \theta) - v_t^*(X_t | X_1)\|^2 \right] dt, \quad X_t = (1-t)X_0 + tX_1, \quad (6)$$

where the target vector field is defined to be $dX_t = v_t^*(X_t | X_1) dt = (X_1 - X_0) dt$. The simplicity of v_t^* is a result of choosing a simple *linear* interpolation path (McCann, 1997) between p_0 and p_1 . OT has recently been used to augment neural ODEs by straightening the sample paths of flows, and speeding up simulations at inference time (Liu et al., 2023; Pooladian et al., 2023; Tong et al., 2024).

4 Counterfactual Identifiability: Theoretical Analysis

We begin by defining the scope of our theoretical analysis in the context of existing counterfactual identifiability results. Detailed proofs for all our theoretical results are provided in Appendix B.

4.1 Problem Statement

Without loss of generality, we focus on the counterfactual identification of the i^{th} causal mechanism f for a multi-dimensional variable X within an SCM \mathfrak{C} , where $\dim(X) = \dim(U) = d > 1$, given only observational data. Further, we are interested in the *Markovian* case where there is no unobserved confounding, that is, U is independent of X 's parents $U \perp\!\!\!\perp \mathbf{PA}_X$ as detailed in Definition 4.1 below.

Definition 4.1 (Markovian SCM). An SCM is said to be Markovian if $U_i \perp\!\!\!\perp U_j$ whenever $i \neq j$. In other words, the exogenous variables in the model are statistically independent of each other, and their joint distribution factorises $P_{\mathbf{U}}(\mathbf{u}) = \prod_{i=1}^n P_{U_i}(u_i)$, where \mathbf{u} is a realisation of \mathbf{U} . Thus, Markovian SCMs induce a unique, factored joint observational distribution: $P_{\mathbf{X}}^{\mathfrak{C}}(\mathbf{x}) = \prod_{i=1}^n P_{X_i|\mathbf{PA}_i}(x_i | \mathbf{pa}_i)$.

Counterfactual identifiability (\mathcal{L}_3 , cf. Definition 4.2) results using only observational (\mathcal{L}_1) data exist for the Markovian case when $d = 1$, by using a strict monotonicity constraint on f . However, results for the $d > 1$ case are still missing, as generalising the monotonicity condition with multi-dimensional (X, U) variables is non-trivial (Nasr-Esfahany et al., 2023), and remains unexplored in counterfactual identifiability literature. In the presence of unobserved confounding (i.e. non-Markovian SCMs), Nasr-Esfahany et al. (2023) established counterfactual identifiability from observational (\mathcal{L}_1) data for: (i) $d = 1$ given a set of Instrumental Variables (IVs)³, \mathbf{I} (Imbens and Angrist, 1994); and (ii) $d \geq 1$ given a set of variables \mathbf{Z} that satisfy the Backdoor Criterion (BC)⁴ (Pearl, 2009), w.r.t. the pair (X, \mathbf{PA}_X) .

Definition 4.2 (Counterfactual Identifiability (Pearl, 2009)). A counterfactual query Q is identifiable if for any pair of SCMs $\mathfrak{C}^{(1)}$ and $\mathfrak{C}^{(2)}$ we have that $Q(\mathfrak{C}^{(1)}) = Q(\mathfrak{C}^{(2)})$, whenever $P_{\mathbf{X}}^{\mathfrak{C}^{(1)}} = P_{\mathbf{X}}^{\mathfrak{C}^{(2)}}$.

Nasr-Esfahany et al. (2023)'s counterfactual identifiability results rely on the bijectivity and monotonicity of the causal mechanism f , except for the BC case where bijectivity alone is shown to be sufficient for $d \geq 1$ given that a *variability* assumption holds. This assumption requires that \mathbf{Z} influence U strongly enough for $P_{U|\mathbf{Z}}$ and its gradient to vary across different values of \mathbf{Z} . In Markovian settings, the independence of U and \mathbf{PA}_X alone is not sufficient for counterfactual identifiability of f . In addition, bijectivity constraints on f are also insufficient when $d > 1$, due to well-known rotational symmetries of the prior on U (Hyvärinen and Pajunen, 1999; Hyvärinen et al., 2024).

In the following, we characterise the set of constraints and assumptions that permit counterfactual identifiability for multi-dimensional variables in Markovian SCMs from observational data. For this, we connect ideas from (dynamic) optimal transport (Benamou and Brenier, 2000; Villani et al., 2008; Santambrogio, 2015) and graphical causality (Pearl, 2009) to build monotone mechanisms for $d > 1$.

³IVs must be $\mathbf{I} \perp\!\!\!\perp \mathbf{U}$ and only influence X through \mathbf{PA}_X .

⁴If \mathbf{Z} blocks all backdoor paths from \mathbf{PA}_X to X ; non-descendancy of \mathbf{Z} is only required for adjustment.

4.2 Dynamic Optimal Transport for Counterfactual Identification

A counterfactual query $X_{\mathbf{pa}^*} | \{X = x, \mathbf{PA} = \mathbf{pa}\}$ can be answered by the deterministic map⁵:

$$f : \mathbb{R}^k \times \mathbb{R}^d \rightarrow \mathbb{R}^d, \quad \forall x, \mathbf{pa}, \mathbf{pa}^* : x^* = f(\mathbf{pa}^*, u), \quad \text{where } u = f^{-1}(\mathbf{pa}, x), \quad (7)$$

with \mathbf{pa}^* denoting the counterfactual parents of x , and f is invertible w.r.t. the exogenous noise u . Therefore, a counterfactual transport map that implicitly abducts the exogenous noise exists:

$$T^* : \mathbb{R}^{2k} \times \mathbb{R}^d \rightarrow \mathbb{R}^d, \quad \forall x, \mathbf{pa}, \mathbf{pa}^* : T^*(\mathbf{pa}^*, \mathbf{pa}, x) = f(\mathbf{pa}^*, f^{-1}(\mathbf{pa}, x)), \quad (8)$$

directly pushing the observational distribution forward to the counterfactual $T^*_{\#} P_{X|\mathbf{PA}=\mathbf{pa}}^{\mathcal{C}}$.

Definition 4.3 (Monotone Operator). A mapping $f : \mathbb{R}^k \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is monotone in u if:

$$\langle f(\mathbf{pa}, u_1) - f(\mathbf{pa}, u_2), u_1 - u_2 \rangle \geq 0, \quad \forall u_1, u_2 \in \mathbb{R}^d, \mathbf{pa} \in \mathbb{R}^k. \quad (9)$$

Proposition 4.4 (Monotone Counterfactual Transport Map). *If a mechanism $f(\mathbf{pa}, u)$ is monotone in u (Def. 4.3), then the respective counterfactual transport map $T^*(\mathbf{pa}^*, \mathbf{pa}, x)$ is monotone in x .*

Remark 4.5. In Appendix A we provide a gentle motivating example in ($d = 1$)-dimension of what monotonicity of T^* entails and why it is important for consistent counterfactual inferences. The subsequent proof provides a generalisation to vectors (i.e., $d > 1$) in the sense of monotone operators.

Monotonicity of the counterfactual transport map T^* w.r.t. x guarantees that, for a given intervention on \mathbf{pa} , the rank order of factual outcomes is preserved in the counterfactuals. This is important (e.g. for *fairness*) as it prevents rank inversions across individuals under a given intervention. However, learning the counterfactual transport map directly from data is challenging, since we (almost) never have access to paired or unpaired samples from both the observational and counterfactual distributions.

As we will show, the dynamic optimal transport specialisation of T^* generalises quantile and rank functions for $d > 1$, ensuring multivariate rank preservation and consistent counterfactual inferences.

Lemma 4.6 (Unique and Monotone Dynamic OT Mechanism). *Let $\dim(X) = \dim(U) = d > 1$, and consider a Markovian setting $U \perp\!\!\!\perp \mathbf{PA}$. Assume P_U and $P_{X|\mathbf{PA}}^{\mathcal{C}}$ are absolutely continuous w.r.t. the Lebesgue measure with strictly positive and bounded densities on bounded, open, convex domains. Let $T : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ be the time-1 map of a dynamic optimal transport flow:*

$$\{T_t : t \in [0, 1]\}, \quad dT_t(u; \mathbf{pa}) = v_t(T_t(u; \mathbf{pa})) dt, \quad T_{\#} P_U = P_{X|\mathbf{PA}}^{\mathcal{C}}. \quad (10)$$

Then, there exists a convex function $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ such that: $T(u; \mathbf{pa}) = \nabla_u \phi(u; \mathbf{pa})$, for $P_U(u)$ -a.e. u , where T is monotone, bijective a.e., and uniquely determined by the pair $(P_U, P_{X|\mathbf{PA}}^{\mathcal{C}})$.

Remark 4.7. We draw on Brenier (1991)’s theorem to show that the causal mechanism is monotone. However, Brenier’s map does not guarantee bijectivity by default. For this, we use Caffarelli (1992)’s standard regularity results to show the OT map is locally diffeomorphic. In practice, the bijectivity condition can be satisfied by smoothing empirical target distributions by adding mild continuous noise (e.g. uniform or Gaussian) to ensure the resulting distribution admits a smooth density.

Since dynamic OT maps are invertible when the velocity field v_t is well-defined (e.g. Lipschitz continuous in space), we can recover the counterfactual transport map by composition (cf. Eq. (8)). By Proposition 4.4, if $T(u; \mathbf{pa})$ is monotone in u then $T^*(\mathbf{pa}^*, \mathbf{pa}, x)$ is monotone in x . In the following section, we discuss the indeterminacy induced by the choice of prior on the exogenous noise distribution P_U and characterise the necessary conditions for strict monotonicity of T^* in x .

4.2.1 Exogenous Prior Indeterminacy

Since the true prior distribution over the exogenous variables P_U is typically unknown, one must either rely on domain expertise to define a prior, choose one for mathematical convenience, or try to learn it directly from data. This choice of prior induces an indeterminacy in counterfactual outcomes.

Next, we show that regardless of the prior P_U we choose, under standard regularity conditions, there exists a unique and optimal function $g^* : \mathbb{R}^d \rightarrow \mathbb{R}^d$ that maps to any other P_U we would have chosen.

⁵We omit the subscripts for simplicity, i.e., $\mathbf{PA} := \mathbf{PA}_X$ and similarly for their realisations: $\mathbf{pa} := \mathbf{pa}_x$.

Definition 4.8 (Transport \mathcal{L}_3 -Equivalence). Let $T^{(1)}, T^{(2)} : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ be transport maps with exogenous priors $P_U^{(1)}, P_U^{(2)}$ on \mathbb{R}^d , and parent domain \mathbb{R}^k . We say they are counterfactually equivalent $\sim_{\mathcal{L}_3}$, if and only if there exists a bijection $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ such that $g_* P_U^{(2)} = P_U^{(1)}$, that is:

$$T^{(1)} \sim_{\mathcal{L}_3} T^{(2)} \iff \exists g : T^{(1)}(u; \mathbf{pa}) = T^{(2)}(g^{-1}(u); \mathbf{pa}) \quad \text{for } P_U^{(1)}\text{-a.e. } u, \forall \mathbf{pa}. \quad (11)$$

Proposition 4.9 (Nasr-Esfahany et al. (2023)). Transport maps $T^{(1)}, T^{(2)} : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ produce the same counterfactuals if and only if they are \mathcal{L}_3 -equivalent in the sense of Definition 4.8:

$$\forall x, \mathbf{pa}, \mathbf{pa}^* : x^* = T^{*(1)}(\mathbf{pa}^*, \mathbf{pa}, x) = T^{*(2)}(\mathbf{pa}^*, \mathbf{pa}, x) \iff T^{(1)} \sim_{\mathcal{L}_3} T^{(2)}. \quad (12)$$

Remark 4.10. Given only observational data (\mathcal{L}_1), we seek a transport map T that is counterfactually equivalent ($\sim_{\mathcal{L}_3}$) to the true transport map T^* underlying the data-generating process.

Lemma 4.11 (Existence of the Prior Transition Map). Let $P_U^{(1)}, P_U^{(2)}$ be probability measures on \mathbb{R}^d with finite second moments, both absolutely continuous w.r.t. the Lebesgue measure. Then, there exists a transport map $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ that is unique $P_U^{(1)}$ -a.e., monotone, and a.e. bijective.

We are now equipped to prove our main counterfactual identifiability result in the sense of Def. 4.8.

Theorem 4.12 (Counterfactual Identifiability in Markovian SCMs). Let $\dim(X) = \dim(U) = d > 1$, and $U \perp\!\!\!\perp \mathbf{PA}$. Assume P_U is the continuous uniform measure on $[0, 1]^d$. Let $T : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ be the time-1 dynamic OT map described in Lemma 4.6, which pushes P_U forward to $P_{X|\mathbf{PA}}^c$. Then, the induced time-1 counterfactual dynamic OT map $T^* : \mathbb{R}^{2k} \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is strictly monotone in x :

$$\langle T^*(\mathbf{pa}^*, \mathbf{pa}, x_1) - T^*(\mathbf{pa}^*, \mathbf{pa}, x_2), x_1 - x_2 \rangle > 0, \quad \forall x_1, x_2 \in \mathbb{R}^d, \mathbf{pa}, \mathbf{pa}^* \in \mathbb{R}^k. \quad (13)$$

Remark 4.13. This shows a dynamic OT flow mechanism (Lemma 4.6) yields a counterfactual optimal transport map T^* that is strictly monotone in x (i.e., monotonic in the vector sense), thereby extending the classical monotone-quantile notion to multivariate ($d > 1$) settings and, under stated Caffarelli (1992) regularity conditions, guaranteeing $\sim_{\mathcal{L}_3}$ identifiability from observational data (\mathcal{L}_1).

4.3 Non-Markovian Counterfactual Identifiability



Figure 1: **Four canonical causal graphs.** From left to right: (i) Markovian, (ii) Instrumental Variable, (iii) Backdoor, and (iv) Frontdoor. Dashed bidirected arcs denote unobserved confounding.

To ensure wide applicability, we extend counterfactual identification from observational data (\mathcal{L}_1) to non-Markovian multivariate ($d > 1$) settings under the following common criteria (Figure 1): (i) Instrumental Variable (IV), (ii) Backdoor Criterion (BC), and (iii) Frontdoor Criterion (FC). Appendix B.3 contains the proofs. Nasr-Esfahany et al. (2023) provided results for $d > 1$ only when BC applies. We expand the IV results to $d > 1$ thanks to the mechanism proposed in Lemma 4.6 being monotone, bijective and uniquely determinable under regularity conditions (Caffarelli, 1992). We also prove $\sim_{\mathcal{L}_3}$ identifiability for FC under similar conditions to BC (Nasr-Esfahany et al., 2023).

5 Counterfactual Transport Maps via Flow Matching

Although bijectivity and variability are sufficient for counterfactual identification under BC settings (see Appendix B.3), Markovian/IV settings require a monotone counterfactual OT map to obtain equivalent guarantees (Theorem 4.12). For the former, we prescribe standard continuous-time flows trained via flow matching, and for the latter, we approximate dynamic OT with these flows.

Counterfactual Inference. Computing counterfactuals with a continuous-time flow model is simple. Using abduction-action-prediction (Pearl, 2009), we first solve the associated ODE backwards in time for abduction $u = T^{-1}(x; \mathbf{pa})$, then forwards in time for prediction $x^* = T(u; \mathbf{pa}^*)$, as follows:

$$u = x - \int_0^1 v_t(x_t; \mathbf{pa}, \theta) dt, \quad \Rightarrow \quad x^* = u + \int_0^1 v_t(x_t; \mathbf{pa}^*, \theta) dt, \quad (14)$$

where \mathbf{pa}^* is obtained from an upstream intervention (i.e. *action*) on one or more nodes in the associated SCM. The Picard-Lindelöf theorem states that both initial value problems admit unique solutions if $v_t(x_t; \mathbf{pa}, \theta)$ is Lipschitz continuous, a condition that is readily satisfiable in practice.

Markovian OT Coupling. Although our theory for Markovian and IV settings is not tied to any particular OT approximation, it remains nontrivial to operationalise at scale with current techniques. To validate our theoretical claims, we offer a flow matching approach with a *bespoke* Markovian Batch-OT coupling that resolves counterfactual consistency issues in the standard formulation. Batch-OT flow matching (Pooladian et al., 2023; Tong et al., 2024) solves the OT problem on batches of source and target samples to form better pairs, using GPU-enabled solvers (Flamary et al., 2021). This asymptotically recovers the global OT map, but requires large batches in practice, especially in high dimensions (Klein et al., 2025). Notably, Mousavi-Hosseini et al. (2025) amortise OT pairing via semidiscrete couplings, reporting improved sample quality with substantially lower pairing cost.

As prescribed by Lemma 4.6, the correct way to formulate OT for Markovian structures must ensure that the marginal P_U remains independent of \mathbf{PA} upon coupling $P_{X|\mathbf{PA}}^c$. A naive application of Batch-OT flow matching to a Markovian setting implicitly entangles the parent variables \mathbf{PA} and the exogenous noise U , which violates the independence requirement $U \perp\!\!\!\perp \mathbf{PA}$. This happens because upon sampling a random batch of exogenous noise $\{u^{(i)}\}_{i=1}^m \sim P_U$, and observations $\{(x^{(j)}, \mathbf{pa}^{(j)})\}_{j=1}^m \sim P_{X,\mathbf{PA}}^c$, solving the OT problem then reassigns each $u^{(i)}$ to a pair $(x^{(j)}, \mathbf{pa}^{(j)})$, but implicitly couples $u^{(i)}$ with $\mathbf{pa}^{(j)}$ by association with $x^{(j)}$. This invalidates the abduction process in Markovian settings as U is no longer strictly exogenous, and the counterfactuals will be incorrect.

To fix this issue, we can instead sample batched data from the *conditional* distribution:

$$\{u^{(i)}\}_{i=1}^m \sim P_U, \quad \mathbf{pa} \sim P_{\mathbf{PA}}^c, \quad \{x^{(j)}\}_{j=1}^m \sim P_{X|\mathbf{PA}=\mathbf{pa}}^c, \quad (15)$$

then solve the Batch-OT problem for each fixed value of \mathbf{pa} in turn. Simply put, the parent values must match across each element in the batch to satisfy the Markovian constraint that $U \perp\!\!\!\perp \mathbf{PA}$.

The objective we optimise can be understood as solving a *family* of OT flow couplings:

$$\min_{\theta} \int_{\mathbb{R}^k} \mathbb{E}_{t \sim \mathcal{U}(0,1), (u,x) \sim \pi^{(m)}(\cdot|\mathbf{pa})} \left[\|v_t(x_t; \mathbf{pa}, \theta) - v_t^*(x_t | x, \mathbf{pa})\|^2 \right] dP_{\mathbf{PA}}^c(\mathbf{pa}), \quad (16)$$

where the flow is $x_t = (1-t)u + tx$. Here $\pi^{(m)}$ denotes the implicit conditional joint distribution:

$$\pi^{(m)}(u, x | \mathbf{pa}) = \frac{1}{m} \sum_{i=1}^m \sum_{j=1}^m \pi_{\mathbf{pa}}^*(i, j) \delta_{u^{(i)}}(u) \delta_{x^{(j)}}(x), \quad (17)$$

induced by the OT coupling $\pi_{\mathbf{pa}}^* \in \mathbb{R}^m \times \mathbb{R}^m$, for m i.i.d. samples drawn according to Eq. (15).

6 Experiments

We conduct two sets of experiments: (i) a constructed scenario where the ground-truth counterfactuals are known and we can, in principle, verify our identifiability claims; (ii) a real-world medical imaging dataset widely used for counterfactual inference. When counterfactual ground truth is not available, we follow Monteiro et al. (2023); Ribeiro et al. (2023) and measure the counterfactual soundness axioms of *composition*, *effectiveness* and *reversibility*. While useful, these metrics alone do not imply identification and should not be construed as evidence of causal validity. For details, see Appendix D.

6.1 Counterfactual Ellipse Generation

For this study, we adapt the counterfactual ellipse generation setup by Nasr-Esfahany et al. (2023). Let $U \in \mathbb{R}^2$ be the semi-major and -minor parameters of an ellipse, $\mathbf{PA} \in (0, 2\pi)$ be an angle specifying a single point on the ellipse, and $X \in \mathbb{R}^2$ be its cartesian coordinates. The data-generating process is: $z \sim P_Z$, $u \sim P_{U|Z=z}$, $\mathbf{pa} \sim P_{\mathbf{PA}|Z=z}$, and $x := f(\mathbf{pa}, u)$. By construction, $U \perp\!\!\!\perp \mathbf{PA} | Z$, and Z satisfies the backdoor criterion (BC) w.r.t. $\mathbf{PA} \rightarrow X$. To induce a Markovian setting, we randomise \mathbf{PA} , yielding $U \perp\!\!\!\perp \mathbf{PA}$. The goal is to learn a map $T : (0, 2\pi) \times \mathbb{R}^2 \rightarrow \mathbb{R}^2$ that can infer the set of counterfactual points $\mathcal{X}^* := \{x^* = T(\mathbf{pa}^*, T^{-1}(\mathbf{pa}, x)) \mid \mathbf{pa}^* \in (0, 2\pi)\}$, which draws the entire ellipse each observed (\mathbf{pa}, x) belongs to. Importantly, since we always know the ground truth \mathcal{X}^* , we can evaluate our counterfactual estimates exactly using the mean average percentage error (μ_{APE}).

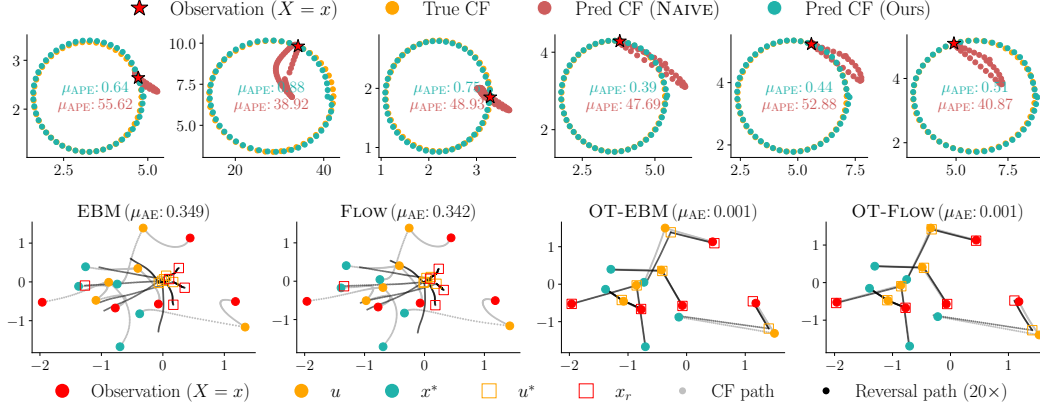


Figure 2: **Counterfactual ellipse generation.** (Top) Comparing our OT coupling flow to the naive approach (Section 5). (Bottom) OT maps exhibit greater counterfactual *reversibility*. A counterfactual $x^* = T_{pa^*} \circ T_{pa}^{-1}(x)$, is reversed by $x_r = T_{pa} \circ T_{pa^*}^{-1}(x^*)$, and a perfect reversal squares the circle.

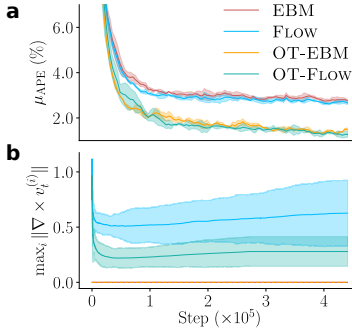


Figure 3: **(a)** CF error; **(b)** *curl* of the vector field during training.

Table 1: Counterfactual ellipse evaluation. As predicted by our theory, monotone flows are consistent in the Markovian setting, and bijectivity alone is sufficient under the front-door criterion.

Baselines (Nasr-Esfahany et al., 2023)					
SCHEME	COND _{PA}	COND _{PA,Z}	Markovian	BC _Z	
$\mu_{APE}(\%) \downarrow$	6607	6582	607	1.0	
(Ours)	NFE	EBM	FLOW	OT-EBM	OT-FLOW
Front-door	2	19.7 \pm .03	19.9 \pm .30	1.64 \pm .19	1.60 \pm .01
	10	5.79 \pm .11	5.80 \pm .08	1.42 \pm .23	1.37 \pm .14
	50	1.79 \pm .08	1.67 \pm .10	1.42 \pm .22	1.35 \pm .18
Markovian	2	34.0 \pm .90	33.6 \pm .23	1.21 \pm .04	1.06 \pm .02
	10	9.41 \pm .24	9.20 \pm .16	0.95 \pm .02	0.78 \pm .01
	50	2.32 \pm .01	2.30 \pm .02	0.93 \pm .02	0.76\pm.01

We build four flow variants: (i) an energy-based model flow (EBM), which is curl-free by design; (ii) a continuous-time flow (Lipman et al., 2023) (FLOW)⁶; (iii) an EBM using the family of OT couplings described in Section 5 (OT-EBM); and (iv) same as (iii) but using a FLOW (denoted OT-FLOW). To show our OT coupling is necessary for correct counterfactual inferences, we compare with the ‘naive’ (NAIVE) version of a Batch-OT flow, which violates Markovianity (cf. Section 5). For all other details regarding architectures, datasets and experimental setup please refer to Appendix E.

Nasr-Esfahany et al. (2023) reports that their spline flow-based model *failed* in the Markovian case, with $\mu_{APE}=607\%$. It only succeeded using the BC_Z scheme (Back-door) with a μ_{APE} of 1% (reproduced at .98%). Learning $P(X | PA)$ or $P(X | PA, Z)$ also failed when Z is a confounder (cf. COND_{PA}, COND_{PA,Z}). Table 1 shows our flows produce near-exact ground-truth counterfactuals, and using just two function evaluations with OT. Counterfactual *reversibility* (Monteiro et al., 2023) is also improved by straighter paths (Figure 2). Further, we experiment with a non-Markovian setting with non-linear *unobserved* confounding where the front-door criterion applies. The results validate our theory in that bijectivity alone is sufficient for consistent counterfactual inference in this case.

6.2 Case Study: Chest X-ray Imaging Counterfactuals

To extend our study to high-dimensional settings, we conduct experiments on MIMIC-CXR (Johnson et al., 2019), a widely used dataset for counterfactual inference. Our assumed causal graph follows the baselines (Ribeiro et al., 2023; Xia et al., 2024), and includes SEX (S), RACE (R), AGE (A) and DISEASE (D) variables, where $A \rightarrow D$, and $PA_X = \{S, R, A, D\}$ cause the X-ray image X . To parameterise our flow models, we use a streamlined version of Dhariwal and Nichol (2021)’s UNet

⁶Equivalent to Sanchez and Tsafaris (2021) if the source distribution is Gaussian (Gao et al., 2025).

Table 2: Counterfactual *effectiveness* on MIMIC Chest X-ray (192×192). $|\Delta_{\text{AUC}}|$ denotes the absolute difference in ROCAUC of counterfactuals relative to the observed data baseline. For each variable, our results (blue shade) appear on the right, and baseline results (Ribeiro et al., 2023) are on the left. Note the large improvements for e.g. RACE. For more comparisons and ablations, see Appendix F.

	SEX (S)		RACE (R)		AGE (A)		DISEASE (D)	
BASELINE	AUC (%) \uparrow		AUC (%) \uparrow		MAE (yr) \downarrow		AUC (%) \uparrow	
Observed data	99.63		95.34		6.197		94.41	
INTERVENTION	$ \Delta_{\text{AUC}} $ (%) \downarrow		$ \Delta_{\text{AUC}} $ (%) \downarrow		Δ_{MAE} (yr) \downarrow		$ \Delta_{\text{AUC}} $ (%) \downarrow	
$do(S = s)$	0.370	0.173 \pm .02	11.44	0.583 \pm .15	0.288	0.333 \pm .06	2.490	0.023 \pm .05
$do(R = r)$	0.070	0.180 \pm .01	8.640	0.050 \pm .07	0.144	0.394 \pm .10	7.010	0.310 \pm .19
$do(A = a)$	0.070	0.187 \pm .03	14.64	1.197 \pm .15	0.446	0.836 \pm .08	2.810	0.347 \pm .09
$do(D = d)$	0.070	0.067 \pm .00	16.04	0.627 \pm .18	0.371	0.435 \pm .05	3.790	2.280 \pm .37
$do(\text{rand})$	0.170	0.150 \pm .02	12.54	0.730 \pm .22	0.300	0.510 \pm .05	0.590	0.640 \pm .17

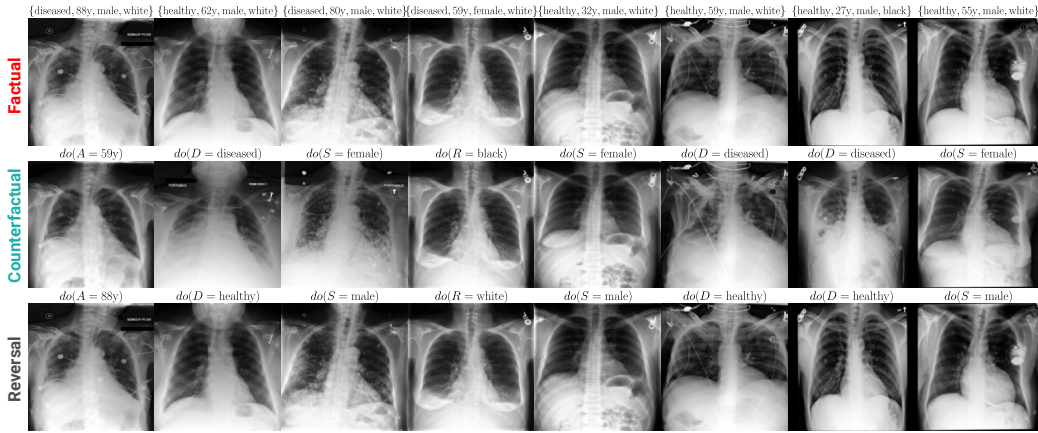


Figure 4: Qualitative counterfactual inference results on MIMIC Chest X-ray. We observe faithful, reversible interventions without requiring counterfactual fine-tuning, or classifier(-free) guidance.

architecture (see Appendix F for details). Table 2 and Figure 4 report our main results. We observe substantial improvements over baselines (Ribeiro et al., 2023; Xia et al., 2024) using our flows, across all three counterfactual soundness axioms, and without requiring any costly counterfactual fine-tuning or classifier(-free) guidance. That said, this alone does not imply causal validity. In Appendix F, we report additional comparisons and ablations. We observe performance trade-offs: for instance, OT-FLOW (which assumes Markovianity) outperforms on race interventions but underperforms FLOW on disease interventions, suggesting non-Markovian interaction effects or a subpar OT approximation. Notably, our Markovian OT coupling substantially improves over the NAIVE OT flow baseline.

7 Conclusion

Causal claims are credible only insofar as their identification is defensible, because observationally equivalent models can imply different answers. This work establishes a foundation for counterfactual identification of high-dimensional, multivariate outcomes (e.g. images) from observational data. We clarify the conditions under which flow matching yields identified counterfactuals for common causal structures, stating all assumptions and constraints explicitly to invite scrutiny and relaxation. Our results address causal validity concerns in prior work and extend to non-Markovian settings under standard criteria. For Markovian and instrumental variable settings, we characterise a continuous flow that is provably unique and monotone, yielding a rank-preserving dynamic OT map and consistent counterfactuals. Using continuous flows, we demonstrate near-exact ground-truth counterfactuals in controlled scenarios and improved axiomatic counterfactual soundness on real images relative to prior methods. Scaling OT to large problems remains a challenge. We conclude by urging practitioners to assess the causal validity of their estimates when using generative models for causal inference.

Acknowledgments and Disclosure of Funding

We thank Aapo Hyvärinen and Charles Jones for helpful insights and discussions. F.R. and B.G. acknowledge the support of the UKRI AI programme, and the EPSRC, for CHAI-EPSRC Causality in Healthcare AI Hub (grant no. EP/Y028856/1). B.G. received support from the Royal Academy of Engineering as part of his Kheiron/RAEng Research Chair.

References

- Michael Samuel Albergo and Eric Vanden-Eijnden. Building normalizing flows with stochastic interpolants. In *The Eleventh International Conference on Learning Representations*, 2023. 2, 4, 26
- Joshua Angrist and Guido Imbens. Identification and estimation of local average treatment effects, 1995. 17
- Michał Balcerak, Tamaz Amiranashvili, Antonio Terpin, Suprosanna Shit, Lea Bogensperger, Sebastian Kaltenbach, Petros Koumoutsakos, and Bjoern Menze. Energy matching: Unifying flow matching and energy-based models for generative modeling. *arXiv preprint arXiv:2504.10612*, 2025. 27
- Elias Bareinboim, Juan D. Correa, Duligur Ibeling, and Thomas Icard. *On Pearl’s Hierarchy and the Foundations of Causal Inference*, pages 507–556. Association for Computing Machinery, 2022. 1, 2, 26
- Jean-David Benamou and Yann Brenier. A computational fluid mechanics solution to the monge-kantorovich mass transfer problem. *Numerische Mathematik*, 84(3):375–393, 2000. 2, 3, 4, 19, 26
- Yann Brenier. Polar factorization and monotone rearrangement of vector-valued functions. *Communications on pure and applied mathematics*, 44(4):375–417, 1991. 2, 3, 5, 18, 19, 21, 25, 26
- Kailash Budhathoki, Lenon Minorics, Patrick Blöbaum, and Dominik Janzing. Causal structure-based root cause analysis of outliers. In *International conference on machine learning*, pages 2357–2369. PMLR, 2022. 1
- Luis A Caffarelli. The regularity of mappings with a convex potential. *Journal of the American Mathematical Society*, 5(1):99–104, 1992. 2, 5, 6, 19, 21, 22, 26
- Guillaume Carlier, Victor Chernozhukov, and Alfred Galichon. Vector quantile regression: an optimal transport approach. *The Annals of Statistics*, pages 1165–1192, 2016. 23, 26
- Daniel C Castro, Ian Walker, and Ben Glocker. Causality matters in medical imaging. *Nature Communications*, 11(1):1–10, 2020. 1
- Ricky TQ Chen, Yulia Rubanova, Jesse Bettencourt, and David K Duvenaud. Neural ordinary differential equations. *Advances in neural information processing systems*, 31, 2018. 2, 4, 22, 26
- Yikang Chen, Lili Tian, et al. Exogenous matching: Learning good proposals for tractable counterfactual estimation. *Advances in Neural Information Processing Systems*, 37:132313–132363, 2024. 2
- Juan Correa, Sanghack Lee, and Elias Bareinboim. Nested counterfactual identification from arbitrary surrogate experiments. *Advances in Neural Information Processing Systems*, 34:6856–6867, 2021. 2
- Fabio De Sousa Ribeiro and Ben Glocker. Demystifying variational diffusion models. *Foundations and Trends in Computer Graphics and Vision*, 17(2):76–170, 2025. 27

- Prafulla Dhariwal and Alexander Nichol. Diffusion models beat gans on image synthesis. *Advances in neural information processing systems*, 34:8780–8794, 2021. 8, 35
- Rémi Flamary, Nicolas Courty, Alexandre Gramfort, Mokhtar Z Alaya, Aurélie Boissunon, Stanislas Chambon, Laetitia Chapel, Adrien Corenflos, Kilian Fatras, Nemo Fournier, et al. Pot: Python optimal transport. *Journal of Machine Learning Research*, 22(78):1–8, 2021. 7
- David Galles and Judea Pearl. An axiomatic characterization of causal counterfactuals. *Foundations of Science*, 3:151–182, 1998. ISSN 1572-8471. doi: 10.1023/A:1009602825894. 28
- Ruiqi Gao, Emiel Hoogetboom, Jonathan Heek, Valentin De Bortoli, Kevin Patrick Murphy, and Tim Salimans. Diffusion models and gaussian flow matching: Two sides of the same coin. In *The Fourth Blogpost Track at ICLR 2025*, 2025. URL <https://openreview.net/forum?id=C8Yyg9wy0s>. 8, 31, 33
- Tomas Geffner, Javier Antoran, Adam Foster, Wenbo Gong, Chao Ma, Emre Kiciman, Amit Sharma, Angus Lamb, Martin Kukla, Nick Pawlowski, et al. Deep end-to-end causal inference. *Transactions on Machine Learning Research*, 2024. ISSN 2835-8856. 2
- Luigi Gresele, Julius Von Kügelgen, Jonas Kübler, Elke Kirschbaum, Bernhard Schölkopf, and Dominik Janzing. Causal inference through the structural causal marginal problem. In *International conference on machine learning*, pages 7793–7824. PMLR, 2022. 2
- Joseph Y. Halpern. Axiomatizing causal reasoning. In *Proceedings of the Fourteenth Conference on Uncertainty in Artificial Intelligence*, UAI’98, pages 202–210, San Francisco, CA, USA, 1998. Morgan Kaufmann Publishers Inc. ISBN 155860555X. 28
- Jason Hartford, Greg Lewis, Kevin Leyton-Brown, and Matt Taddy. Deep iv: A flexible approach for counterfactual prediction. In *International Conference on Machine Learning*, pages 1414–1423. PMLR, 2017. 2
- Jonathan Ho and Tim Salimans. Classifier-free diffusion guidance. *arXiv preprint arXiv:2207.12598*, 2022. 34
- Patrik Hoyer, Dominik Janzing, Joris M Mooij, Jonas Peters, and Bernhard Schölkopf. Nonlinear causal discovery with additive noise models. *Advances in neural information processing systems*, 21, 2008. 2
- Aapo Hyvärinen and Petteri Pajunen. Nonlinear independent component analysis: Existence and uniqueness results. *Neural networks*, 12(3):429–439, 1999. 2, 4
- Aapo Hyvärinen, Hiroaki Sasaki, and Richard Turner. Nonlinear ica using auxiliary variables and generalized contrastive learning. In *The 22nd international conference on artificial intelligence and statistics*, pages 859–868. PMLR, 2019. 2
- Aapo Hyvärinen, Ilyes Khemakhem, and Ricardo Monti. Identifiability of latent-variable and structural-equation models: from linear to nonlinear. *Annals of the Institute of Statistical Mathematics*, 76(1):1–33, 2024. 1, 4, 26, 27
- Guido W Imbens and Joshua D Angrist. Identification and estimation of local average treatment effects. *Econometrica*, 62(2):467–475, 1994. ISSN 00129682, 14680262. 4
- Alexander Immer, Christoph Schultheiss, Julia E Vogt, Bernhard Schölkopf, Peter Bühlmann, and Alexander Marx. On the identifiability and estimation of causal location-scale noise models. In *International Conference on Machine Learning*, pages 14316–14332. PMLR, 2023. 2
- Adrián Javaloy, Pablo Sánchez-Martín, and Isabel Valera. Causal normalizing flows: from theory to practice. *Advances in Neural Information Processing Systems*, 36:58833–58864, 2023. 2
- Alistair EW Johnson, Tom J Pollard, Seth J Berkowitz, Nathaniel R Greenbaum, Matthew P Lungren, Chih-ying Deng, Roger G Mark, and Steven Horng. Mimic-cxr, a de-identified publicly available

- database of chest radiographs with free-text reports. *Scientific data*, 6(1):1–8, 2019. 8
- Amir-Hossein Karimi, Julius Von Kügelgen, Bernhard Schölkopf, and Isabel Valera. Algorithmic recourse under imperfect causal knowledge: a probabilistic approach. *Advances in neural information processing systems*, 33:265–277, 2020. 1
- Ilyes Khemakhem, Ricardo Monti, Robert Leech, and Aapo Hyvarinen. Causal autoregressive flows. In *International conference on artificial intelligence and statistics*, pages 3520–3528. PMLR, 2021. 2, 27
- Michal Klein, Alireza Mousavi-Hosseini, Stephen Zhang, and Marco Cuturi. On fitting flow models with large sinkhorn couplings. *arXiv preprint arXiv:2506.05526*, 2025. 7, 35, 36, 38
- Aneesh Komanduri, Chen Zhao, Feng Chen, and Xintao Wu. Causal diffusion autoencoders: Toward counterfactual generation via diffusion probabilistic models. In *ECAI 2024*, pages 2516–2523. IOS Press, 2024. 2
- Amar Kumar, Anita Kriz, Mohammad Havaei, and Tal Arbel. PRISM: High-resolution & precise counterfactual medical image generation using language-guided stable diffusion. In *Medical Imaging with Deep Learning*, 2025. 2
- Matt J Kusner, Joshua Loftus, Chris Russell, and Ricardo Silva. Counterfactual fairness. *Advances in neural information processing systems*, 30, 2017. 1
- Yaron Lipman, Ricky TQ Chen, Heli Ben-Hamu, Maximilian Nickel, and Matthew Le. Flow matching for generative modeling. In *The Eleventh International Conference on Learning Representations*, 2023. 2, 4, 8, 33
- Xingchao Liu et al. Flow straight and fast: Learning to generate and transfer data with rectified flow. In *The Eleventh International Conference on Learning Representations*, 2023. 2, 4
- Francesco Locatello, Stefan Bauer, Mario Lucic, Gunnar Raetsch, Sylvain Gelly, Bernhard Schölkopf, and Olivier Bachem. Challenging common assumptions in the unsupervised learning of disentangled representations. In *international conference on machine learning*, pages 4114–4124. PMLR, 2019. 2
- Chaochao Lu, Biwei Huang, Ke Wang, José Miguel Hernández-Lobato, Kun Zhang, and Bernhard Schölkopf. Sample-efficient reinforcement learning via counterfactual-based data augmentation. *arXiv preprint arXiv:2012.09092*, 2020. 2
- Charles F. Manski. Monotone treatment response. *Econometrica*, 65(6):1311–1334, 1997. ISSN 00129682, 14680262. 17
- Robert J McCann. A convexity principle for interacting gases. *Advances in mathematics*, 128(1): 153–179, 1997. 4, 26
- Raghav Mehta, Fabio De Sousa Ribeiro, Tian Xia, Mélanie Roschewitz, Ainkaran Santhirasekaram, Dominic C Marshall, and Ben Glocker. Cf-seg: Counterfactuals meet segmentation. In *International Conference on Medical Image Computing and Computer-Assisted Intervention*, pages 117–127. Springer, 2025. 1
- Valentyn Melnychuk, Dennis Frauen, and Stefan Feuerriegel. Partial counterfactual identification of continuous outcomes with a curvature sensitivity model. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023. 2
- Miguel Monteiro, Fabio De Sousa Ribeiro, Nick Pawlowski, Daniel C Castro, and Ben Glocker. Measuring axiomatic soundness of counterfactual image models. In *The Eleventh International Conference on Learning Representations*, 2023. 7, 8, 28, 31, 37
- Alireza Mousavi-Hosseini, Stephen Y Zhang, Michal Klein, and Marco Cuturi. Flow matching with semidiscrete couplings. *arXiv preprint arXiv:2509.25519*, 2025. 7, 35, 38

- Arash Nasr-Esfahany and Emre Kiciman. Counterfactual non-identifiability of learned structural causal models. *arXiv preprint arXiv:2301.09031*, 2023. 2, 26
- Arash Nasr-Esfahany, Mohammad Alizadeh, and Devavrat Shah. Counterfactual identifiability of bijective causal models. In *International Conference on Machine Learning*, pages 25733–25754. PMLR, 2023. 2, 4, 6, 7, 8, 20, 23, 24, 25, 26, 27, 29, 34
- Yushu Pan and Elias Bareinboim. Counterfactual image editing. In *International Conference on Machine Learning*, pages 39087–39101. PMLR, 2024. 2
- Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. Pytorch: An imperative style, high-performance deep learning library. *Advances in Neural Information Processing Systems*, 2019. 29
- Nick Pawlowski, Daniel C Castro, and Ben Glocker. Deep structural causal models for tractable counterfactual inference. *Advances in Neural Information Processing Systems*, 33:857–869, 2020. 2, 35
- Judea Pearl. Causal diagrams for empirical research. *Biometrika*, 82(4):669–688, 1995. 1, 2
- Judea Pearl. The logic of counterfactuals in causal inference. *Journal of American Statistical Association*, 95, 2000. Discussion of Causal Inference Without Counterfactuals by A.P. Dawid. 1
- Judea Pearl. Direct and indirect effects. In *Proceedings of the Seventeenth Conference on Uncertainty in Artificial Intelligence*, UAI’01, pages 411–420, San Francisco, CA, USA, 2001. Morgan Kaufmann Publishers Inc. ISBN 1558608001. 2
- Judea Pearl. *Causality*. Cambridge university press, 2009. 1, 2, 3, 4, 6, 23, 26, 28
- Judea Pearl and Elias Bareinboim. *External Validity: From Do-Calculus to Transportability Across Populations*, page 451–482. Association for Computing Machinery, New York, NY, USA, 1 edition, 2022. ISBN 9781450395861. 26
- Judea Pearl and Dana Mackenzie. *The book of why: the new science of cause and effect*. Basic books, 2018. 2
- Fernando Pérez-García, Sam Bond-Taylor, Pedro P. Sanchez, Boris van Breugel, Daniel C. Castro, Harshita Sharma, Valentina Salvatelli, Maria T. A. Wetscherek, Hannah Richardson, Matthew P. Lungren, Aditya Nori, Javier Alvarez-Valle, Ozan Oktay, and Maximilian Ilse. Radedit: Stress-testing biomedical vision models via diffusion image editing. In *Computer Vision – ECCV 2024*, pages 358–376, Cham, 2025. Springer Nature Switzerland. ISBN 978-3-031-73254-6. 42
- Jonas Peters, Joris M Mooij, Dominik Janzing, and Bernhard Schölkopf. Causal discovery with continuous additive noise models. *The Journal of Machine Learning Research*, 15(1):2009–2053, 2014. 2
- Jonas Peters, Dominik Janzing, and Bernhard Schölkopf. *Elements of causal inference: foundations and learning algorithms*. The MIT Press, 2017. 1
- Gabriel Peyré, Marco Cuturi, et al. Computational optimal transport: With applications to data science. *Foundations and Trends® in Machine Learning*, 11(5-6):355–607, 2019. 2, 3
- Silviu Pitis, Elliot Creager, Ajay Mandlekar, and Animesh Garg. Mocoda: Model-based counterfactual data augmentation. *Advances in Neural Information Processing Systems*, 35:18143–18156, 2022. 1
- Aram-Alexandre Pooladian, Heli Ben-Hamu, Carles Domingo-Enrich, Brandon Amos, Yaron Lipman, and Ricky TQ Chen. Multisample flow matching: Straightening flows with minibatch couplings. In *International Conference on Machine Learning*, pages 28100–28127. PMLR, 2023. 2, 4, 7, 27, 35, 36

- Rajat R Rasal, Avinash Kori, Fabio De Sousa Ribeiro, Tian Xia, and Ben Glocker. Diffusion counterfactual generation with semantic abduction. In *Forty-second International Conference on Machine Learning*, 2025. 2
- Fabio De Sousa Ribeiro, Tian Xia, Miguel Monteiro, Nick Pawlowski, and Ben Glocker. High fidelity image counterfactuals with probabilistic causal models. In *International Conference on Machine Learning*, pages 7390–7425. PMLR, 2023. 2, 7, 8, 9, 28, 35, 36, 37, 39, 40
- Mélanie Roschewitz, Fabio De Sousa Ribeiro, Tian Xia, Galvin Khara, and Ben Glocker. Counterfactual contrastive learning: robust representations via causal image synthesis. In *MICCAI Workshop on Data Engineering in Medical Imaging*, pages 22–32. Springer, 2024. 1
- Pedro Sanchez and Sotirios A Tsafaris. Diffusion causal models for counterfactual estimation. In *First Conference on Causal Learning and Reasoning*, 2021. 2, 8, 33
- Pablo Sánchez-Martin, Miriam Rateike, and Isabel Valera. Vaca: Designing variational graph autoencoders for causal queries. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pages 8159–8168, 2022. 2
- Filippo Santambrogio. *Optimal transport for applied mathematicians*, volume 87. Springer, 2015. 2, 3, 4
- Bernhard Schölkopf. *Causality for Machine Learning*, pages 765–804. Association for Computing Machinery, New York, NY, USA, 1 edition, 2022. ISBN 9781450395861. 1
- Bernhard Schölkopf, Francesco Locatello, Stefan Bauer, Nan Rosemary Ke, Nal Kalchbrenner, Anirudh Goyal, and Yoshua Bengio. Toward causal representation learning. *Proceedings of the IEEE*, 109(5):612–634, 2021. 1
- Shohei Shimizu, Patrik O Hoyer, Aapo Hyvärinen, Antti Kerminen, and Michael Jordan. A linear non-gaussian acyclic model for causal discovery. *Journal of Machine Learning Research*, 7(10), 2006. 2
- Ilya Shpitser and Judea Pearl. What counterfactuals can be tested. In *23rd Conference on Uncertainty in Artificial Intelligence, UAI 2007*, pages 352–359, 2007. 2
- Jin Tian and Judea Pearl. Probabilities of causation: Bounds and identification. *Annals of Mathematics and Artificial Intelligence*, 28(1):287–313, 2000. 2
- Alexander Tong, Kilian Fatras, Nikolay Malkin, Guillaume Hugué, Yanlei Zhang, Jarrid Rector-Brooks, Guy Wolf, and Yoshua Bengio. Improving and generalizing flow-based generative models with minibatch optimal transport. *Transactions on Machine Learning Research*, 2024. ISSN 2835-8856. 2, 4, 7, 27, 35
- Stratis Tsirtsis and Manuel Rodriguez. Finding counterfactually optimal action sequences in continuous state spaces. *Advances in Neural Information Processing Systems*, 36:3220–3247, 2023. 1
- Cédric Villani et al. *Optimal transport: old and new*, volume 338. Springer, 2008. 2, 3, 4, 19
- Athanasios Vlontzos, Bernhard Kainz, and Ciarán M Gilligan-Lee. Estimating categorical counterfactuals via deep twin networks. *Nature Machine Intelligence*, 5(2):159–168, 2023. 2
- Yulun Wu, Louis McConnell, and Claudia Iriondo. Counterfactual generative modeling with variational causal inference. In *The Thirteenth International Conference on Learning Representations*, 2025. 2
- Kevin Xia, Yushu Pan, and Elias Bareinboim. Neural causal models for counterfactual identification and estimation. In *The Eleventh International Conference on Learning Representations*, 2023. 2, 26

- Tian Xia, Mélanie Roschewitz, Fabio De Sousa Ribeiro, Charles Jones, and Ben Glocker. Mitigating attribute amplification in counterfactual image generation. In *International Conference on Medical Image Computing and Computer-Assisted Intervention*, pages 546–556. Springer, 2024. [8](#), [9](#), [35](#), [36](#)
- Tian Xia, Fabio De Sousa Ribeiro, Rajat R Rasal, Avinash Kori, Raghav Mehta, and Ben Glocker. Decoupled classifier-free guidance for counterfactual diffusion models. *arXiv preprint arXiv:2506.14399*, 2025. [2](#)
- Junzhe Zhang and Elias Bareinboim. Fairness in decision-making—the causal explanation formula. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 32, 2018. [2](#)
- Kun Zhang and Aapo Hyvärinen. On the identifiability of the post-nonlinear causal model. In *Proceedings of the Twenty-Fifth Conference on Uncertainty in Artificial Intelligence*, pages 647–655, 2009. [2](#)

Appendices

Table of Contents

A Motivating Example: Monotonicity Requirement	16
B Proofs: Counterfactual Identifiability	18
B.1 Optimal Transport for Counterfactual Identification	18
B.2 Exogenous Prior Indeterminacy	20
B.3 Non-Markovian Counterfactual Identifiability	23
B.4 Assumptions: Summary & Plausibility	26
C Energy Based Models: Curl-free Flows	27
D Counterfactual Soundness Axioms	28
E Counterfactual Ellipse: Extra Results	29
E.1 Dataset Details	29
E.2 Architecture and Experimental Setup	29
E.3 Qualitative Results	30
E.4 Ablation Studies: Priors & Assumption Violations	34
F MIMIC Chest X-ray: Extra Results	35
F.1 Dataset Details	35
F.2 Architecture and Experimental Setup	35
F.3 Additional Comparisons and Ablation Studies	36
F.4 Qualitative Results	39

A Motivating Example: Monotonicity Requirement

We start with a simple instructive example in one dimension ($d = 1$). Suppose we have two causal mechanisms $T^{(1)}$ and $T^{(2)}$ defined as follows:

$$X = T^{(1)}(\mathbf{PA}, U) = \mathbf{PA} + U, \quad (18)$$

$$X = T^{(2)}(\mathbf{PA}, U) = \mathbf{PA} + 1 - U, \quad (19)$$

where $\mathbf{PA} \sim \mathcal{B}(0.5)$ is Bernoulli distributed, and $U \sim \mathcal{U}(0, 1)$ is continuous uniform. One can verify that both $T^{(1)}$ and $T^{(2)}$ induce the same conditional observational distribution:

$$P(X \mid \mathbf{PA} = 0) = \mathcal{U}(0, 1), \quad P(X \mid \mathbf{PA} = 1) = \mathcal{U}(1, 2). \quad (20)$$

Without loss of generality, consider the counterfactual query

$$X_{\mathbf{pa}^* := 1} \mid \{\mathbf{PA} = 0, X = 0.8\}. \quad (21)$$

In the abduction step, $T^{(1)}$ and $T^{(2)}$ infer *different* exogenous noise values:

$$u^{(1)} = (T^{(1)})^{-1}(\mathbf{pa}, x) = x - \mathbf{pa} = 0.8 - 0 = 0.8, \quad (22)$$

$$u^{(2)} = (T^{(2)})^{-1}(\mathbf{pa}, x) = \mathbf{pa} + 1 - x = 0 + 1 - 0.8 = 0.2. \quad (23)$$

Nonetheless, both mechanisms produce the same counterfactuals:

$$x^{*(1)} = T^{(1)}(\mathbf{pa}^*, u^{(1)}) = \mathbf{pa}^* + u^{(1)} = 1 + 0.8 = 1.8, \quad (24)$$

$$x^{*(2)} = T^{(2)}(\mathbf{pa}^*, u^{(2)}) = \mathbf{pa}^* + 1 - u^{(2)} = 1 + 1 - 0.2 = 1.8. \quad (25)$$

Even if $u^{(1)} \neq u^{(2)}$, both $T^{(1)}$ and $T^{(2)}$ can return the same counterfactual outcomes because they assign the same **rank** u (i.e., cumulative probability or quantile level) to the observed value x .

Concretely, since $T^{(1)}, T^{(2)}$ define the same observational distribution $P(X \mid \mathbf{PA})$, their conditional CDFs $F_{X \mid \mathbf{PA}} : \mathbb{R} \rightarrow [0, 1]$ match, and we can use them to perform abduction:

$$u = F_{X \mid \mathbf{PA}=0}(x) \quad (26)$$

$$= P(X \leq x \mid \mathbf{PA} = 0) \quad (27)$$

$$= \frac{x - a}{b - a} = \frac{0.8 - 0}{1 - 0} = 0.8, \quad (28)$$

where $(a, b) = (0, 1)$ since $P(X \mid \mathbf{PA} = 0) = \mathcal{U}(0, 1)$.

Then, we compute the counterfactual using the quantile function $F_{X \mid \mathbf{PA}=\mathbf{pa}^*}^{-1} : (0, 1) \rightarrow \mathbb{R}$, that is, the inverse conditional CDF under intervention:

$$x^* = F_{X \mid \mathbf{PA}=\mathbf{pa}^*}^{-1}(u) = a + u(b - a) = 1 + 0.8(1) = 1.8, \quad (29)$$

where $(a, b) = (1, 2)$, since we set $\mathbf{pa}^* := 1$ and $P(X \mid \mathbf{PA} = 1) = \mathcal{U}(1, 2)$.

The key here is the **strict monotonicity** of $T^{(1)}, T^{(2)}$ in U , that is for any $u^{(1)} < u^{(2)} \in \mathbb{R}$, we have

$$T^{(1)}(\cdot, u^{(1)}) < T^{(1)}(\cdot, u^{(2)}) \quad \text{and} \quad T^{(2)}(\cdot, u^{(1)}) > T^{(2)}(\cdot, u^{(2)}). \quad (30)$$

To illustrate the importance of this property, consider a third mechanism $T^{(3)}$ that induces the same conditional observational distribution:

$$X = T^{(3)}(\mathbf{PA}, U) = \begin{cases} U & \text{if } \mathbf{PA} = 0 \\ 2 - U & \text{if } \mathbf{PA} = 1 \end{cases}, \quad U \sim \mathcal{U}(0, 1). \quad (31)$$

However, we can see that $T^{(3)}$ produces a different counterfactual for the same query used before:

$$u^{(3)} = (T^{(3)})^{-1}(\mathbf{pa}, x) = x = 0.8, \quad (32)$$

$$x^{*(3)} = T^{(3)}(\mathbf{pa}^*, u^{(3)}) = 2 - u^{(3)} = 1.2. \quad (33)$$

One can verify that, unlike for $T^{(1)}, T^{(2)}$, the rank is not being preserved under intervention:

$$F_{X \mid \mathbf{PA}=0}(x) = 0.8 > F_{X \mid \mathbf{PA}=\mathbf{pa}^*}(x^{*(3)}) = 0.2. \quad (34)$$

For a consistent counterfactual inference model, we would expect the inferred rank u (i.e., the cumulative probability or quantile level) of an observed outcome x given its parents \mathbf{pa} to map to a counterfactual outcome x^* that lies at the same rank in the counterfactual distribution:

$$x^* = F_{X \mid \mathbf{PA}=\mathbf{pa}^*}^{-1}(F_{X \mid \mathbf{PA}=\mathbf{pa}}(x)). \quad (35)$$

The mismatch observed previously occurs because $T^{(3)}$ is not monotonic in U across different values of the parents \mathbf{PA} ⁷. As a result, $T^{(3)}$ fails to preserve the rank order of outcomes across different interventions, thereby breaking counterfactual consistency and identifiability.

This rank-preservation condition can be viewed as the continuous analogue of the *monotone treatment response* (Manski, 1997; Angrist and Imbens, 1995) used in epidemiological studies, which rules out so-called ‘defiers’: units for whom exposure to disease risk factors would actually *reduce* disease risk. In both cases, monotonicity ensures that counterfactuals respect the domain knowledge-based intuition that exposure should not make disease less likely. As is often the case in causal analysis, the appropriateness of this condition is contingent on the particular context in which it is applied.

With the above $d = 1$ example in mind, in the following sections, we characterise the set of constraints on the map T which permit (point-wise) counterfactual identification of causal mechanisms for multi-dimensional variables (i.e. $d > 1$); a key gap in existing literature. To achieve this, we connect ideas from dynamic optimal transport theory and graphical causality in ways previously unexplored.

⁷Note that $T^{(3)}$ is monotonic in U for each fixed value of \mathbf{PA} , but not globally across both settings.

B Proofs: Counterfactual Identifiability

B.1 Optimal Transport for Counterfactual Identification

Proposition B.1 (Monotone Counterfactual Transport Map). *If a mechanism $x := f(\mathbf{pa}, u)$ is monotone in u , then the respective counterfactual transport map $T^*(\mathbf{pa}^*, \mathbf{pa}, x)$ is monotone in x .*

Proof. If $f(\mathbf{pa}, u_1) < f(\mathbf{pa}, u_2)$ for all $u_1 < u_2$, then its inverse must be monotonic in x given \mathbf{pa} :

$$\forall x_1, x_2 : x_1 < x_2 \Rightarrow f^{-1}(\mathbf{pa}, x_1) < f^{-1}(\mathbf{pa}, x_2). \quad (36)$$

Applying the same logic given \mathbf{pa}^* , we have that their composition is also monotonic in x :

$$\forall x_1, x_2 : x_1 < x_2 \Rightarrow T^*(\mathbf{pa}^*, \mathbf{pa}, x_1) < T^*(\mathbf{pa}^*, \mathbf{pa}, x_2). \quad (37)$$

To generalise to multiple dimensions ($d > 1$), assume $f : \mathbb{R}^k \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is monotone in u :

$$\forall u_1, u_2 : \langle f(\mathbf{pa}, u_1) - f(\mathbf{pa}, u_2), u_1 - u_2 \rangle \geq 0, \quad (38)$$

and let

$$x_1 - x_2 = f(\mathbf{pa}, u_1) - f(\mathbf{pa}, u_2), \quad u_1 - u_2 = f^{-1}(\mathbf{pa}, x_1) - f^{-1}(\mathbf{pa}, x_2). \quad (39)$$

By substituting in the above, we have that:

$$\langle f(\mathbf{pa}, u_1) - f(\mathbf{pa}, u_2), u_1 - u_2 \rangle = \langle x_1 - x_2, f^{-1}(\mathbf{pa}, x_1) - f^{-1}(\mathbf{pa}, x_2) \rangle \geq 0, \quad (40)$$

which by symmetry of the dot product, shows f^{-1} is monotone in x . Lastly, to show when the counterfactual transport map $T^*(\mathbf{pa}^*, \mathbf{pa}, x) = f(\mathbf{pa}^*, f^{-1}(\mathbf{pa}, x))$ is also monotone in x (for $d > 1$), suppose that the causal mechanism f is equal to the gradient of a convex function:

$$\phi : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}, \quad \forall u, \mathbf{pa} : f(\mathbf{pa}, u) = \nabla_u \phi(u; \mathbf{pa}). \quad (41)$$

Recall that gradients of convex functions are monotone:

$$\forall u_1, u_2, \mathbf{pa} : \langle \nabla_u \phi(u_1; \mathbf{pa}) - \nabla_u \phi(u_2; \mathbf{pa}), u_1 - u_2 \rangle \geq 0, \quad (42)$$

and therefore, the following must hold:

$$\forall x, \mathbf{pa}, \mathbf{pa}^* : T^*(\mathbf{pa}^*, \mathbf{pa}, x) = \nabla_u \phi(u; \mathbf{pa}^*)|_{u=f^{-1}(\mathbf{pa}, x)}, \quad (43)$$

$$\implies \forall x_1, x_2 : \langle T^*(\mathbf{pa}^*, \mathbf{pa}, x_1) - T^*(\mathbf{pa}^*, \mathbf{pa}, x_2), x_1 - x_2 \rangle_x \geq 0, \quad (44)$$

where $\langle v, w \rangle_x := v^\top \partial_x f^{-1}(\mathbf{pa}, x)w$, concluding the proof. \square

Remark B.2. Monotonicity of the counterfactual transport map T^* w.r.t. x guarantees that, for a given intervention, the rank order of factual outcomes is preserved in the counterfactuals. This is important for, e.g. *fairness*, as it prevents rank inversions across individuals under intervention. Euclidean monotonicity of T^* (for $d > 1$) is guaranteed if the symmetric part of its Jacobian $\partial_x T^* = \partial_u f \partial_x f^{-1}$ is positive semi-definite; this holds, for example, if the two Jacobian components commute.

Next, we present Brenier’s theorem, a celebrated result in optimal transport theory that we draw from in our counterfactual identifiability analysis of dynamic OT-based causal mechanisms.

Theorem B.3 (Brenier (1991)). *Let μ, ν be probability measures on $\Omega \subset \mathbb{R}^d$ with finite second moments, and suppose μ is absolutely continuous w.r.t. Lebesgue measure. Then, for the quadratic cost function $c(x, T(x)) = \|x - T(x)\|^2$, the Monge problem admits a unique optimal transport map $T : \Omega \rightarrow \Omega$ pushing μ forward to ν , i.e., $T_\# \mu = \nu$. Moreover, this optimal map is the gradient of a convex function, $T = \nabla \phi$, and is monotone in the sense that:*

$$\forall x_1, x_2 : \langle T(x_1) - T(x_2), x_1 - x_2 \rangle \geq 0. \quad (45)$$

Remark B.4. This result provides a powerful geometric insight: under regularity conditions, the most efficient way of transporting mass from a source to a target distribution is by pushing it along the gradient of a convex function. The gradient structure ensures that the map does not ‘fold’, and the monotonicity condition reflects directional consistency in the sense that points which are initially close tend to remain close under the map, thereby preserving order and preventing overlaps.

Lemma B.5 (Unique and Monotone Dynamic OT Mechanism). *Let $\dim(X) = \dim(U) = d > 1$, and consider the Markovian setting $U \perp\!\!\!\perp \mathbf{PA}$. Assume P_U and $P_{X|\mathbf{PA}}^{\mathcal{C}}$ are absolutely continuous w.r.t. the Lebesgue measure with strictly positive and bounded densities on bounded, open, convex domains. Let $T : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ be the time-1 map of a dynamic OT flow satisfying:*

$$\{T_t : t \in [0, 1]\}, \quad dT_t(u; \mathbf{pa}) = v_t(T_t(u; \mathbf{pa})) dt, \quad T_{\sharp} P_U = P_{X|\mathbf{PA}}^{\mathcal{C}}. \quad (46)$$

Then, there exists a convex function $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ such that: $T(u; \mathbf{pa}) = \nabla_u \phi(u; \mathbf{pa})$, for $P_U(u)$ -a.e. u , where T is monotone, bijective a.e., and uniquely determined by the pair $(P_U, P_{X|\mathbf{PA}}^{\mathcal{C}})$.

Proof. First, we invoke standard Caffarelli (1992) regularity conditions for OT (see Theorem 12.50 in Villani et al. (2008) for a helpful summary). Let $\Omega, \Lambda \subset \mathbb{R}^d$ be bounded, open, convex sets. The source P_U and target $P_{X|\mathbf{PA}}^{\mathcal{C}}$ are absolutely continuous w.r.t. Lebesgue measure, with densities ρ_U and $\rho_{X|\mathbf{PA}}^{\mathcal{C}}$ bounded above and below by positive constants on $\overline{\Omega}$ and $\overline{\Lambda}$, respectively. These conditions cover the strictest version of our results; weaker conclusions follow under standard relaxations.

According to Benamou and Brenier (2000)'s dynamic formulation of optimal transport, the time-1 map T of a flow $\{T_t : t \in [0, 1]\}$ minimising the kinetic energy

$$\inf_{(\rho_t, v_t)} \int_0^1 \int_{\mathbb{R}^d \times \mathbb{R}^k} \|v_t(u; \mathbf{pa})\|^2 \rho_t(u, \mathbf{pa}) du d\mathbf{pa} dt \quad (47)$$

subject to the continuity equation

$$\partial_t \rho_t + \operatorname{div}(\rho_t v_t) = 0, \quad \rho_0 = \rho_U, \quad \rho_1 = \rho_{X|\mathbf{PA}}^{\mathcal{C}}, \quad (48)$$

solves the Monge problem:

$$T^* = \arg \min_{T(\cdot; \mathbf{PA})_{\sharp} P_U = P_{X|\mathbf{PA}}^{\mathcal{C}}} \int \|u - T(u; \mathbf{pa})\|^2 dP_U(u). \quad (49)$$

Since $P_U \ll \mathcal{L}^d$ (i.e. absolutely continuous w.r.t. the Lebesgue measure), Brenier (1991)'s theorem (cf. Theorem B.3) applies, and implies that the optimal transport map T^* is of the form:

$$T^*(u; \mathbf{pa}) = \nabla_u \phi(u; \mathbf{pa}), \quad (50)$$

where ϕ is convex on Ω . Further, this gradient map is well-defined P_U -almost everywhere and is uniquely determined by P_U and $P_{X|\mathbf{PA}}^{\mathcal{C}}$. Moreover, since $\nabla \phi$ pushes P_U forward to $P_{X|\mathbf{PA}}^{\mathcal{C}}$, this implies that for almost every $u \in \Omega$, it satisfies the Monge-Ampère equation:

$$\rho_U(u) = \rho_{X|\mathbf{PA}}^{\mathcal{C}}(\nabla_u \phi(u; \mathbf{pa})) \det D_u^2 \phi(u; \mathbf{pa}). \quad (51)$$

If ϕ is differentiable and strictly convex, then $\nabla \phi$ is strictly monotone and therefore injective:

$$\langle \nabla_u \phi(u^{(1)}; \mathbf{pa}) - \nabla_u \phi(u^{(2)}; \mathbf{pa}), u^{(1)} - u^{(2)} \rangle > 0 \quad \text{for } u^{(1)} \neq u^{(2)}. \quad (52)$$

In particular, $\nabla_u \phi(u^{(1)}; \mathbf{pa}) = \nabla_u \phi(u^{(2)}; \mathbf{pa})$ implies $u^{(1)} = u^{(2)}$, and thus T is injective almost everywhere. Moreover, since $T_{\sharp} P_U = P_{X|\mathbf{PA}}^{\mathcal{C}}$, no Borel set $A \subset \Lambda$ of positive $P_{X|\mathbf{PA}}^{\mathcal{C}}$ -measure can be missed by T and must satisfy $P_U(T^{-1}(A)) > 0$, hence T is onto Λ up to null sets.

The regularity of ϕ now follows from the theory of elliptic partial differential equations, specifically from Caffarelli (1992)'s well-known interior and global regularity results for convex solutions to the Monge-Ampère equation. If ρ_U and $\rho_{X|\mathbf{PA}}^{\mathcal{C}}$ are bounded above and below by positive constants on $\overline{\Omega}, \overline{\Lambda}$ and are C^α , then by Caffarelli (1992)'s theory the convex potential $\phi \in C^{2,\alpha}(\overline{\Omega})$; in particular, $D_u^2 \phi(u; \mathbf{pa})$ is almost everywhere positive definite and $\nabla \phi$ is locally a diffeomorphism. Hence, we conclude that $T(u; \mathbf{pa}) = \nabla_u \phi(u; \mathbf{pa})$, P_U -almost everywhere, and that T is monotone, almost everywhere bijective, and uniquely determined by the pair $(P_U, P_{X|\mathbf{PA}}^{\mathcal{C}})$. \square

Remark B.6. We draw on Brenier (1991)'s theorem to show that the causal mechanism is monotone. However, Brenier's map does not guarantee bijectivity by default. For this, we must invoke Caffarelli (1992)'s standard regularity results for OT, to ensure the map is locally diffeomorphic. In practice, this condition is often satisfied by smoothing empirical target distributions by adding mild continuous noise (e.g. uniform or Gaussian) to ensure the resulting distribution admits a density.

B.2 Exogenous Prior Indeterminacy

Given only observational data (\mathcal{L}_1), our goal is to find a transport map T that is counterfactually equivalent ($\sim_{\mathcal{L}_3}$) to the true transport map T^* underlying the data-generating process.

Definition B.7 (Transport \mathcal{L}_3 -Equivalence). Let $T^{(1)}, T^{(2)} : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ be transport maps with exogenous priors $P_U^{(1)}, P_U^{(2)}$ on \mathbb{R}^d , and parent domain \mathbb{R}^k . We say they are counterfactually equivalent $\sim_{\mathcal{L}_3}$, if and only if there exists a bijection $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ such that $g_{\#} P_U^{(2)} = P_U^{(1)}$, that is:

$$T^{(1)} \sim_{\mathcal{L}_3} T^{(2)} \iff \exists g : T^{(1)}(u; \mathbf{pa}) = T^{(2)}(g^{-1}(u); \mathbf{pa}) \text{ for } P_U^{(1)}\text{-a.e. } u, \forall \mathbf{pa}. \quad (53)$$

Proposition B.8 (Nasr-Esfahany et al. (2023)). Transport maps $T^{(1)}, T^{(2)} : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ produce the same counterfactuals if and only if they are \mathcal{L}_3 -equivalent in the sense of Definition B.7:

$$\forall x, \mathbf{pa}, \mathbf{pa}^* : x^* = T^{*(1)}(\mathbf{pa}^*, \mathbf{pa}, x) = T^{*(2)}(\mathbf{pa}^*, \mathbf{pa}, x) \iff T^{(1)} \sim_{\mathcal{L}_3} T^{(2)}. \quad (54)$$

Proof. We provide a proof here for completeness. An arbitrary counterfactual query $X_{\mathbf{pa}^*} \mid \{X = x, \mathbf{PA} = \mathbf{pa}\}$, where $\{X = x, \mathbf{PA} = \mathbf{pa}\}$ is the observed evidence, is answerable by any two equivalent transport maps $T^{(1)}, T^{(2)} : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ via abduction-action-prediction.

We first prove \Leftarrow .

In the abduction step, both maps use the observed evidence to infer the exogenous noise:

$$u^{(1)} = (T^{(1)})^{-1}(x; \mathbf{pa}), \quad u^{(2)} = (T^{(2)})^{-1}(x; \mathbf{pa}), \quad (55)$$

and their equivalence (cf. Definition B.7) implies that:

$$\exists g : u^{(1)} = g(u^{(2)}). \quad (56)$$

In the action-prediction step, for any intervention on the parents, we have that:

$$T^{(1)}(u^{(1)}; \mathbf{pa}^*) = T^{(1)}(g(u^{(2)}); \mathbf{pa}^*) = T^{(2)}(g^{-1}(u^{(1)}); \mathbf{pa}^*) = T^{(2)}(u^{(2)}; \mathbf{pa}^*), \quad (57)$$

thus both maps produce the same counterfactual outcomes:

$$\forall x, \mathbf{pa}, \mathbf{pa}^* : x^* = T^{(1)}(\mathbf{pa}^*, \mathbf{pa}, x) = T^{(2)}(\mathbf{pa}^*, \mathbf{pa}, x). \quad (58)$$

We now prove \Rightarrow .

Suppose, for the sake of contradiction, that the function g depends on the parents \mathbf{pa} , then:

$$\forall u^{(1)}, \mathbf{pa} : T^{(1)}(u^{(1)}; \mathbf{pa}) = T^{(2)}(g^{-1}(u^{(1)}; \mathbf{pa}); \mathbf{pa}). \quad (59)$$

Since $T^{(1)}, T^{(2)}$ produce identical counterfactuals, they must agree for any fixed \mathbf{pa}^* :

$$T^{(1)}(u^{(1)}; \mathbf{pa}^*) = T^{(2)}(g^{-1}(u^{(1)}; \mathbf{pa}); \mathbf{pa}^*), \quad (60)$$

where the abduction step is given by:

$$g^{-1}(u^{(1)}; \mathbf{pa}) = u^{(2)} = (T^{(2)})^{-1}(x; \mathbf{pa}). \quad (61)$$

Since Eq. (59) also holds when $\mathbf{pa} := \mathbf{pa}^*$, we have that:

$$T^{(1)}(u^{(1)}; \mathbf{pa}^*) = T^{(2)}(g^{-1}(u^{(1)}; \mathbf{pa}^*); \mathbf{pa}^*) \quad (62)$$

$$\implies T^{(2)}(g^{-1}(u^{(1)}; \mathbf{pa}); \mathbf{pa}^*) = T^{(2)}(g^{-1}(u^{(1)}; \mathbf{pa}^*); \mathbf{pa}^*). \quad (63)$$

Since $T^{(2)}$ is injective (i.e. bijective in $u^{(2)}$ by construction), the above implies that:

$$\forall \mathbf{pa}, \mathbf{pa}^* : g^{-1}(u^{(1)}; \mathbf{pa}) = g^{-1}(u^{(1)}; \mathbf{pa}^*), \quad (64)$$

$$\implies \forall \mathbf{pa} : g^{-1}(u^{(1)}; \mathbf{pa}) = g^{-1}(u^{(1)}). \quad (65)$$

This contradicts the assumption that g depends on \mathbf{pa} , completing the proof. \square

Lemma B.9 (Existence of the Prior Transition Map). *Let $P_U^{(1)}, P_U^{(2)}$ be probability measures on \mathbb{R}^d with finite second moments, both absolutely continuous w.r.t. the Lebesgue measure. Then, there exists a transport map $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ that is unique $P_U^{(1)}$ -a.e., monotone, and a.e. bijective:*

$$\inf_{g_\# P_U^{(1)} = P_U^{(2)}} \int_{\mathbb{R}^d} c(u, g(u)) dP_U^{(1)}(u), \quad c(u, g(u)) := \|u - g(u)\|^2. \quad (66)$$

Proof. If $P_U^{(1)}, P_U^{(2)}$ have finite second moments and $P_U^{(1)} \ll \mathcal{L}^d$, by [Brenier \(1991\)](#) (Theorem B.3), there exists a unique $P_U^{(1)}$ -a.e., monotone, map $g = \nabla \phi$. Since $P_U^{(2)} \ll \mathcal{L}^d$, the map is a.e. bijective. Under standard [Caffarelli \(1992\)](#) regularity conditions (bounded densities and convex domains), we can upgrade a.e. invertibility to a homeomorphism/diffeomorphism between supports.

To fix a common reference, we invoke the higher-dimensional Probability Integral Transform (PIT), known as the Rosenblatt transform. It states that any absolutely continuous probability measure P_U on \mathbb{R}^d (with $d > 1$) whose density is strictly positive almost everywhere can be represented as the push-forward of the uniform $\mathcal{U}([0, 1]^d)$ via a measurable and almost everywhere invertible map.

More concretely, first consider the one-dimensional case ($d = 1$). For any random variable $X \in \mathbb{R}$, with cumulative distribution function (CDF) $F_X : \mathbb{R} \rightarrow [0, 1]$, the PIT states that:

$$U = F_X(X), \quad X = F_X^{-1}(U), \quad (67)$$

where U is uniformly distributed on $[0, 1]$. To extend this to higher dimensions ($d > 1$), we use a recursive component-wise construction known as the Rosenblatt transform, explained below.

Let $U \sim \mathcal{U}([0, 1]^d)$, and define a map $T : [0, 1]^d \rightarrow \mathbb{R}^d$ component-wise in a triangular manner. Further, write (u_1, \dots, u_d) for coordinates in $[0, 1]^d$, and let $X = (X_1, \dots, X_d)$ be a random vector distributed according to P_U . Now set $T_1(u_1) = F_{X_1}^{-1}(u_1)$.

For each $k = 2, \dots, d$, let $F_{X_k|X_1, \dots, X_{k-1}}$ be the conditional CDF of X_k given (X_1, \dots, X_{k-1}) , then define:

$$T_k(u_1, \dots, u_k) = [F_{X_k|X_1, \dots, X_{k-1}}(\cdot \mid T_1(u_1), \dots, T_{k-1}(u_1, \dots, u_{k-1}))]^{-1}(u_k). \quad (68)$$

Under mild continuity assumptions on each conditional CDF (which follow from strict positivity of the density of P_U), this construction is well-defined for almost every $(u_1, \dots, u_d) \in [0, 1]^d$.

The resulting map

$$T(u_1, \dots, u_d) = (T_1(u_1), T_2(u_1, u_2), \dots, T_d(u_1, \dots, u_d)) \quad (69)$$

is measurable and invertible almost everywhere. Since $U \sim \mathcal{U}([0, 1]^d)$, one can verify that $T(U)$ has law P_U , or equivalently that $T_\# \mathcal{U}([0, 1]^d) = P_U$. Finally, for any two distinct absolutely continuous probability measures $P_U^{(1)}$ and $P_U^{(2)}$ on \mathbb{R}^d , one may similarly construct maps $T^{(1)}, T^{(2)} : [0, 1]^d \rightarrow \mathbb{R}^d$ such that:

$$T_\#^{(1)} \mathcal{U}([0, 1]^d) = P_U^{(1)}, \quad T_\#^{(2)} \mathcal{U}([0, 1]^d) = P_U^{(2)}. \quad (70)$$

With an almost-everywhere inverse $(T^{(2)})^{-1}$ (i.e. $(T^{(2)})^{-1} \circ T^{(2)} = \text{id}$ a.e.), it follows that the transport map

$$g = (T^{(2)})^{-1} \circ T^{(1)}, \quad \text{satisfies} \quad g_\# P_U^{(1)} = P_U^{(2)}. \quad (71)$$

Thus, both measures $P_U^{(1)}$ and $P_U^{(2)}$ can be considered push-forwards of the same uniform measure on $[0, 1]^d$, via different invertible maps, showing that any particular choice of P_U is essentially arbitrary. Without loss of generality, we may therefore fix the exogenous prior as $P_U = \mathcal{U}([0, 1]^d)$, and interpret all subsequent distributions as push-forwards thereof, concluding the proof. \square

Remark B.10. We use the Rosenblatt transform only to fix a common reference for the result; any absolutely continuous law can be written as $T_\# \mathcal{U}([0, 1]^d)$ for a measurable, a.e.-invertible triangular T . This does not imply that T is the quadratic-cost OT (Brenier) map. Note that the Rosenblatt transform depends on the chosen coordinate order, meaning that different permutations yield different triangular maps (each still pushes $\mathcal{U}([0, 1]^d)$ to the same target law). This indicates that rank-preserving continuous-time flows without OT are realisable by, for example, assuming a coordinate order and parameterising the flow with a component-wise autoregressive model. By contrast, the Brenier OT map is order-invariant and is determined solely by the two measures and the quadratic cost.

Theorem B.11 (Counterfactual Identifiability in Markovian SCMs). *Let $\dim(X) = \dim(U) = d > 1$, and $U \perp\!\!\!\perp \mathbf{PA}$. Assume P_U is the continuous uniform measure on $[0, 1]^d$. Let $T : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ be the time-1 dynamic OT map described in Lemma 4.6, which pushes P_U forward to $P_{X|\mathbf{PA}}^c$. Then, the induced time-1 counterfactual dynamic OT map $T^* : \mathbb{R}^{2k} \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is strictly monotone in x :*

$$\langle T^*(\mathbf{pa}^*, \mathbf{pa}, x_1) - T^*(\mathbf{pa}^*, \mathbf{pa}, x_2), x_1 - x_2 \rangle > 0, \quad \forall x_1, x_2 \in \mathbb{R}^d, \mathbf{pa}, \mathbf{pa}^* \in \mathbb{R}^k. \quad (72)$$

Proof. We present a generalised notion of the monotonicity requirement for multi-dimensional causal mechanisms ($d > 1$), and show counterfactual identifiability can be achieved using the dynamic OT map described in Lemma B.5.

Let $\dim(X) = \dim(U) = d \geq 1$, and $U \perp\!\!\!\perp \mathbf{PA}$. Let P_U be a uniform measure $\mathcal{U}([0, 1]^d)$, and assume $P_{X|\mathbf{PA}}^c$ is absolutely continuous w.r.t. the Lebesgue measure. Let $T : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ be the time-1 map of a dynamic OT flow $\{T_t : t \in [0, 1]\}$ described in Lemma B.5, that is:

$$dT_t(u; \mathbf{pa}) = v_t(T_t(u; \mathbf{pa})) dt, \quad T(\cdot; \mathbf{PA})_{\#} P_U = P_{X|\mathbf{PA}}^c. \quad (73)$$

By Theorem B.3, there exists an optimal map that minimises quadratic transport cost:

$$T(u; \mathbf{pa}) = \nabla_u \phi(u; \mathbf{pa}), \quad (74)$$

where $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is a convex function. Importantly, T is well-defined P_U -almost everywhere and is uniquely determined by P_U and $P_{X|\mathbf{PA}}^c$. This gradient map generalises the notion of one-dimensional monotonicity, as it is ‘vector monotonic’ in the sense that:

$$\forall u_1, u_2, \mathbf{pa} : \langle T(u_1; \mathbf{pa}) - T(u_2; \mathbf{pa}), u_1 - u_2 \rangle \geq 0. \quad (75)$$

Since $P_{X|\mathbf{PA}}^c$ is assumed to be absolutely continuous, under Caffarelli (1992) regularity conditions (Lemma B.5), the map T is also bijective. Then, it follows that:

$$T^{-1}(T(u; \mathbf{pa}); \mathbf{pa}) = u, \quad u \in [0, 1]^d, \quad (76)$$

where the respective maps are realised by solving the associated ODE backwards in time for abduction:

$$u_0 = T^{-1}(x; \mathbf{pa}) = x - \int_0^1 v_t(T_t(u; \mathbf{pa})) dt, \quad (77)$$

and forwards in time for prediction of x^* , for instance, under a chosen intervention \mathbf{pa}^* :

$$x^* = T(u_0; \mathbf{pa}^*) = u_0 + \int_0^1 v_t(T_t(u; \mathbf{pa}^*)) dt. \quad (78)$$

By the Picard-Lindelöf theorem, both initial value problems admit unique solutions if the associated velocity field is Lipschitz continuous, which is readily satisfiable in practice (Chen et al., 2018).

Under Caffarelli (1992)’s standard regularity and smoothness conditions (Lemma B.5), the time-1 dynamic transport map T arises as the gradient of a strictly convex potential $T(u; \mathbf{pa}) = \nabla_u \phi(u; \mathbf{pa})$, and its Jacobian $\partial_u T(u; \mathbf{pa}) = \nabla_u^2 \phi(u; \mathbf{pa})$ is symmetric positive-definite (SPD).

The Jacobian of the counterfactual transport map

$$T^*(\mathbf{pa}^*, \mathbf{pa}, x) := T(T^{-1}(x; \mathbf{pa}); \mathbf{pa}^*) \quad (79)$$

is thus given by the product of two SPD factors:

$$\partial_x T^*(\mathbf{pa}^*, \mathbf{pa}, x) = \partial_u T(u; \mathbf{pa}^*)|_{u=T^{-1}(x; \mathbf{pa})} \cdot \partial_x T^{-1}(x; \mathbf{pa}). \quad (80)$$

For two distinct points $x_1, x_2 \in \Omega$, define the straight line segment

$$\forall t \in [0, 1], \quad x_t = (1 - t)x_2 + tx_1, \quad dx_t = (x_1 - x_2) dt =: z dt, \quad (81)$$

where $z \neq 0$. Applying the fundamental theorem of calculus, then the chain rule, we get:

$$T^*(\mathbf{pa}^*, \mathbf{pa}, x_1) - T^*(\mathbf{pa}^*, \mathbf{pa}, x_2) = \int_0^1 \frac{d}{dt} [T^*(\mathbf{pa}^*, \mathbf{pa}, x_t)] dt \quad (82)$$

$$= \int_0^1 \partial_{x_t} T^*(\mathbf{pa}^*, \mathbf{pa}, x_t) z dt. \quad (83)$$

Taking the inner product with z in the form $\langle v, w \rangle_x := v^\top \partial_x T^{-1}(x; \mathbf{pa}) w$ yields:

$$\langle T^*(\mathbf{pa}^*, \mathbf{pa}, x_1) - T^*(\mathbf{pa}^*, \mathbf{pa}, x_2), z \rangle = \int_0^1 \langle \partial_{x_t} T^* z, z \rangle_{x_t} dt, \quad (84)$$

$$= \int_0^1 z^\top (\partial_{x_t} T^{-1} \partial_u T \partial_{x_t} T^{-1}) z dt \quad (85)$$

$$= \int_0^1 (\partial_{x_t} T^{-1} z)^\top \partial_u T (\partial_{x_t} T^{-1} z) dt > 0, \quad (86)$$

because $\partial_u T$ is SPD and $\partial_{x_t} T^{-1} z \neq 0$ for each $t \in [0, 1]$ (since $\partial_x T^{-1}$ is SPD). Hence the integral is strictly positive and the counterfactual transport map T^* is strictly monotone in x , as required. \square

Remark B.12. An intuition for the above result is provided next. Since the time-1 transport map $T : [0, 1]^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ exists, is uniquely optimal, and (Brenier-)monotone, it generalises the notion of a scalar quantile function to vector-valued outcomes (Carlier et al., 2016). Further, since the inverse map $T^{-1} : \mathbb{R}^d \times \mathbb{R}^k \rightarrow [0, 1]^d$ also exists and shares these properties, it serves as a vector rank function, and can be used to uniquely recover u analogously to the $d = 1$ case in Appendix A.

The proof above establishes that T^* is strictly monotone in x , and this represents the multivariate (Brenier/OT) notion of monotonicity and is sufficient for rank preservation (Carlier et al., 2016). If one additionally wants coordinate-wise (product-order) monotonicity, it holds under extra structure. For example, when $\nabla_u^2 \phi(u; \mathbf{pa})$ has nonnegative off-diagonal entries, so $T(\cdot; \mathbf{pa})$ is coordinate-wise increasing. If, for both \mathbf{pa} and \mathbf{pa}^* , the map $T(\cdot; \mathbf{pa})$ is an order-isomorphism for the product order (hence $T^{-1}(\cdot; \mathbf{pa})$ is also coordinate-wise increasing), then the composition of the two $T^*(\mathbf{pa}^*, \mathbf{pa}, x) = T(T^{-1}(x; \mathbf{pa}); \mathbf{pa}^*)$ is coordinate-wise increasing in x .

Importantly, for quadratic cost with an absolutely continuous source, the OT map is unique a.e. and does not depend on a coordinate ordering; its monotonicity is in the Brenier/OT sense (i.e., it is the gradient of a convex potential). This sidesteps the non-uniqueness inherent in coordinate-wise (product) orders, or Rosenblatt transforms, which depend on an arbitrary permutation of coordinates.

B.3 Non-Markovian Counterfactual Identifiability

In the following, we extend our theoretical analysis to non-Markovian settings. We provide counterfactual identifiability results from observational data under the following standard criteria: (i) Forward Criterion (FC); (ii) Instrumental Variable(s) (IV); (iii) Backdoor Criterion (BC). The proofs for BC ($d \geq 1$) and IV ($d = 1$) criteria are provided by Nasr-Esfahany et al. (2023). We provide a proof for FC ($d \geq 1$) and extend Nasr-Esfahany et al. (2023)’s IV result to $d > 1$.

B.3.1 Frontdoor Criterion Setting

A setting in which counterfactual identifiability under an unobserved confounding U on (A, X) is possible (under stated assumptions) is through the frontdoor criterion, using a mediator variable Z (Pearl, 2009). For FC to apply, the following must hold: (i) Z intercepts all directed paths from A to X ; (ii) no backdoor path from A to Z exists; (iii) A blocks all backdoor paths from Z to X . The \mathcal{L}_3 -equivalence result presented below also applies to the multi-dimensional ($d > 1$) setting.

Lemma B.13 (FC \mathcal{L}_3 -Equivalence). *Consider two FC models T and \hat{T} with the same observational joint law (A, Z, X) , where $A \rightarrow Z \rightarrow X$ and the pair (A, X) is confounded by U , and \hat{U} , respectively. The bijective structural assignments are*

$$T(u; a) = (T_Z(a), T_X(u; T_Z(a))), \quad \text{and} \quad \hat{T}(\hat{u}; a) = (\hat{T}_Z(a), \hat{T}_X(\hat{u}; \hat{T}_Z(a))). \quad (87)$$

The maps T and \hat{T} are counterfactually equivalent ($\sim_{\mathcal{L}_3}$) if

1. (Frontdoor Criterion):

$$U \perp\!\!\!\perp Z \mid A \text{ and } \hat{U} \perp\!\!\!\perp Z \mid A, \quad X \perp\!\!\!\perp A \mid \{U, Z\} \text{ and } X \perp\!\!\!\perp A \mid \{\hat{U}, Z\}. \quad (88)$$

2. (Regularity) For every z , the derivatives $\nabla_z |\det \mathbf{J}_{T_X^{-1}}(\cdot; z)|$ and $\nabla_z |\det \mathbf{J}_{\hat{T}_X}(\cdot; z)|$ exist.

3. (Variability) For every u , there exist $d + 1$ points a_1, \dots, a_{d+1} such that

$$M(u; a_1, \dots, a_{d+1}) = \begin{bmatrix} \rho_{U|A}(u | a_1) & \nabla_u \rho_{U|A}(u | a_1) \\ \vdots & \vdots \\ \rho_{U|A}(u | a_{d+1}) & \nabla_u \rho_{U|A}(u | a_{d+1}) \end{bmatrix} \quad (89)$$

is full rank, i.e. $\det M \neq 0$.

Proof. If $Z | A$ is *deterministic* in both models, then matching the joint law of (A, Z) forces:

$$Z = T_Z(A), \quad Z = \hat{T}_Z(A) \Rightarrow T_Z(A) = \hat{T}_Z(A) \text{ a.s.} \quad (90)$$

If A is discrete with $P(A = a) > 0$, or has density strictly positive on an open \mathcal{A} and T_Z, \hat{T}_Z are continuous on \mathcal{A} , then $T_Z(a) = \hat{T}_Z(a)$ for all a . If $Z | A$ is instead *stochastic*, with bijective maps w.r.t. noise variables W, \hat{W} , counterfactual equivalence (Definition B.7) states that:

$$T_Z \sim_{\mathcal{L}_3} \hat{T}_Z \iff \exists h, \forall w, a : T_Z(w; a) = \hat{T}_Z(h^{-1}(w); a), \quad (91)$$

where h is a bijection. By Lemma B.9, h exists, therefore, $T_Z \sim_{\mathcal{L}_3} \hat{T}_Z$ holds.

Next, we prove $T_X \sim_{\mathcal{L}_3} \hat{T}_X$ under similar conditions to [Nasr-Esfahany et al. \(2023\)](#)'s BC result. First, define a link function of both transport maps on the exogenous noise channel:

$$g(\cdot; z) := T_X^{-1}(\cdot; z) \circ \hat{T}_X(\cdot; z), \quad u = g(\hat{u}; z), \quad (92)$$

which, by the change-of-variables formula:

$$\rho_{\hat{U}|A,Z}(\hat{u} | a, z) = \rho_{U|A,Z}(g(\hat{u}; z) | a, z) |\det \mathbf{J}_g(\hat{u}; z)|. \quad (93)$$

Under FC (condition 1), we have that $U \perp\!\!\!\perp Z | A$ and $\hat{U} \perp\!\!\!\perp Z | A$, respectively:

$$\rho_{\hat{U}|A}(\hat{u} | a) = \rho_{U|A}(g(\hat{u}; z) | a) |\det \mathbf{J}_g(\hat{u}; z)|. \quad (94)$$

Given *regularity* (condition 2), differentiate both sides of Eq. (94) w.r.t. z_i :

$$0 = (\nabla_u \rho_{U|A}(u | a))^\top \frac{\partial g(\hat{u}; z)}{\partial z_i} |\det \mathbf{J}_g(\hat{u}; z)| + \rho_{U|A}(u | a) \frac{\partial}{\partial z_i} |\det \mathbf{J}_g(\hat{u}; z)|, \quad (95)$$

and write in block form:

$$\begin{bmatrix} \rho_{U|A}(u | a) & (\nabla_u \rho_{U|A}(u | a))^\top \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial z_i} |\det \mathbf{J}_g(\hat{u}; z)| \\ \frac{\partial g(\hat{u}; z)}{\partial z_i} |\det \mathbf{J}_g(\hat{u}; z)| \end{bmatrix} = 0. \quad (96)$$

Stacking the respective equations for a_1, a_2, \dots, a_{d+1} then yields:

$$M(u; a_1, \dots, a_{d+1}) \Big|_{u=g(\hat{u}; z)} \begin{bmatrix} \frac{\partial}{\partial z_i} |\det \mathbf{J}_g(\hat{u}; z)| \\ \frac{\partial g(\hat{u}; z)}{\partial z_i} |\det \mathbf{J}_g(\hat{u}; z)| \end{bmatrix} = \mathbf{0}, \quad (97)$$

because M must be full rank by *variability* (condition 3) we have that, for all indices $i \in \{1, \dots, d\}$, $\partial g(\hat{u}; z)/\partial z_i = 0$ and $\partial/\partial z_i |\det \mathbf{J}_g(\hat{u}; z)| = 0$. Therefore, $g(\hat{u}; z)$ does not depend on z , and can be written as $g(\hat{u}; z) = g(\hat{u})$, proving T_X and \hat{T}_X differ only by a bijection of the exogenous noise.

Finally, combining the above $\sim_{\mathcal{L}_3}$ -equivalence results, there exist bijections g and h such that:

$$\forall u, w, a : T_X(u; T_Z(w; a)) = \hat{T}_X(g^{-1}(u); \hat{T}_Z(h^{-1}(w); a)), \quad (98)$$

and for the deterministic $Z | A$ case we have

$$\forall u, a : T_X(u; T_Z(a)) = \hat{T}_X(g^{-1}(u); \hat{T}_Z(a)), \quad (99)$$

hence T and \hat{T} produce the same counterfactuals, concluding the proof. \square

B.3.2 Instrumental Variable Setting

Even when an unobserved confounder is present, counterfactual identifiability can still be recovered from purely observational (\mathcal{L}_1) data, provided we can locate suitable instrumental variables. Here, an instrumental variable is any variable (or set of variables) that is: (i) statistically independent of the latent noise U ; and (ii) influences the outcome X exclusively through its effect on its parents \mathbf{PA} .

Lemma B.14 (IV \mathcal{L}_3 -Equivalence (Nasr-Esfahany et al., 2023)). *Let the instrument take values in the finite set $\mathbf{I} = \{i_1, \dots, i_n\}$ and the endogenous parents of X take values in $\mathbf{PA} = \{\mathbf{pa}_1, \dots, \mathbf{pa}_n\}$. Two bijective models T and \hat{T} yield the same counterfactuals (i.e. are equivalent in the sense that they coincide up to a reparameterisation of the latent noise), whenever the following conditions hold:*

1. (Instrumental Variable) $\mathbf{I} \perp\!\!\!\perp U$ and $\mathbf{I} \perp\!\!\!\perp \hat{U}$.
2. For all $\mathbf{pa} \in \mathbf{PA}$, the maps $T^{-1}(\cdot; \mathbf{pa})$ and $\hat{T}(\cdot; \mathbf{pa})$ are strictly monotone (either strictly increasing or strictly decreasing) and twice continuously differentiable.
3. The density $\rho_{\hat{U}}(\cdot)$ is continuously differentiable.
4. For every i, \mathbf{pa} the joint density $\rho_{\mathcal{D}}(i, \mathbf{pa}, \cdot)$ is continuously differentiable in its latent coordinate.
5. (Positivity) $\forall u, \hat{u}$ and every $\mathbf{pa} \in \mathbf{PA}$, $\rho_{U, \mathbf{PA}}(u, \mathbf{pa}) > 0$ and $\rho_{\hat{U}, \mathbf{PA}}(\hat{u}, \mathbf{pa}) > 0$.
6. (Variability) For every fixed u , the matrix

$$M_{\mathcal{D}}(u, \mathbf{I}) := \begin{bmatrix} \rho_{\mathcal{D}}(\mathbf{pa}_1 | u, i_1) & \cdots & \rho_{\mathcal{D}}(\mathbf{pa}_n | u, i_1) \\ \vdots & & \vdots \\ \rho_{\mathcal{D}}(\mathbf{pa}_1 | u, i_n) & \cdots & \rho_{\mathcal{D}}(\mathbf{pa}_n | u, i_n) \end{bmatrix} \quad (100)$$

satisfies $|\det M_{\mathcal{D}}(u, \mathbf{I})| \geq c$, for some constant $c > 0$, that does not depend on u .

Proof. The proof (for $d = 1$) is given by Nasr-Esfahany et al. (2023). Since T and \hat{T} are assumed to be strictly monotone only in the scalar setting, counterfactual identifiability is established for $d = 1$ only. Theorem B.11 shows (drawing on Brenier (1991)'s Theorem) that if there exists a convex function $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$, where $T(u; \mathbf{pa}, i) = \nabla_u \phi(u; \mathbf{pa}, i)$, then T, \hat{T} are strictly monotone (rank-preserving) in u in the multi-dimensional case. Therefore, by Theorem B.11, we now generalise the above IV counterfactual identifiability result for $d > 1$, concluding the proof. \square

B.3.3 Backdoor Criterion Setting

Another scenario in which counterfactual identification from observational (\mathcal{L}_1) data is achievable (under stated assumptions), despite the presence of confounding, is when there exists a set of variables \mathbf{Z} that satisfies the backdoor criterion (BC) w.r.t. the pair (\mathbf{PA}, X) , where \mathbf{PA} are X 's parents. That is, \mathbf{Z} blocks all backdoor paths between \mathbf{PA} and X , where each such path includes an arrow pointing into \mathbf{PA} . The role of \mathbf{Z} is to account for all the spurious associations between \mathbf{PA} and U .

Lemma B.15 (BC \mathcal{L}_3 -Equivalence (Nasr-Esfahany et al., 2023)). *Let T and \hat{T} be two distinct bijective models that induce identical joint distributions over the endogenous variables $\{\mathbf{PA}, X\}$. Then T and \hat{T} are counterfactually equivalent ($\sim_{\mathcal{L}_3}$) if the following conditions hold:*

1. (Backdoor Criterion) $U \perp\!\!\!\perp \mathbf{PA} \mid \mathbf{Z}$ and $\hat{U} \perp\!\!\!\perp \mathbf{PA} \mid \mathbf{Z}$.
2. For every \mathbf{pa} , the derivatives $\nabla_{\mathbf{pa}} |\det \mathbf{J}_{T^{-1}}(\cdot; \mathbf{pa})|$ and $\nabla_{\mathbf{pa}} |\det \mathbf{J}_{\hat{T}}(\cdot; \mathbf{pa})|$ both exist.
3. (Variability) For every u , there exist instances $\mathbf{z}_1, \dots, \mathbf{z}_{d+1}$ such that

$$|\det M(u, \mathbf{z}_1, \dots, \mathbf{z}_{d+1})| > 0, \quad (101)$$

where

$$M(u, \mathbf{z}_1, \dots, \mathbf{z}_{d+1}) := \begin{bmatrix} \rho_{U|\mathbf{Z}}(u | \mathbf{z}_1) & \nabla_u \rho_{U|\mathbf{Z}}(u | \mathbf{z}_1) \\ \vdots & \vdots \\ \rho_{U|\mathbf{Z}}(u | \mathbf{z}_{d+1}) & \nabla_u \rho_{U|\mathbf{Z}}(u | \mathbf{z}_{d+1}) \end{bmatrix}. \quad (102)$$

Remark B.16. The proof for Lemma B.15 is provided by [Nasr-Esfahany et al. \(2023\)](#) and already applies to the multi-dimensional setting ($d \geq 1$), showing that bijectivity of T, \hat{T} is sufficient for counterfactual equivalence when the BC is satisfied and the *variability* assumption holds.

Intuition. Because BC makes the change-of-variables identity independent of the parents, differentiating w.r.t. \mathbf{PA} and stacking across $d + 1$ values of \mathbf{Z} yields a full-rank (variability) linear system whose only solution is zero; hence the link $g(\cdot; \mathbf{pa}) := T^{-1}(\cdot; \mathbf{pa}) \circ \hat{T}(\cdot; \mathbf{pa})$ cannot depend on \mathbf{pa} , so $g(u; \mathbf{pa}) = g(u)$ and T and \hat{T} are counterfactually equivalent ($\sim_{\mathcal{L}_3}$) in the sense that they produce the same counterfactuals.

B.4 Assumptions: Summary & Plausibility

We open with [Pearl and Bareinboim \(2022\)](#):

“Assumptions are self-destructive in their honesty. The more explicit the assumption, the more criticism it invites. [...] Researchers therefore prefer to declare ‘threats’ in public and make assumptions in private.”

Our work counters this practice: we intend to make our assumptions and constraints explicit so they can be better understood, challenged, and ultimately relaxed in light of new evidence or insight.

Markovian SCMs. The Markovianity assumption is standard in causality literature and is also the default assumption in many causal representation learning frameworks ([Pearl, 2009](#); [Hyvärinen et al., 2024](#)). The assumption that there is no unobserved confounding is strong in most real-world scenarios. However, it is widely known that Markovianity alone is insufficient for counterfactual identifiability ([Xia et al., 2023](#); [Bareinboim et al., 2022](#); [Nasr-Esfahany and Kiciman, 2023](#)). Thus, further assumptions and/or restrictions on the functional class are necessary, such as monotonicity in the $d = 1$ case ([Nasr-Esfahany et al., 2023](#)). This is the gap our work fills, particularly for $d > 1$.

OT Regularity Assumptions. We assume that $\dim(X) = \dim(U) \geq 1$ as is commonplace in flow-based generative models. This is straightforward to enforce in practice by embedding lower-dimensional latents using dummy coordinates. For our strictest results, we assume quadratic cost and that the source P_U and target $P_{X|\mathbf{PA}}^c$ are absolutely continuous w.r.t. Lebesgue measure, with densities ρ_U and $\rho_{X|\mathbf{PA}}^c$ bounded above and below by positive constants on bounded convex supports.

These are standard assumptions in the literature, particularly in OT, which ensure that the measures P_U and $P_{X|\mathbf{PA}}$ admit well-behaved densities, guaranteeing the existence and uniqueness of an OT map ([Brenier, 1991](#); [Caffarelli, 1992](#)). However, they may not always hold, and are often stronger than strictly necessary in practice. In practice, when working with empirical distributions, it is often advantageous to approximate them by smoothing with small continuous uniform or Gaussian noise so that the resulting distribution admits a density. Real-world data are often normalised and then modelled with smooth densities on (possibly truncated) compact supports, making these assumptions a common modelling choice. Optionally, if the densities are $C^{1,\alpha}$ and satisfy standard two-sided bounds on a convex domain, this yields improved regularity, e.g. an interior $C^{2,\alpha}$ Brenier potential.

We require that there exist a velocity field v_t solving $\partial_t \rho_t + \nabla \cdot (\rho_t v_t) = 0$ where $\rho_0 = P_U$, and $\rho_1 = P_{X|\mathbf{PA}}$, with v_t Lipschitz in x and in $L^2([0, 1] \times \Omega)$ ([Benamou and Brenier, 2000](#)). Neural ODE parameterisations with spectral normalisation or weight clipping satisfy global Lipschitz bounds, and so do classical kernels with bounded derivatives ([Chen et al., 2018](#)). Uniqueness of the associated ODE’s solution is satisfied by the Lipschitz condition under Picard-Lindelöf’s theorem. We note that in practice the time-dependent density ρ_t is often fixed by choice of interpolant (e.g. linear ([McCann, 1997](#))). By further optimising the interpolant, it is possible to solve Eq. (47) under mild assumptions on the Benamou-Brenier density ([Albergo and Vanden-Eijnden, 2023](#)).

For our most general result, which generalises scalar quantiles/ranks to $d > 1$, we assume that the prior P_U be a uniform measure, e.g. $\mathcal{U}([0, 1]^d)$. This was chosen for PIT-type reasons. However, a uniform on a d -dimensional cube is not strictly necessary for rank-preservation; other choices like the standard normal or the uniform on a ball are available provided regularity conditions for OT are met ([Carlier et al., 2016](#)). In any case, weaker counterfactual equivalence relations may be obtained by relaxing the conditions under which point-wise identification holds. Such relaxations are

often admissible in practice without completely sacrificing the utility of the method; this is in the spirit of many existing identifiability results (Khemakhem et al., 2021; Nasr-Esfahany et al., 2023; Hyvärinen et al., 2024). Finally, the experiments we ran to validate our theory rely on Batch-OT to recover the global OT map in practice, which Pooladian et al. (2023); Tong et al. (2024) provide convergence proofs for. However, Batch-OT is known to underperform for smaller batch sizes. Therefore, improving high-dimensional OT in terms of accuracy and efficiency remains key.

To summarise: with quadratic cost, (i) finite second moments ensure existence of an optimal coupling; (ii) if the source is absolutely continuous and $\dim(U) = \dim(X)$, the OT is (a.e.) unique and given by Brenier’s gradient map; (iii) two-sided density bounds on convex domains are standard, useful regularity assumptions, but are not always strictly necessary in practice; and (iv) a Lipschitz velocity field yields a unique, invertible Benamou-Brenier flow solving the continuity equation. When embedded in a Markovian SCM with independent noise, this flow provides a unique, rank-preserving transport representation of the causal mechanism, generalising the notion of scalar quantiles to $d > 1$, and under our stated assumptions, supporting identifiability of multi-dimensional counterfactuals from observational data.

C Energy Based Models: Curl-free Flows

Proposition C.1 (Curl-free Flows.). *Let $(\rho_t, v_t)_{t \in [0,1]}$ be an admissible curve for the dynamic OT map in Lemma B.5, with $v_t \in C^1(\Omega; \mathbb{R}^d)$ for each fixed $\mathbf{pa} \in \mathbb{R}^k$. Write the Helmholtz-Hodge decomposition $v_t = \nabla \psi_t + s_t$, where s_t is the curl component. Since $\operatorname{div}(\rho_t s_t) = 0$ by construction, the pair $(\rho_t, \nabla \psi_t)$ satisfies $\partial_t \rho_t + \operatorname{div}(\rho_t \nabla \psi_t) = 0$. Then, the Benamou-Brenier action \mathcal{A} is:*

$$\mathcal{A}(\rho, v) - \mathcal{A}(\rho, \nabla \psi) = \frac{1}{2} \int_0^1 \int_{\Omega} \|s_t(u; \mathbf{pa})\|^2 \rho_t(u; \mathbf{pa}) \, du \, dt \geq 0, \quad (103)$$

hence replacing v_t by its curl-free component $\nabla \psi$ never increases the dynamic OT cost.

Proof. For each $t \in [0, 1]$ the Helmholtz-Hodge decomposition provides a unique split

$$v_t = \nabla \psi_t + s_t, \quad \int_{\Omega} \rho_t(u, \mathbf{pa}) s_t(u, \mathbf{pa}) \cdot \nabla \eta(u, \mathbf{pa}) \, du = 0, \quad \forall \eta \in H_N^1(\Omega). \quad (104)$$

Orthogonality in $L^2(\rho_t)$ then implies

$$\|v_t\|^2 = \|\nabla \psi_t\|^2 + \|s_t\|^2 \quad (105)$$

hence

$$\mathcal{A}(\rho, v) = \mathcal{A}(\rho, \nabla \psi) + \frac{1}{2} \int_0^1 \int_{\Omega} \|s_t(u; \mathbf{pa})\|^2 \rho_t(u, \mathbf{pa}) \, du \, dt. \quad (106)$$

The integral above is non-negative and vanishes iff $s_t \equiv 0$, and therefore, $\mathcal{A}(\rho, v) \geq \mathcal{A}(\rho, \nabla \psi)$, with strict inequality for every non-conservative field. \square

Remark C.2. The unique minimiser of the dynamic OT problem is curl-free, as its time-1 map is the gradient of a convex potential. Thus, the above result suggests that an energy-based model (EBM) parameterisation of v_t (e.g. see De Sousa Ribeiro and Glocker (2025); Balcerak et al. (2025)) could prove to be a useful inductive bias for some problems, as it restricts the search space to curl-free vector fields. In practice, we operationalise this model by simply taking the sum of a neural network’s output as the energy, then taking gradients w.r.t the input x , yielding a curl-free vector field. We use this model class primarily for the constructed counterfactual ellipse scenarios, as it can be quite computationally intensive for high-dimensional images, given our resources. We consider scalable curl-free flow models fertile ground for future work.

D Counterfactual Soundness Axioms

When counterfactual ground truth is not available, we follow prior work (Monteiro et al., 2023; Ribeiro et al., 2023) and measure counterfactual *composition*, *effectiveness* and *reversibility*, which are axiomatic soundness properties of counterfactual functions that must hold true in all causal models (Halpern, 1998; Galles and Pearl, 1998; Pearl, 2009). We provide a gentle introduction next for completeness; for a more detailed treatment, please refer to Monteiro et al. (2023).

We point out that, while certainly useful diagnostic tools, the following metrics alone do not imply identification and should not be construed as evidence of causal validity.

1. The **composition** axiom states that intervening on a variable to have a value it would have had without the intervention should leave the system unchanged. In practice, composition is often measured using reconstruction error under a null-intervention on the parents:

$$\mathbb{E}_{(x, \mathbf{pa}) \sim P_{\text{data}}} \left[\|x - T(\mathbf{pa}, \mathbf{pa}, x)\|_1 \right]. \quad (107)$$

We report this metric to enable fair comparisons with prior work. For a more stringent measure of composition that tests path independence of intervention sequences, we suggest:

$$\mathbb{E}_{(x, \mathbf{pa}) \sim P_{\text{data}}} \left[\|T(\mathbf{pa}_2^*, \mathbf{pa}_1^*, T(\mathbf{pa}_1^*, \mathbf{pa}, x)) - T(\mathbf{pa}_2^*, \mathbf{pa}, x)\|_1 \right]. \quad (108)$$

Other *composition* tests could include comparing outcomes of one-by-one sequential interventions against equivalent simultaneous ones.

2. The **effectiveness** axiom states that intervening on a variable to have a specific value will cause the variable to take on that value. Effectiveness is typically the most challenging axiom to obtain an unbiased measure of in practice, as ideally one needs access to an *oracle* to tell us when/if our interventions are faithful. In practice, pseudo-oracles in the form of parent predictor models are used to determine whether interventions are successful:

$$\mathbb{E}_{(x, \mathbf{pa}) \sim P_{\text{data}}} \left[d(\mathcal{O}(T(\mathbf{pa}^*, \mathbf{pa}, x)), \mathbf{pa}^*) \right], \quad (109)$$

where $\mathcal{O}(\cdot)$ is a pseudo-oracle function that returns the value of the parent(s) given the observation. Here $d(\cdot)$ is an appropriate distance function dependent on the parent type. It is common practice to also apply the same metric to variables that are *not* descendants of the intervened-on variable, as invariance there serves as a diagnostic measure of *minimality*.

3. The **reversibility** axiom precludes multiple solutions due to feedback loops, and follows directly from composition in recursive systems such as DAGs. This can be intuitively understood as measuring cycle consistency w.r.t. interventions on the parents:

$$\mathbb{E}_{(x, \mathbf{pa}) \sim P_{\text{data}}} \left[\|x - T(\mathbf{pa}, \mathbf{pa}^*, T(\mathbf{pa}^*, \mathbf{pa}, x))\|_1 \right]. \quad (110)$$

Using less cluttered notation, we measure the extent to which the reversal x_r matches the observation x after $n \geq 1$ intervention cycles, where each cycle is given by:

$$x^* = T_{\mathbf{pa}^*} \circ T_{\mathbf{pa}}^{-1}(x), \quad x_r = T_{\mathbf{pa}} \circ T_{\mathbf{pa}^*}^{-1}(x^*). \quad (111)$$

Although often too costly in practice, recursive measurement of all the above metrics can yield more fine-grained insight into the faithfulness of interventions, biases of the associated counterfactual function, and incremental loss of identity w.r.t. the original observation (Monteiro et al., 2023).

E Counterfactual Ellipse: Extra Results

E.1 Dataset Details

As outlined in the main text, our ellipse dataset is built on [Nasr-Esfahany et al. \(2023\)](#)’s setup. We reiterate here for completeness. Let $U \in \mathbb{R}^2$ be the semi-major and -minor parameters of an ellipse, $PA \in (0, 2\pi)$ be an angle specifying a single point on the ellipse, and $X \in \mathbb{R}^2$ be its cartesian coordinates. The data-generating process is defined as follows:

$$\begin{aligned}
Z &:= \epsilon_z, & \epsilon_z &\sim \text{Uniform}(-0.5, 0.5) \\
PA &:= (1.44254843z + 0.59701923 + \epsilon_{pa}) \bmod (2\pi), & \epsilon_{pa} &\sim \mathcal{N}(0, 1) \\
U_0 &:= \exp(1.64985274z + 0.2656131) + \epsilon_{u_0} & \epsilon_{u_0} &\sim \text{Beta}(1, 1) \\
U_1 &:= U_0(1 + \epsilon_{u_1} \exp(1.61323358z - 0.18070237)) & \epsilon_{u_1} &\sim \text{Exponential}(1) \\
X_0 &:= U_0(2 + \sin(PA)) \\
X_1 &:= U_1(2 + \cos(PA)).
\end{aligned}$$

By construction, $U \perp\!\!\!\perp PA \mid Z$, and Z satisfies the backdoor criterion (BC) w.r.t. $PA \rightarrow X$. To induce a Markovian setting, we simply randomise PA , yielding marginal independence $U \perp\!\!\!\perp PA$.

For the front-door criterion (FC) to apply, we modify the data-generating process slightly to include a mediator variable M , such that $PA \rightarrow M \rightarrow X$:

$$\begin{aligned}
Z &:= \epsilon_z, & \epsilon_z &\sim \text{Uniform}(-0.5, 0.5) \\
PA &:= (1.44254843z + 0.59701923 + \epsilon_{pa}) \bmod (2\pi), & \epsilon_{pa} &\sim \mathcal{N}(0, 1) \\
M_0 &:= \beta \cdot (\sin(PA) + \epsilon_{m_0}) & \epsilon_{m_0} &\sim \mathcal{N}(0, 0.01) \\
M_1 &:= \beta \cdot (\cos(PA) + \epsilon_{m_1}) & \epsilon_{m_1} &\sim \mathcal{N}(0, 0.01) \\
U_0 &:= \exp(1.64985274z^2 + 0.2656131) + \epsilon_{u_0} & \epsilon_{u_0} &\sim \text{Beta}(1, 1) \\
U_1 &:= U_0(1 + \epsilon_{u_1} \exp(1.61323358z^2 - 0.18070237)) & \epsilon_{u_1} &\sim \text{Exponential}(1) \\
X_0 &:= U_0(2 + M_0) \\
X_1 &:= U_1(2 + M_1),
\end{aligned}$$

where $\beta = 1/\sqrt{m_0^2 + m_1^2}$ projects the noised points back onto the unit circle. Note the non-linear confounding $PA \leftarrow Z \rightarrow U \rightarrow X$. This dataset is only used for the front-door criterion experiments, where we intentionally omit the unobserved confounder Z when building the model.

In all cases, we split our datasets into 70/10/20% for training, validation and testing, respectively.

E.2 Architecture and Experimental Setup

For all our model variants, we used the following simple residual multi-layer perceptron (MLP) to parameterise the (conditional) vector field. We start with a linear projection layer which takes as input the concatenation of x , pa and a time index $t \in [0, 1]$. The input dimension is therefore $\dim(X) + \dim(PA) + 1 = 4$. We then have 3 of the following (residual) blocks:

$$x \mapsto \text{LINEAR} \circ \text{SiLU} \circ \text{LINEAR} \circ \text{LAYERNORM}(x). \quad (112)$$

The hidden dimension of these blocks is 256. The head of the MLP consists of a final layer norm and a linear projection to the output dimension $\dim(X) = 2$. The energy-based flow model variants were built by taking the mean of the MLP output, then taking gradients w.r.t. the input x .

We used PyTorch ([Paszke et al., 2019](#)) to train all our modes for 500k steps, under identical hyperparameter setups. These were determined with a light sweep over the learning rate and network width. We used the AdamW optimizer with a learning rate of 10^{-4} , weight decay of 10^{-4} , $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$, and batch size 256. The best model was selected based on the counterfactual error (μ_{APE}) on the validation set during training. Final performance is reported on the test set.

E.3 Qualitative Results

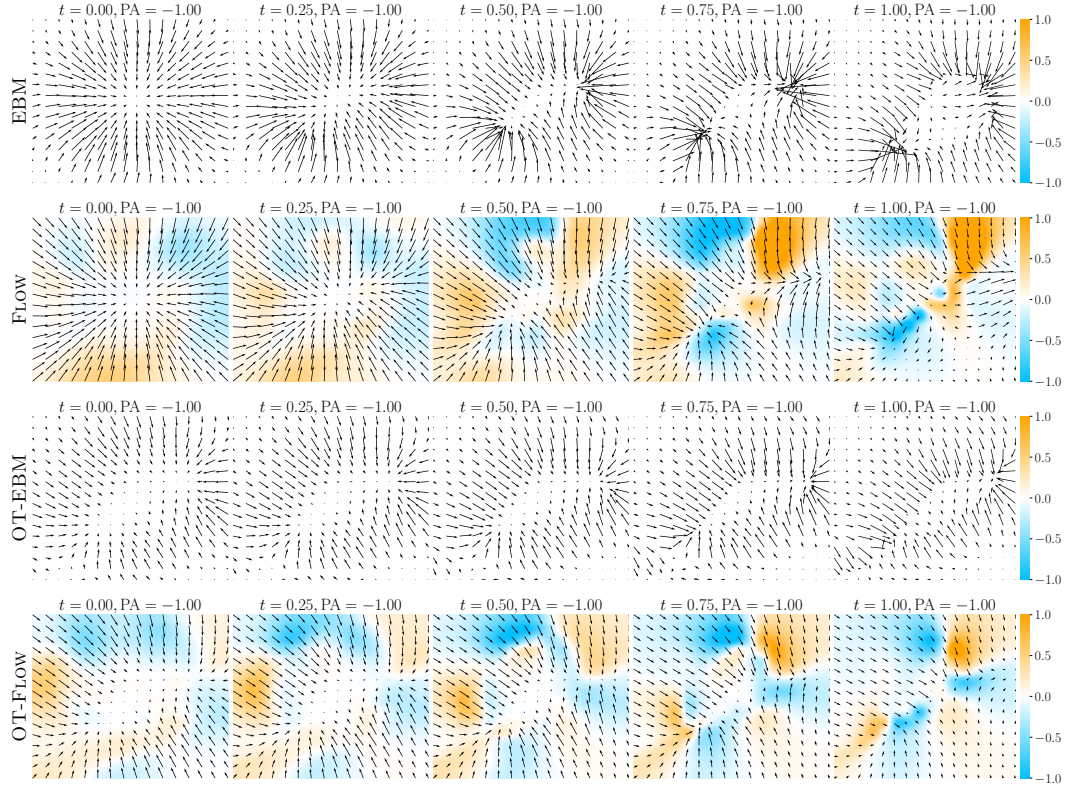


Figure 5: Visualising the curl ($\nabla \times v_t$) of the learned vector field of different models over time (scaled to $[-1, 1]$), for a given intervention on the parents $PA = -1$. We can see that the EBM variants are curl-free (irrotational) by design, as the vector field is given by the gradient of a scalar potential. We also see that the OT vector fields are smoother and OT-FLOW exhibits milder ‘rotations’ compared to FLOW. This is consistent with convergence to the Brenier map, which is itself curl-free.

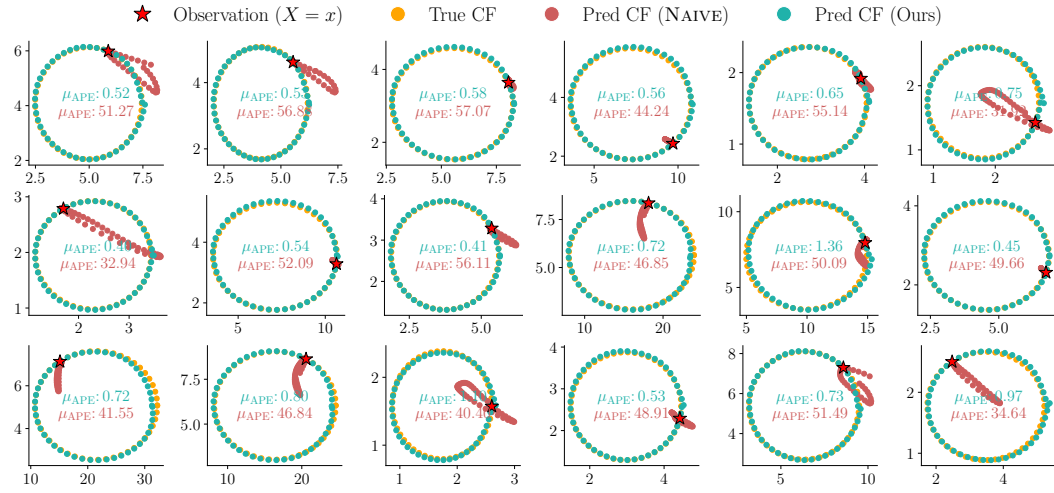


Figure 6: Inferred counterfactual (CF) ellipses using our OT coupling flow vs. the naive OT coupling approach explained in Section 5. Not cherry-picked.

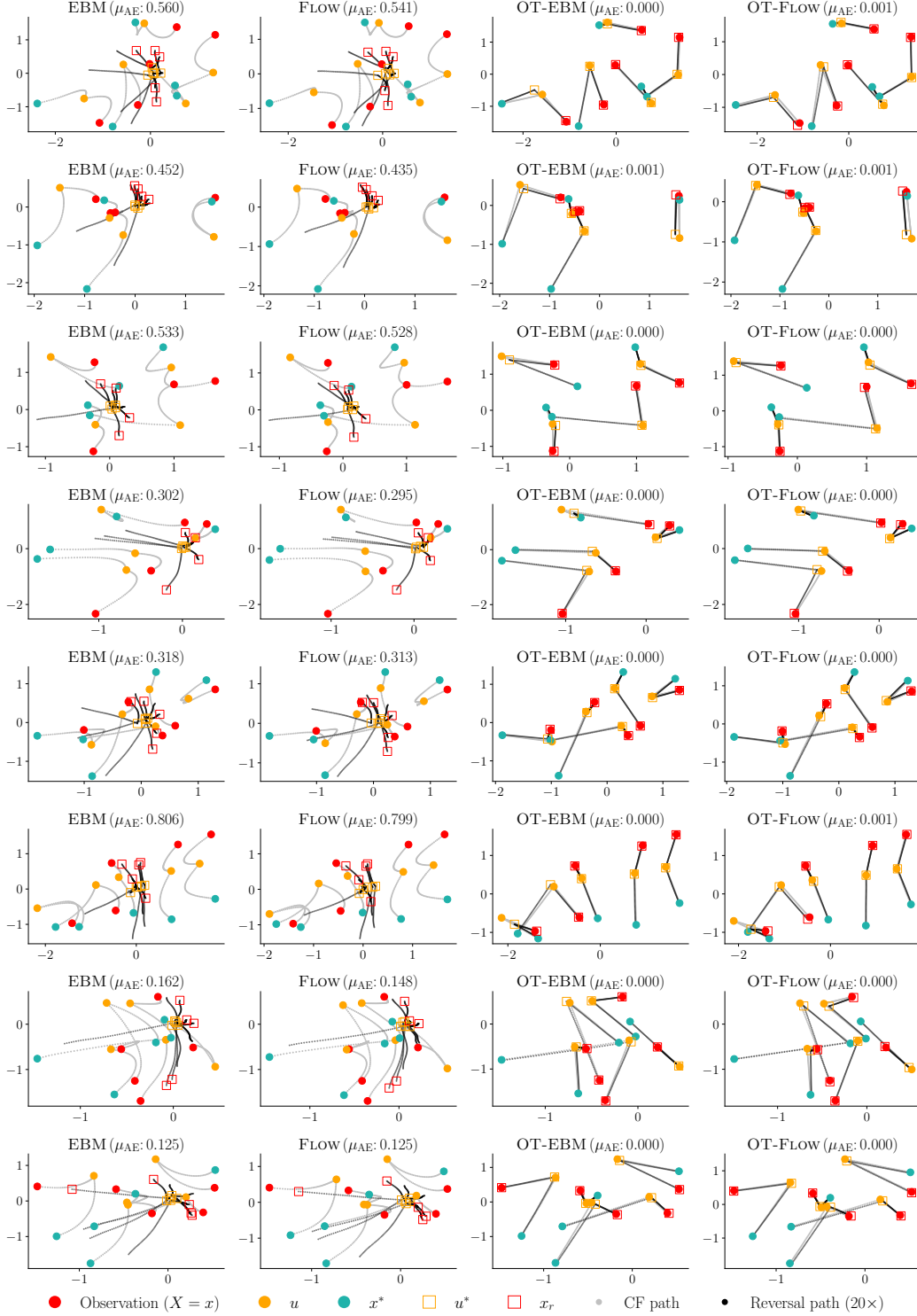


Figure 7: Extra counterfactual *reversibility* results (not cherry-picked). Our OT coupling flow exhibits near-perfect counterfactual reversibility, satisfying the soundness axiom (Monteiro et al., 2023). Conversely, standard flows (and diffusion models, which are equivalent (Gao et al., 2025)) exhibit comparatively poor reversibility upon repeated cycles, with u^* often collapsing to a single point for any initial observation x . In simple terms, straight paths are reversible; therefore, one ought to learn straight paths induced by OT in order to satisfy axiomatic reversibility of counterfactual functions.

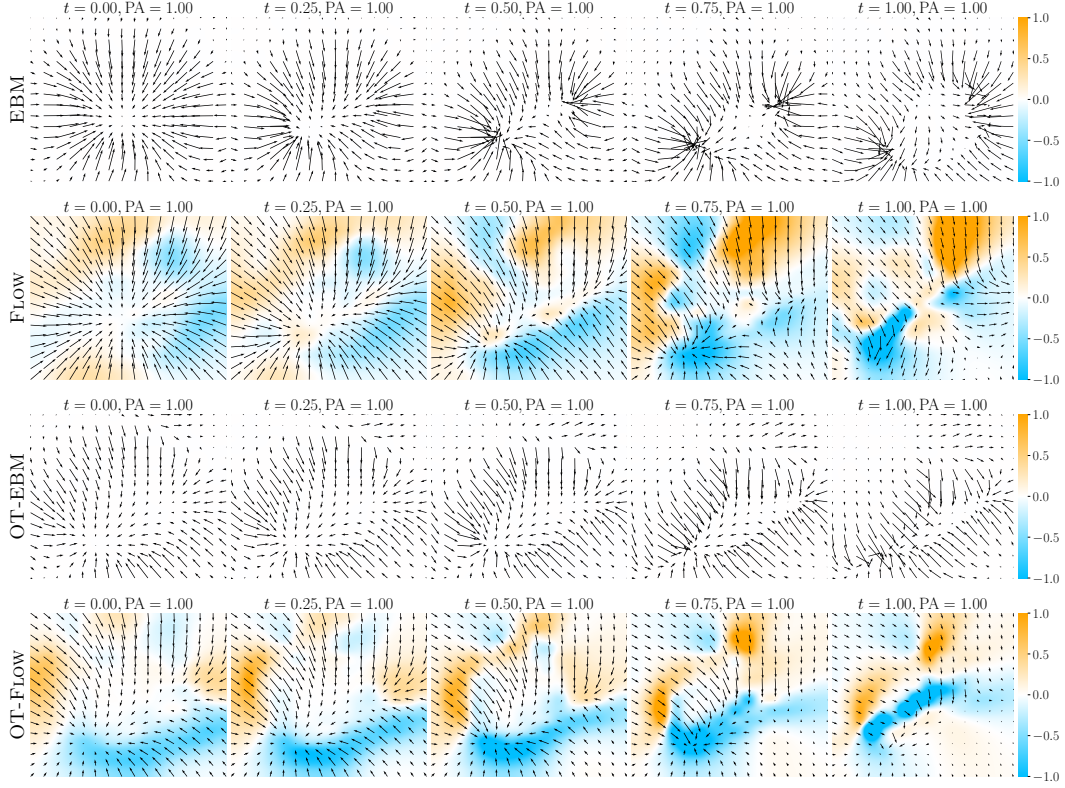


Figure 8: Visualising the curl ($\nabla \times v_t$) of the learned vector field of different models over time (scaled to $[-1, 1]$), for a given intervention on the parents $PA = 1$. We can see that the EBM variants are curl-free (irrotational) by design, as the vector field is given by the gradient of a scalar potential. We also see that the OT vector fields are smoother and OT-FLOW exhibits milder ‘rotations’ compared to FLOW. This is consistent with convergence to the Brenier map, which is itself curl-free.

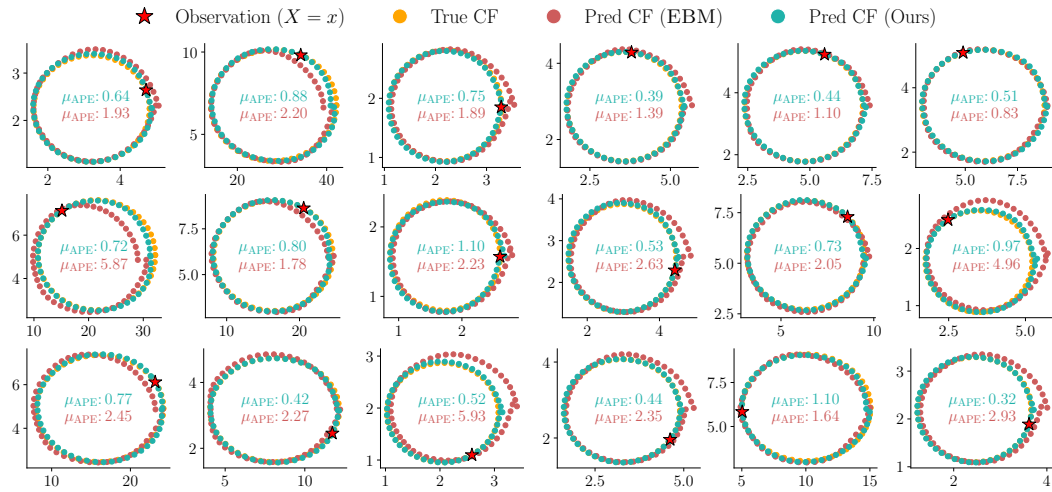


Figure 9: Inferred counterfactual (CF) ellipses using our (Markovian) OT coupling flow vs. an energy-based (curl-free) parameterisation of a flow-based model. Not cherry-picked.

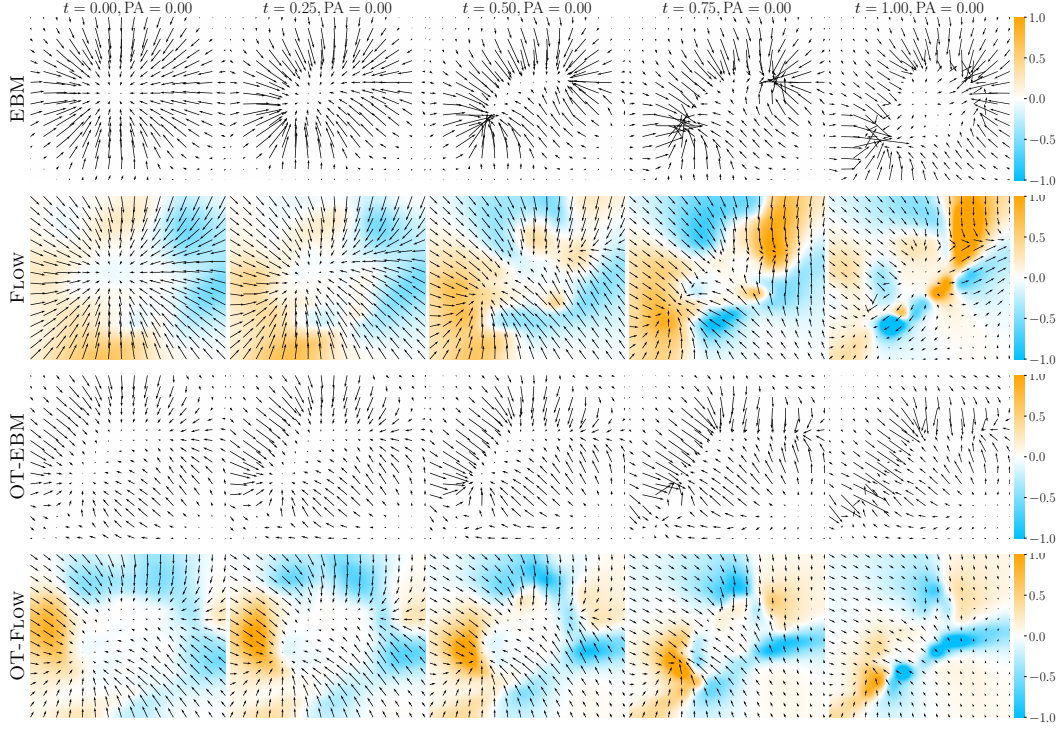


Figure 10: Visualising the $\text{curl} (\nabla \times v_t)$ of the learned vector field of different models over time (scaled to $[-1, 1]$), for a given intervention on the parents $PA = -1$. We can see that the EBM variants are curl-free (irrotational) by design, as the vector field is given by the gradient of a scalar potential. We also see that the OT vector fields are smoother and OT-Flow exhibits milder ‘rotations’ compared to FLOW. This is consistent with convergence to the Brenier map, which is itself curl-free.

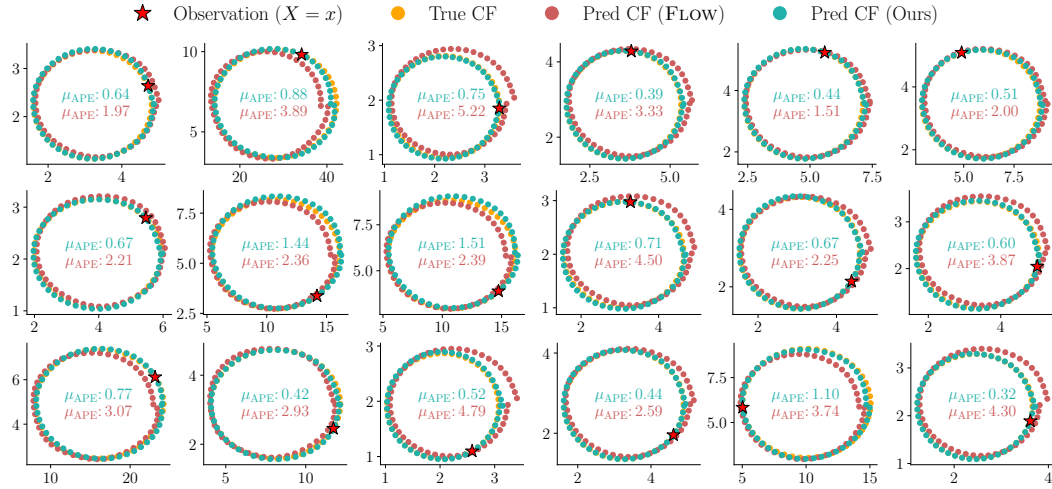


Figure 11: Inferred counterfactual (CF) ellipses using our (Markovian) OT coupling flow vs. a continuous-time flow (Lipman et al., 2023). We note that a standard continuous-time flow is equivalent to a diffusional model (Gao et al., 2025); thus, this baseline is also representative of Sanchez and Tsafaris (2021)’s diffusion-based counterfactual inference model. Not cherry-picked.

E.4 Ablation Studies: Priors & Assumption Violations

Table 3: Ablation of complex data-generating processes (DGP) on CF error $\mu_{\text{APE}} (\%) \downarrow$.

DGP P_U	Counterfactual Ellipse			
	EBM	FLOW	OT-EBM	OT-FLOW
Original	2.32 \pm .01	2.30 \pm .02	0.93 \pm .02	0.76 \pm .01
Bimodal	5.11 \pm .03	5.01 \pm .01	1.73 \pm .09	1.49 \pm .06
Multimodal	7.94 \pm .26	7.69 \pm .20	2.29 \pm .02	2.03 \pm .03

More Complex P_U . Intuitively, a more complex data-generating process is expected to be harder to model. To test this hypothesis, we created new datasets with multimodal P_U . We use an indicator $s_i \sim \text{Bernoulli}(0.5)$ to induce a non-linear, bimodal shift into $\mu_i \in \{-2, 2\}$ into U 's mechanism. We also use a categorical shift $\mu_i \in \{-4, -2, 2, 4\}$, with respective shift probabilities (0.3, 0.2, 0.2, 0.3), to generate another multimodal setting. As reported in Table 3, we confirm that more complex P_U 's can affect generation, but importantly, the relative rank of our models remains consistent. Naturally, we expect larger models to reduce performance gaps for complicated P_U 's.

Table 4: Ablation of monotonicity violation.

MODEL	Monotone	Counterfactual Ellipse		
		COMPOSITION \downarrow	REVERSIBILITY \downarrow	$\mu_{\text{APE}} (\%) \downarrow$
Nasr-Esfahany et al. (2023)	N	-	-	607 \pm N/A
EBM	N	27.86 \pm .369	39.15 \pm .349	2.319 \pm .006
FLOW	N	27.99 \pm .096	39.39 \pm .229	2.295 \pm .020
OT-EBM	Y	0.659 \pm .020	1.056 \pm .072	0.925 \pm .019
OT-FLOW	Y	0.618 \pm .046	1.016 \pm .090	0.763 \pm .014

Monotonicity Violation. We ran a new set of experiments to evaluate different methods under a monotonicity violation. In addition to measuring counterfactual error, we inspect *composition* and *reversibility* counterfactual soundness axioms, in order to reveal possible performance disparities. For evaluation, we use 50/250 steps for ODE/SDE solving, and 20 cycles for composition and reversibility measurements. As reported in Table 4, models which are not ‘vector-monotone’ exhibit substantially inferior counterfactual soundness. The results confirm the intuition that straighter paths lead to improved reversal capabilities. That said, whether this generalises to much higher dimensions is entirely dependent on the quality of the dynamic OT approximation being used.

Table 5: Ablation of bijectivity violation.

MODEL	Bijective	Counterfactual Ellipse		
		COMPOSITION \downarrow	REVERSIBILITY \downarrow	$\mu_{\text{APE}} (\%) \downarrow$
SDE Abduction	N	2.950 \pm .013	4.173 \pm .019	3.064 \pm .011
SDE Prediction	N	3.006 \pm .015	4.276 \pm .019	3.126 \pm .007
CFG ($w = 1.05$)	N	0.032 \pm .004	0.487 \pm .010	2.174 \pm .070
CFG ($w = 1.15$)	N	0.032 \pm .004	1.499 \pm .013	6.081 \pm .069
CFG ($w = 1.25$)	N	0.032 \pm .004	2.598 \pm .024	9.809 \pm .078
OT-FLOW	Y	0.032 \pm .004	0.056 \pm .009	0.763 \pm .014

Bijectivity Violation. In this experiment, we use three strategies to stress-test bijectivity violations: (i) stochastic *abduction* by solving an SDE instead of an ODE; (ii) stochastic *prediction* by solving an SDE; (iii) classifier-free guidance (CFG) (Ho and Salimans, 2022). One cycle was used for measuring composition and reversibility. As reported in Table 5, bijectivity violations affect reversibility and composition substantially; this is likely due to the ground-truth mechanism being bijective.

Table 6: Ablation of Markovianity violation. The NAIVE OT coupling baseline corresponds to Batch-OT flow matching (Pooladian et al., 2023; Tong et al., 2024).

OT Coupling	Markovian	Counterfactual Ellipse		
		COMPOSITION ↓	REVERSIBILITY ↓	$\mu_{\text{APE}} (\%) \downarrow$
NAIVE	N	0.063 \pm .005	0.346 \pm .012	47.01 \pm .016
Ours	Y	0.032 \pm .004	0.056 \pm .009	0.763 \pm .015

Markovianity Violation. In this experiment, we demonstrate the importance of using the correct model specification that reflects our causal assumptions. As explained in the main text, the naive Batch-OT coupling violates the Markovianity assumption, so it should not be used for counterfactual inference as if the assumption were to hold. As reported in Table 6, we observe that composition and reversibility are reasonable for the NAIVE OT coupling version, as the map remains bijective. However, the counterfactual error is substantially higher for the NAIVE version compared to our proposed Markovian OT coupling, since the Markovianity violation leads to inconsistent counterfactuals.

F MIMIC Chest X-ray: Extra Results

F.1 Dataset Details

We reproduce the dataset setup used by our baselines, i.e. Ribeiro et al. (2023) and Xia et al. (2024). The chest X-ray images were resized to 192×192 resolution. From the associated metadata, we focused on four key attributes: SEX (S), RACE (R), AGE (A) and DISEASE (D). The assumed causal graph follows prior work (Ribeiro et al., 2023) in that $A \rightarrow D$ and $\mathbf{PA} = \{S, R, A, D\}$ are the causal parents of the chest X-ray image X . We also focus our scope to only pleural effusion for the disease, to keep comparisons fair. As a result, the final dataset includes only individuals who were either diagnoses with pleural effusion (diseased) or reported as having no findings (i.e. healthy). We then divided the dataset into 62,336 subjects for training, 9,968 for validation and 30,535 for testing, again following the exact same protocol as both Ribeiro et al. (2023) and Xia et al. (2024).

F.2 Architecture and Experimental Setup

The causal mechanisms for all variables $\mathbf{PA} = \{S, R, A, D\}$ and X were learned from observed data. For \mathbf{PA} , standard discrete-time flow-based modelling was used following Pawlowski et al. (2020); Ribeiro et al. (2023). For X , we use a scaled-up version of our most successful model analysed in the counterfactual ellipse experiments, namely OT-FLOW, which includes our specialised family of batch TO couplings to satisfy the Markovianity requirement (cf. Section 5). With that said, we recognise that using large batch sizes is best for accurate batch OT approximations in high dimensions (Klein et al., 2025). Given current resource constraints, we encourage future work to explore more accurate and efficient OT approximations at scale, possibly along the lines of Mousavi-Hosseini et al. (2025).

All models are trained in continuous time using our Markovian Batch-OT coupling. Since the AGE (A) attribute is continuous, we use an age binning strategy to ensure we sample from the conditional distribution $P_{X|\mathbf{PA}}^c$ as explained in Section 5. The effect is that each sample in each batch has the same parents, except for age, which may deviate slightly depending on the bin size. Table 12 reports an ablation study on the age bin size; we find negligible performance differences across bin sizes.

To parameterise the (conditional) vector field for all our models and ablation study variants, we used the same streamlined version of the UNet proposed by Dhariwal and Nichol (2021). To condition the model on the parent variables, we simply learn a separate embedding vector for each parent and sum them all together. This joint parent embedding is then combined with the time embedding to condition each block in the UNet, following Dhariwal and Nichol (2021). The hyperparameters are given in Table 7. The model has just 22M trainable parameters. For training, we used the AdamW optimiser with a learning rate of 10^{-4} , weight decay of 10^{-4} , $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$, and a batch size of 64. We use a linear learning rate warmup of 2000 steps. No extensive hyperparameter sweep was necessary to obtain sufficiently good performance. We trained our models for a maximum of 300 epochs. Since our evaluation is focused on the counterfactual soundness axioms, which are

quite costly to evaluate, we instead performed model selection using the validation set loss achieved by an exponential moving average (EMA) of the model parameters (EMA rate of 0.9999). Further improvements in performance are expected from using standard sample quality metrics for model selection. We conducted three runs with different random seeds. All our models were trained on L40 GPUs, with the full model fitting entirely on a single GPU.

F.3 Additional Comparisons and Ablation Studies

Tables 8 and 9 report additional comparative results against the baselines (Ribeiro et al., 2023; Xia et al., 2024). We again find that our method is superior for all three measured counterfactual soundness axioms, often by large margins, without requiring any costly counterfactual fine-tuning or classifier(-free) guidance strategies. We also conduct ablation studies on our proposed modifications, and the results are reported in Tables 10, 11 and 12. In summary, we observe significant improvements from using our OT coupling compared to the NAIVE non-Markovian approach. As outlined in the main text, we find different performance trade-offs between OT-FLOW and FLOW for different interventions, suggesting either Markovianity violation or a subpar OT approximation (due to small batch size of 64). We expect further improvements from increasing model capacity and batch size significantly (Klein et al., 2025), to better approximate the global OT map (Pooladian et al., 2023).

Table 7: UNet hyperparameters.

MIMIC Chest X-ray	
image shape	(1, 192, 192)
model channels	32
channel mult	[1, 2, 4, 6, 8]
residual blocks	2
attention resolutions	[-1]
heads	1
head channels	64
dropout	0.1

Table 8: Measuring counterfactual *effectiveness* on MIMIC Chest X-ray. $|\Delta_{\text{AUC}}|$ denotes the absolute difference in ROCAUC of inferred counterfactuals relative to the observed data baseline. For each variable, our results (blue shade) appear on the right, and baseline results are on the left. Unlike the baselines, which rely on a costly fine-tuning stage with classifiers/regressors for each variable, our approach does not require any form of classifier or classifier-free guidance to perform well.

MIMIC Chest X-ray (192×192)									
	SEX (S)		RACE (R)		AGE (A)		DISEASE (D)		
BASELINE	AUC (%) \uparrow		AUC (%) \uparrow		MAE (yr) \downarrow		AUC (%) \uparrow		
Observed data	99.63		95.34		6.197		94.41		
(w/o CF fine-tuning Ribeiro et al. (2023))									
INTERVENTION	$ \Delta_{\text{AUC}} $ (%) \downarrow		$ \Delta_{\text{AUC}} $ (%) \downarrow		Δ_{MAE} (yr) \downarrow		$ \Delta_{\text{AUC}} $ (%) \downarrow		
$do(S = s)$	7.430	0.173 $\pm_{.02}$	20.84	0.583 $\pm_{.15}$	0.486	0.333 $\pm_{.06}$	1.310	0.023 $\pm_{.05}$	
$do(R = r)$	0.130	0.180 $\pm_{.01}$	36.94	0.050 $\pm_{.07}$	0.229	0.394 $\pm_{.10}$	7.810	0.310 $\pm_{.19}$	
$do(A = a)$	0.130	0.187 $\pm_{.03}$	20.44	1.197 $\pm_{.15}$	3.872	0.836 $\pm_{.08}$	6.110	0.347 $\pm_{.09}$	
$do(D = d)$	0.030	0.067 $\pm_{.00}$	20.14	0.627 $\pm_{.18}$	0.560	0.435 $\pm_{.05}$	22.01	2.280 $\pm_{.37}$	
$do(\text{rand})$	1.330	0.150 $\pm_{.02}$	24.14	0.730 $\pm_{.22}$	1.166	0.510 $\pm_{.05}$	7.010	0.640 $\pm_{.17}$	
(Soft CF fine-tuning Xia et al. (2024))									
INTERVENTION	$ \Delta_{\text{AUC}} $ (%) \downarrow		$ \Delta_{\text{AUC}} $ (%) \downarrow		Δ_{MAE} (yr) \downarrow		$ \Delta_{\text{AUC}} $ (%) \downarrow		
$do(S = s)$	0.070	0.173 $\pm_{.02}$	2.040	0.583 $\pm_{.15}$	-	0.333 $\pm_{.06}$	0.090	0.023 $\pm_{.05}$	
$do(R = r)$	0.130	0.180 $\pm_{.01}$	3.360	0.050 $\pm_{.07}$	-	0.394 $\pm_{.10}$	0.110	0.310 $\pm_{.19}$	
$do(D = d)$	0.030	0.067 $\pm_{.00}$	1.540	0.627 $\pm_{.18}$	-	0.435 $\pm_{.05}$	3.690	2.280 $\pm_{.37}$	

Table 9: Measuring counterfactual *reversibility* and *composition* properties (Monteiro et al., 2023). The baseline results are reproduced exactly according to Ribeiro et al. (2023). We use an Euler ODE solver or dropi5 (1e-5 tol). A single reverse cycle was used for computing *reversibility*. Three randomly seeded subsets of 1000 test samples were used, and the results were averaged. Similar initial performance was observed for FLOW, thus improving OT further is expected to boost performance.

MIMIC Chest X-ray (192×192)			
METHOD	NFE	COMPOSITION MAE (px) ↓	REVERSIBILITY MAE (px) ↓
HVAE (Ribeiro et al., 2023)	N/A	3.09543 ± 0.0536	2.89816 ± 0.4153
OT-FLOW (Ours)	50	2.70379 ± 0.1151	20.6228 ± 0.6492
	250	0.55289 ± 0.0280	1.22693 ± 0.1630
	dopri5	0.18352 ± 0.0276	0.49485 ± 0.1549

Table 10: Ablation study of our conditional OT coupling on counterfactual *effectiveness*. The baseline is the standard OT coupling (NAIVE) described in Section 5, which violates the Markovian requirement. The results show our approach boosts counterfactual effectiveness, especially for disease and race interventions. The most notable improvements are highlighted using shaded blue areas.

MIMIC Chest X-ray (192×192)					
INTERVENTION	OT Coupling	SEX (<i>S</i>) AUC (%) ↑	RACE (<i>R</i>) AUC (%) ↑	AGE (<i>A</i>) MAE (yr) ↓	DISEASE (<i>D</i>) AUC (%) ↑
N/A (Observed data)	N/A	99.63	95.34	6.197	94.41
$do(S = s)$	NAIVE	99.42	93.85	6.602	94.47
	Ours	99.45±.02	94.76±.15	6.529±.06	94.39±.05
$do(R = r)$	NAIVE	99.56	88.03	6.482	94.24
	Ours	99.45±.06	95.29±.73	6.590±.10	94.10±.19
$do(A = a)$	NAIVE	99.53	93.95	7.723	93.88
	Ours	99.44±.03	94.14±.16	7.032±.07	94.76±.09
$do(D = d)$	NAIVE	99.58	93.66	6.630	88.35
	Ours	99.53±.01	94.71±.19	6.632±.05	92.13±.37
$do(\text{rand})$	NAIVE	99.55	92.75	6.844	92.62
	Ours	99.48±.02	94.61±.23	6.706±.04	93.77±.17

Table 11: Ablation study of Batch-OT on counterfactual *effectiveness*. We observe different performance trade-offs for different models; e.g., the OT-FLOW performs better for race interventions while performing worse than FLOW for disease, suggesting possible non-Markovian interactions. We note that a batch size of 64 was used for training due to our current GPU memory constraints. Larger performance differences are expected with larger batch sizes (Klein et al., 2025), or by adopting more accurate and scalable OT approximations (Mousavi-Hosseini et al., 2025).

MIMIC Chest X-ray (192×192)					
INTERVENTION	OT	SEX (S) AUC (%) \uparrow	RACE (R) AUC (%) \uparrow	AGE (A) MAE (yr) \downarrow	DISEASE (D) AUC (%) \uparrow
N/A (Observed data)	N/A	99.63	95.34	6.197	94.41
$do(S = s)$	N	99.58	94.64	6.495	94.72
	Y	99.45 \pm .02	94.76 \pm .15	6.529 \pm .06	94.39 \pm .05
$do(R = r)$	N	99.56	93.09	6.460	94.59
	Y	99.45 \pm .06	95.29 \pm .73	6.590 \pm .10	94.10 \pm .19
$do(A = a)$	N	99.54	94.40	6.855	95.23
	Y	99.44 \pm .03	94.14 \pm .16	7.032 \pm .07	94.76 \pm .09
$do(D = d)$	N	99.56	94.26	6.589	92.95
	Y	99.53 \pm .01	94.71 \pm .19	6.632 \pm .05	92.13 \pm .37
$do(\text{rand})$	N	99.56	94.17	6.596	94.48
	Y	99.48 \pm .02	94.61 \pm .23	6.706 \pm .04	93.77 \pm .17

Table 12: Ablation study of AGE (A) bin widths on counterfactual *effectiveness*. We observe minimal differences in performance across different bin sizes. This is encouraging as it demonstrates our OT coupling strategy can still work well for continuous parent variables.

MIMIC Chest X-ray (192×192)					
INTERVENTION	Bin	SEX (S) AUC (%) \uparrow	RACE (R) AUC (%) \uparrow	AGE (A) MAE (yr) \downarrow	DISEASE (D) AUC (%) \uparrow
N/A (Observed data)	N/A	99.63	95.34	6.197	94.41
$do(S = s)$	2	99.48 \pm .10	94.49 \pm .34	6.580 \pm .02	94.37 \pm .21
	3	99.45 \pm .02	94.76 \pm .15	6.529 \pm .06	94.39 \pm .05
	5	99.41 \pm .02	94.85 \pm .16	6.600 \pm .04	94.44 \pm .05
$do(R = r)$	2	99.50 \pm .05	94.49 \pm 1.1	6.605 \pm .05	94.07 \pm .18
	3	99.45 \pm .06	95.29 \pm .73	6.590 \pm .10	94.10 \pm .19
	5	99.43 \pm .02	94.97 \pm .33	6.625 \pm .02	94.03 \pm .09
$do(A = a)$	2	99.50 \pm .03	94.06 \pm .09	7.137 \pm .06	94.67 \pm .35
	3	99.44 \pm .03	94.14 \pm .16	7.032 \pm .07	94.76 \pm .09
	5	99.43 \pm .06	93.89 \pm .14	7.159 \pm .05	94.62 \pm .02
$do(D = d)$	2	99.56 \pm .02	94.44 \pm .11	6.675 \pm .89	91.72 \pm .54
	3	99.53 \pm .01	94.71 \pm .19	6.632 \pm .05	92.13 \pm .37
	5	99.52 \pm .02	94.70 \pm .23	6.676 \pm .03	91.66 \pm .02
$do(\text{rand})$	2	99.49 \pm .03	94.35 \pm .48	6.755 \pm .03	93.77 \pm .24
	3	99.48 \pm .02	94.61 \pm .23	6.706 \pm .04	93.77 \pm .17
	5	99.46 \pm .03	94.53 \pm .19	6.760 \pm .03	93.66 \pm .15

F.4 Qualitative Results

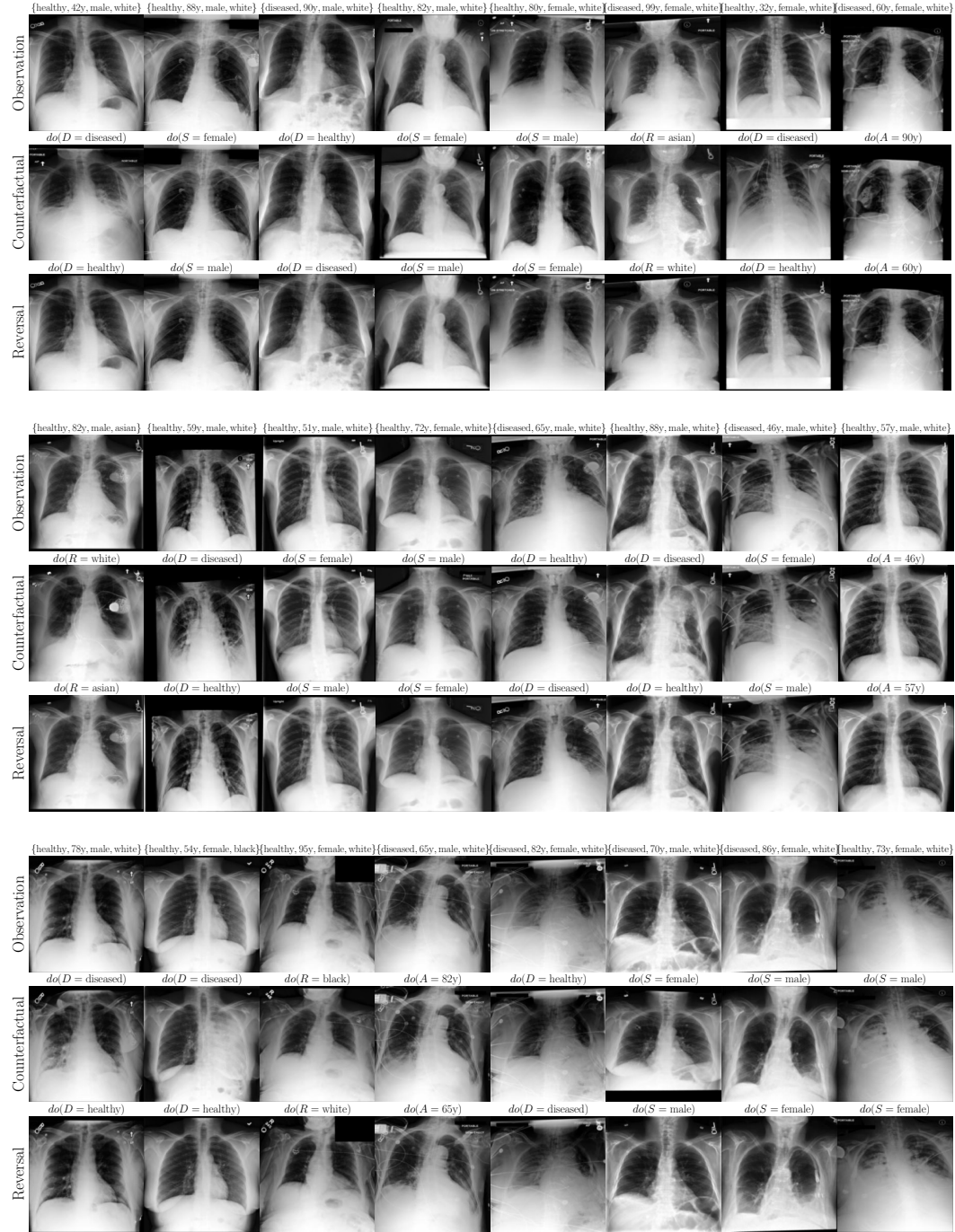


Figure 12: Qualitative counterfactual inference and *reversibility* results (500 ODE Euler solver steps) using our Markovian OT-FLOW model. Despite the small model size, we observe faithful, reasonably identity-preserving interventions, as well as impressive counterfactual reversibility. Importantly, no costly counterfactual fine-tuning (Ribeiro et al., 2023), or classifier(-free) strategies were required.

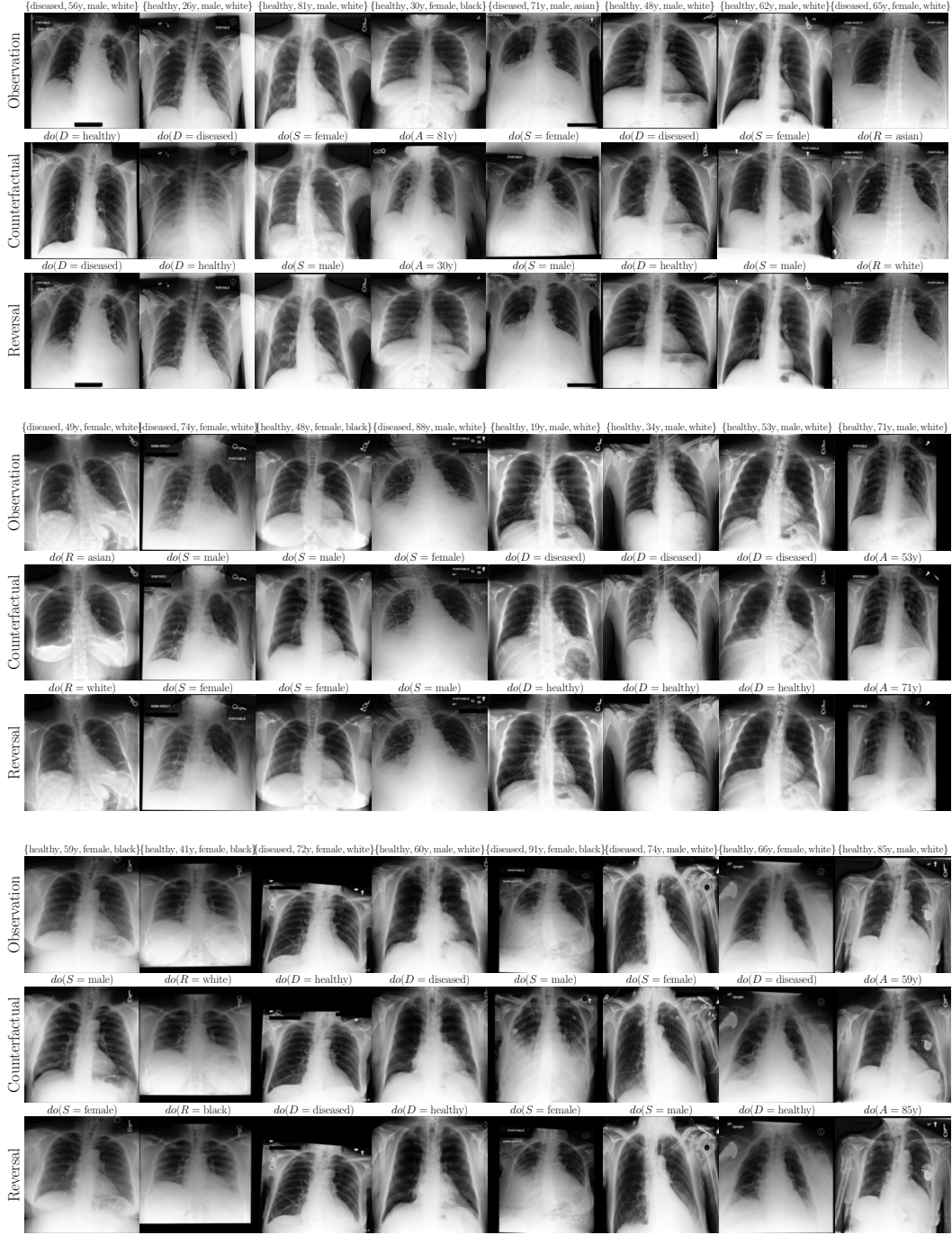


Figure 13: Qualitative counterfactual inference and *reversibility* results (500 ODE Euler solver steps) using our Markovian OT-FLOW model. Despite the small model size, we observe faithful, reasonably identity-preserving interventions, as well as impressive counterfactual reversibility. Importantly, no costly counterfactual fine-tuning (Ribeiro et al., 2023), or classifier(-free) strategies were required.

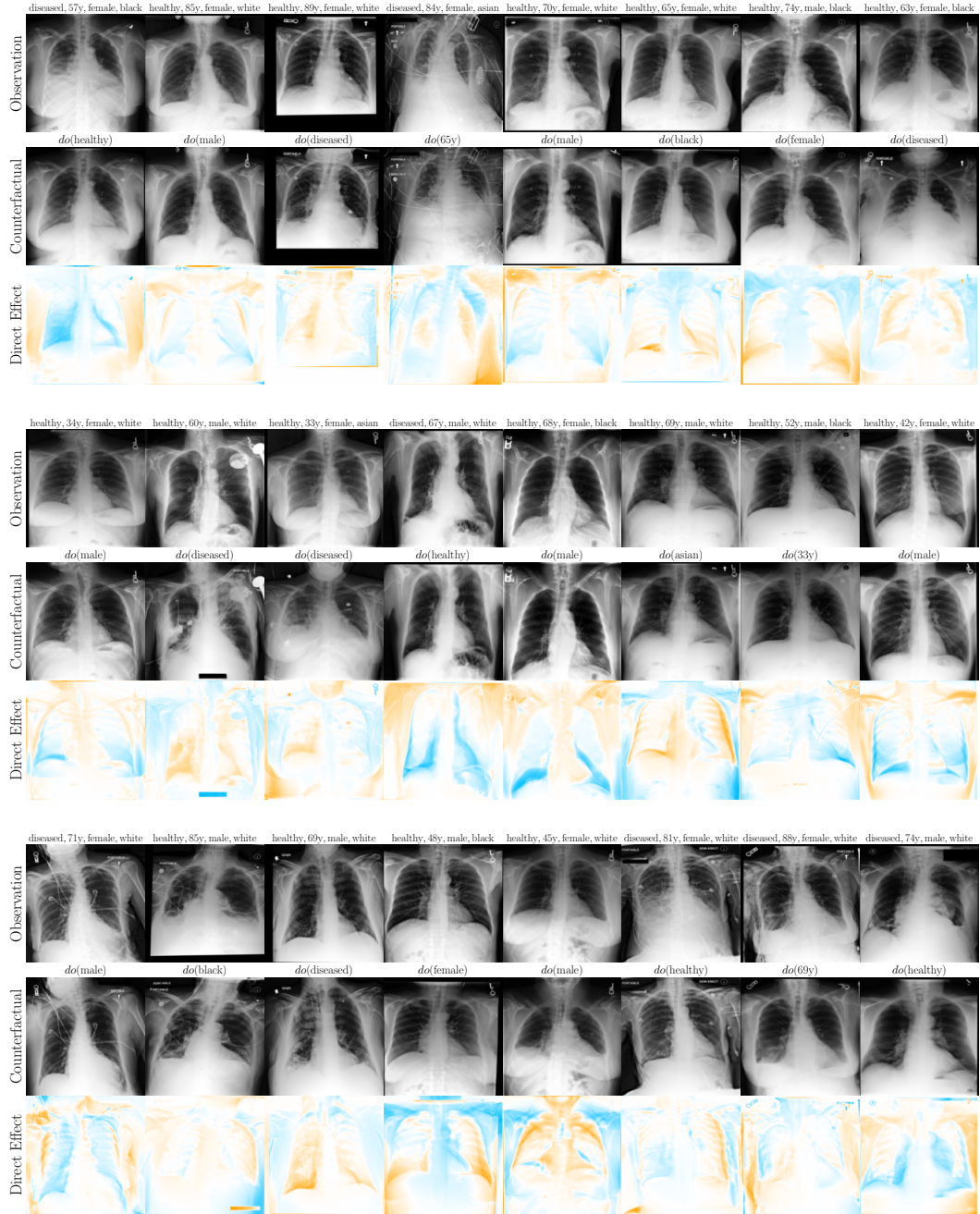


Figure 14: Extra qualitative counterfactual inference results with direct effect maps (500 ODE Euler solver steps). We observe fairly good identity-preservation overall, but counterfactual *effectiveness* appears to be somewhat prioritised by the model. We anticipate that identity preservation can be further improved using inference time guidance strategies without having to retrain the model.

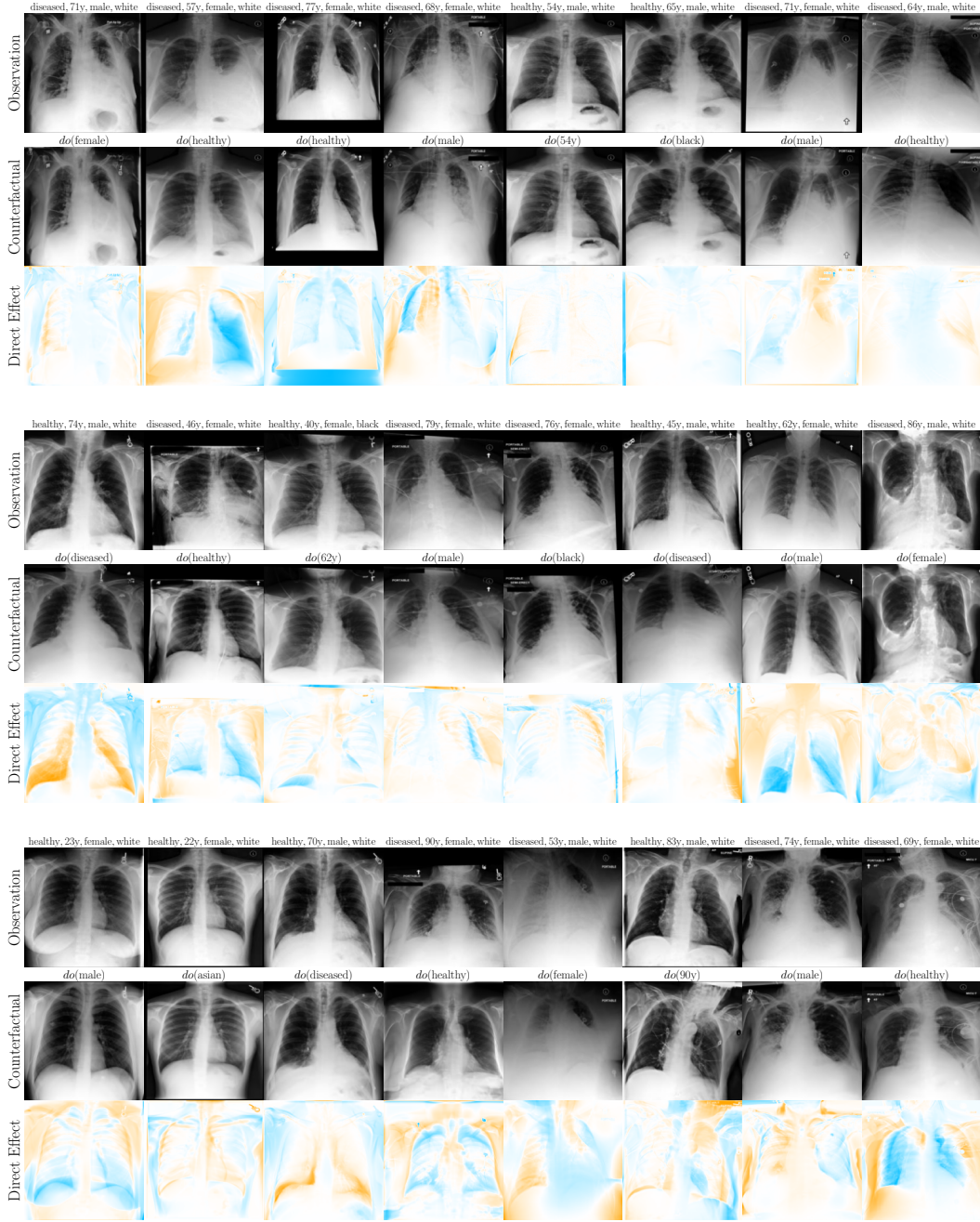


Figure 15: Qualitative counterfactual inference results with only 50 ODE Euler solver steps. We observe decent results considering the small number of ODE solving steps used (classical diffusion models would use, e.g. 1000). However, we find that identity preservation is more challenging in this regime, and spurious associations (e.g. background, artefacts (Pérez-García et al., 2025)) tend to be more prevalent. We expect inference-time classifier(-free) guidance to further improve the results.

NeurIPS Paper Checklist

1. Claims

Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

Answer: [\[Yes\]](#)

Justification: We claim counterfactual identifiability for multi-dimensional variables in Markovian SCMs using our prescribed model, and we validate our theoretical result experimentally using a carefully constructed scenario.

Guidelines:

- The answer NA means that the abstract and introduction do not include the claims made in the paper.
- The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
- The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
- It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

2. Limitations

Question: Does the paper discuss the limitations of the work performed by the authors?

Answer: [\[Yes\]](#)

Justification: We urge practitioners to consider the ethical implications of their causal assumptions when applying this framework in safety-critical settings.

Guidelines:

- The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
- The authors are encouraged to create a separate "Limitations" section in their paper.
- The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
- The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
- The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting. Or a speech-to-text system might not be used reliably to provide closed captions for online lectures because it fails to handle technical jargon.
- The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
- If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
- While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. The authors should use their best judgment and recognize that individual actions in favor of transparency play an important role in developing norms that preserve the integrity of the community. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

3. Theory assumptions and proofs

Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [\[Yes\]](#)

Justification: We provide a detailed appendix with both motivating examples and proofs for all our theoretical claims.

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.
- Inversely, any informal proof provided in the core of the paper should be complemented by formal proofs provided in appendix or supplemental material.
- Theorems and Lemmas that the proof relies upon should be properly referenced.

4. Experimental result reproducibility

Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

Answer: [\[Yes\]](#)

Justification: We provide all the details required to reproduce our results, both: (i) methodology-wise in the main manuscript (Sections 4, 5 and 6); and (ii) all implementation details in terms of neural architecture and hyperparameters are provided in the appendix.

Guidelines:

- The answer NA means that the paper does not include experiments.
- If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important, regardless of whether the code and data are provided or not.
- If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
- Depending on the contribution, reproducibility can be accomplished in various ways. For example, if the contribution is a novel architecture, describing the architecture fully might suffice, or if the contribution is a specific model and empirical evaluation, it may be necessary to either make it possible for others to replicate the model with the same dataset, or provide access to the model. In general, releasing code and data is often one good way to accomplish this, but reproducibility can also be provided via detailed instructions for how to replicate the results, access to a hosted model (e.g., in the case of a large language model), releasing of a model checkpoint, or other means that are appropriate to the research performed.
- While NeurIPS does not require releasing code, the conference does require all submissions to provide some reasonable avenue for reproducibility, which may depend on the nature of the contribution. For example
 - (a) If the contribution is primarily a new algorithm, the paper should make it clear how to reproduce that algorithm.
 - (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
 - (c) If the contribution is a new model (e.g., a large language model), then there should either be a way to access this model for reproducing the results or a way to reproduce the model (e.g., with an open-source dataset or instructions for how to construct the dataset).
 - (d) We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

5. Open access to data and code

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [No]

Justification: We only use publicly available datasets (Ellipse and MIMIC-CXR). We are working on an open-source version of the code and guarantee that it will be made publicly available.

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so “No” is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- The authors should provide instructions on data access and preparation, including how to access the raw data, preprocessed data, intermediate data, and generated data, etc.
- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

6. Experimental setting/details

Question: Does the paper specify all the training and test details (e.g., data splits, hyperparameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer: [Yes]

Justification: We provide the primary details in the experiments section, and the remaining details can be found in the appendix.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

7. Experiment statistical significance

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [Yes]

Justification: We ran experiments with multiple random seeds and report the mean and standard deviation of the results.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.

- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).
- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).
- It should be clear whether the error bar is the standard deviation or the standard error of the mean.
- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

8. Experiments compute resources

Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

Answer: [Yes]

Justification: GPU details are provided in the appendix.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
- The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.
- The paper should disclose whether the full research project required more compute than the experiments reported in the paper (e.g., preliminary or failed experiments that didn't make it into the paper).

9. Code of ethics

Question: Does the research conducted in the paper conform, in every respect, with the NeurIPS Code of Ethics <https://neurips.cc/public/EthicsGuidelines>?

Answer: [Yes]

Justification: We have taken steps to ensure that this is the case.

Guidelines:

- The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
- If the authors answer No, they should explain the special circumstances that require a deviation from the Code of Ethics.
- The authors should make sure to preserve anonymity (e.g., if there is a special consideration due to laws or regulations in their jurisdiction).

10. Broader impacts

Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

Answer: [Yes]

Justification: We warn users to carefully consider the impact of their technical and causal assumptions when drawing causal conclusions from our model in real-world settings.

Guidelines:

- The answer NA means that there is no societal impact of the work performed.

- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.
- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.
- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.
- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

11. Safeguards

Question: Does the paper describe safeguards that have been put in place for responsible release of data or models that have a high risk for misuse (e.g., pretrained language models, image generators, or scraped datasets)?

Answer: [No]

Justification: We only use publicly available data, and our models are small-scale by modern standards. We don't believe they present additional risks relative to the systems already available or warrant specialised safeguards.

Guidelines:

- The answer NA means that the paper poses no such risks.
- Released models that have a high risk for misuse or dual-use should be released with necessary safeguards to allow for controlled use of the model, for example by requiring that users adhere to usage guidelines or restrictions to access the model or implementing safety filters.
- Datasets that have been scraped from the Internet could pose safety risks. The authors should describe how they avoided releasing unsafe images.
- We recognize that providing effective safeguards is challenging, and many papers do not require this, but we encourage authors to take this into account and make a best faith effort.

12. Licenses for existing assets

Question: Are the creators or original owners of assets (e.g., code, data, models), used in the paper, properly credited and are the license and terms of use explicitly mentioned and properly respected?

Answer: [Yes]

Justification: We cite all relevant sources and only make use of publicly available academic material and datasets.

Guidelines:

- The answer NA means that the paper does not use existing assets.
- The authors should cite the original paper that produced the code package or dataset.
- The authors should state which version of the asset is used and, if possible, include a URL.
- The name of the license (e.g., CC-BY 4.0) should be included for each asset.

- For scraped data from a particular source (e.g., website), the copyright and terms of service of that source should be provided.
- If assets are released, the license, copyright information, and terms of use in the package should be provided. For popular datasets, paperswithcode.com/datasets has curated licenses for some datasets. Their licensing guide can help determine the license of a dataset.
- For existing datasets that are re-packaged, both the original license and the license of the derived asset (if it has changed) should be provided.
- If this information is not available online, the authors are encouraged to reach out to the asset's creators.

13. New assets

Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

Answer: [NA]

Justification: No new assets are provided at this time.

Guidelines:

- The answer NA means that the paper does not release new assets.
- Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.
- The paper should discuss whether and how consent was obtained from people whose asset is used.
- At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

14. Crowdsourcing and research with human subjects

Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

Answer: [NA]

Justification: We did not conduct such studies in our work.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Including this information in the supplemental material is fine, but if the main contribution of the paper involves human subjects, then as much detail as possible should be included in the main paper.
- According to the NeurIPS Code of Ethics, workers involved in data collection, curation, or other labor should be paid at least the minimum wage in the country of the data collector.

15. Institutional review board (IRB) approvals or equivalent for research with human subjects

Question: Does the paper describe potential risks incurred by study participants, whether such risks were disclosed to the subjects, and whether Institutional Review Board (IRB) approvals (or an equivalent approval/review based on the requirements of your country or institution) were obtained?

Answer: [NA]

Justification: We did not conduct such studies in our work.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.

- Depending on the country in which research is conducted, IRB approval (or equivalent) may be required for any human subjects research. If you obtained IRB approval, you should clearly state this in the paper.
- We recognize that the procedures for this may vary significantly between institutions and locations, and we expect authors to adhere to the NeurIPS Code of Ethics and the guidelines for their institution.
- For initial submissions, do not include any information that would break anonymity (if applicable), such as the institution conducting the review.

16. **Declaration of LLM usage**

Question: Does the paper describe the usage of LLMs if it is an important, original, or non-standard component of the core methods in this research? Note that if the LLM is used only for writing, editing, or formatting purposes and does not impact the core methodology, scientific rigorousness, or originality of the research, declaration is not required.

Answer: [NA]

Justification: LLMs were occasionally used for help with formatting and writing plotting code.

Guidelines:

- The answer NA means that the core method development in this research does not involve LLMs as any important, original, or non-standard components.
- Please refer to our LLM policy (<https://neurips.cc/Conferences/2025/LLM>) for what should or should not be described.