Counterfactual Cocycles: Noise Invariant and Coherent Transport-based Couplings

Hugh Dance[1], Benjamin Bloem-Reddy[2]

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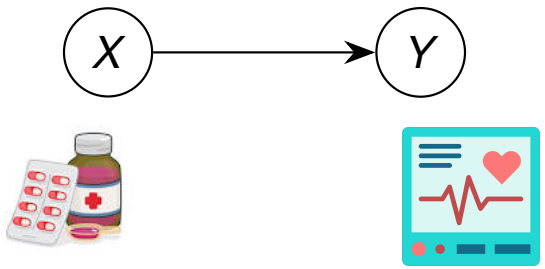
RCT as the “gold-standard” for marginal counterfactual inference

Goal: Assess effectiveness of medication $X \in \{0, 1\}$ on symptoms $Y := (Y_1, \ldots, Y_p)$.



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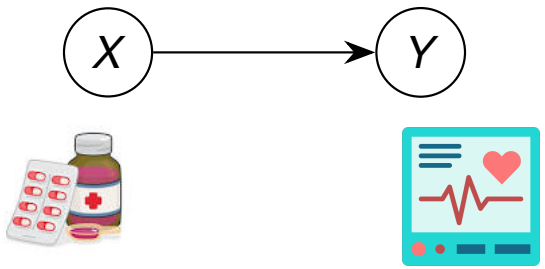

Randomized Control Trial (RCT)

- Observe treatment units $\{Y^{(i)}(1)\}_{i=1}^{n_1}$ and control units $\{Y^{(i)}(0)\}_{i=n_1+1}^{n_1+n_0}$.
- Potential outcomes satisfy $Y^{(i)}(x) \sim \mathbb{P}_{Y|X=x}$

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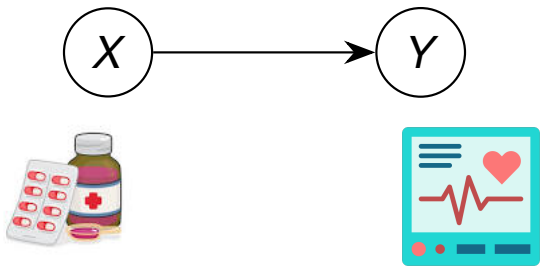

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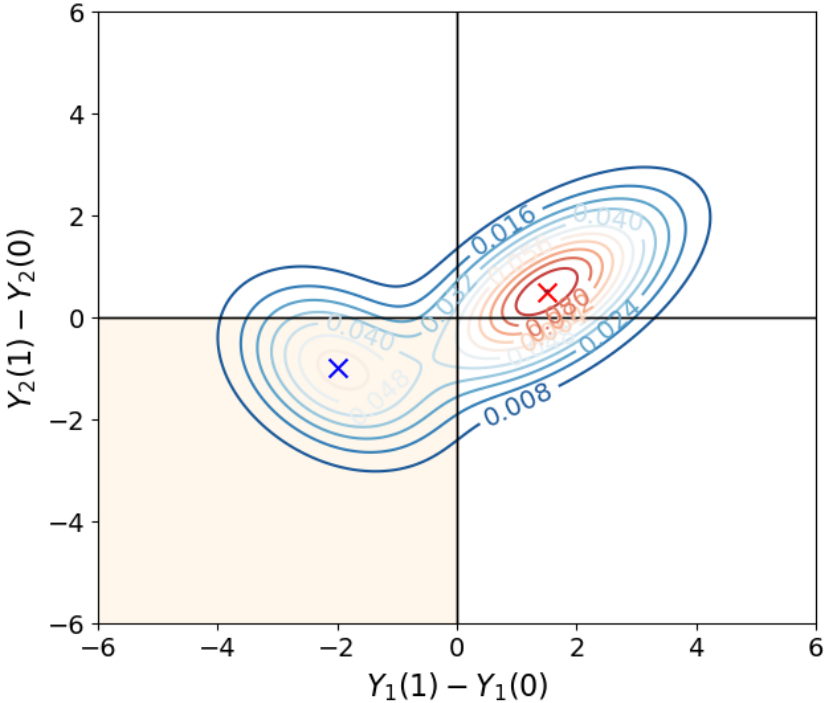
- Potential outcomes satisfy $Y^{(i)}(x) \sim \mathbb{P}_{Y|X=x}$

$$\text{ATE} = \mathbb{E}[Y(1)] - \mathbb{E}[Y(0)] \implies \widehat{ATE} = \frac{1}{n_1}\sum_{i=1}^{n_1} Y^{(i)}(1) - \frac{1}{n_0}\sum_{i=n_1+1}^{n_0} Y^{(i)}(0)$$

When is the “gold-standard” not enough?

Goal: Quantify possible treatment harms



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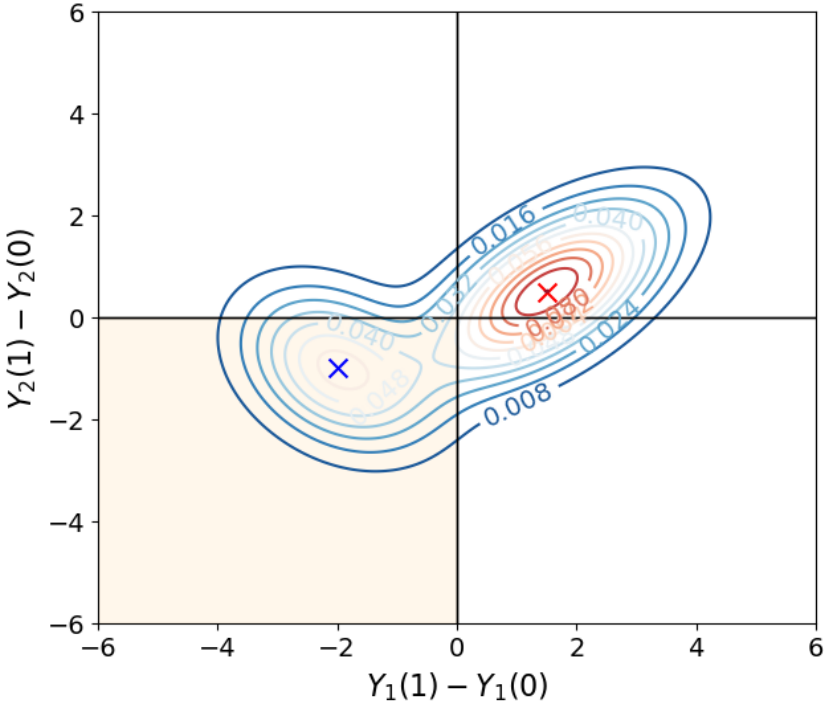

Treatment Harm Rate (THR)[3] $:= \mathbb{P}(Y(1) \prec Y(0)) = \mathbb{P}(\{Y_1(1) \prec Y_1(0)\} \cap \{Y_2(1) - Y_2(0)\})$

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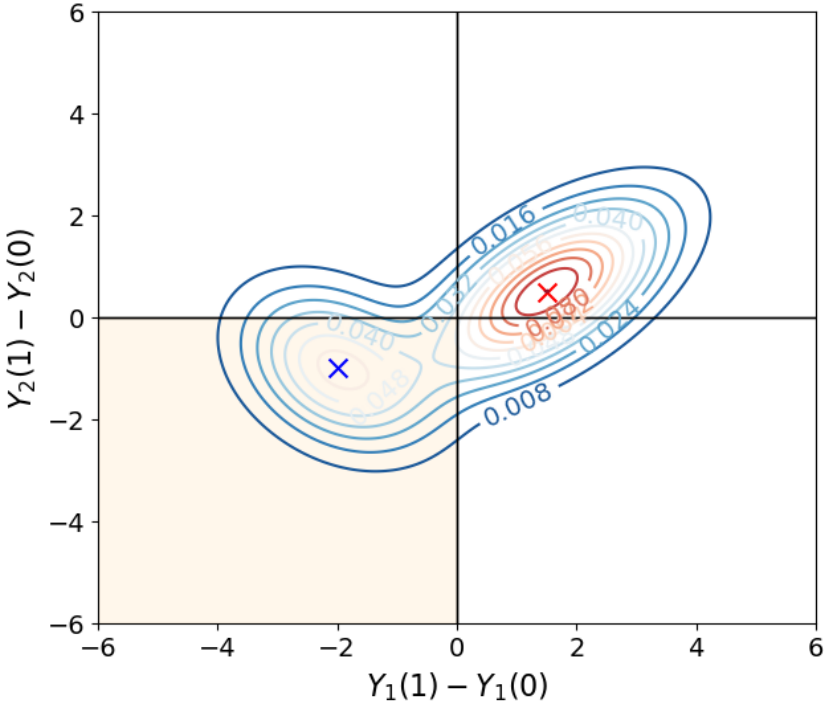

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Issue: Only observe $Y^{(i)}(0)$ or $Y^{(i)}(1)$ for each unit - cannot estimate THR from data!

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The Need for Counterfactual Couplings

Underlying issue: need coupling $\mathbb{P}_{Y(1),Y(0)}$ to estimate $\mathbb{P}_{Y(1)-Y(0)}$

$$\text{THR} := \iint \mathbf{1}\{y_1 - y_0 \leq 0\} \, d\mathbb{P}_{Y(1),Y(0)}(y_1, y_0)$$

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Other Examples

- Median Treatment Effect (MTE)[4]: $\text{Med}(Y(1) - Y(0))$
- Conditional Value at Risk (CVar)[5]: $\mathbb{E}[Y(1) - Y(0) | Y(1) - Y(0) \leq q_\alpha]$
- Treatment Benefit Rate (TBR)[6]: $\mathbb{P}(Y(1) \succ Y(0))$

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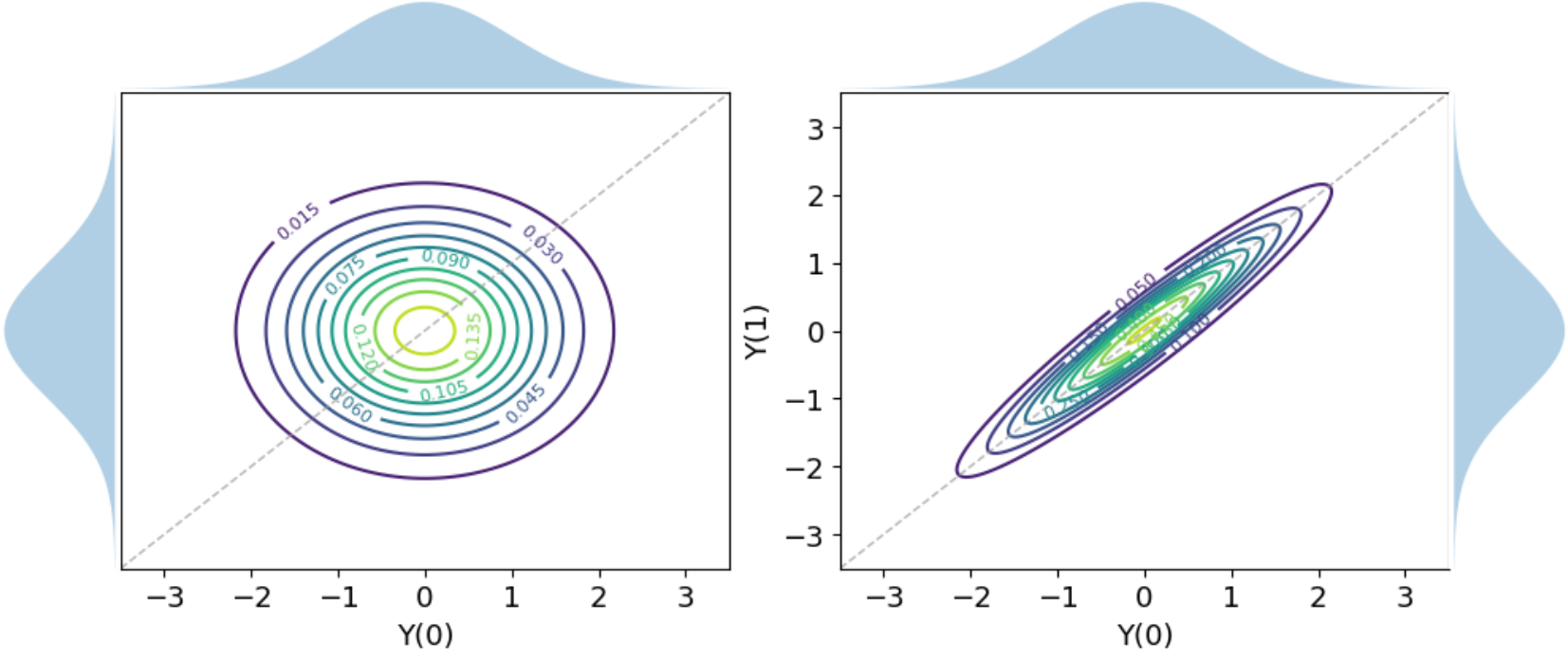
Counterfactual Couplings: Identification Challenge

- Infinitely many admissible couplings $\pi \in \Pi(\mathbb{P}_{Y(1)}, \mathbb{P}_{Y(0)})$
- Can never observe joint samples $(Y(1), Y(0))$



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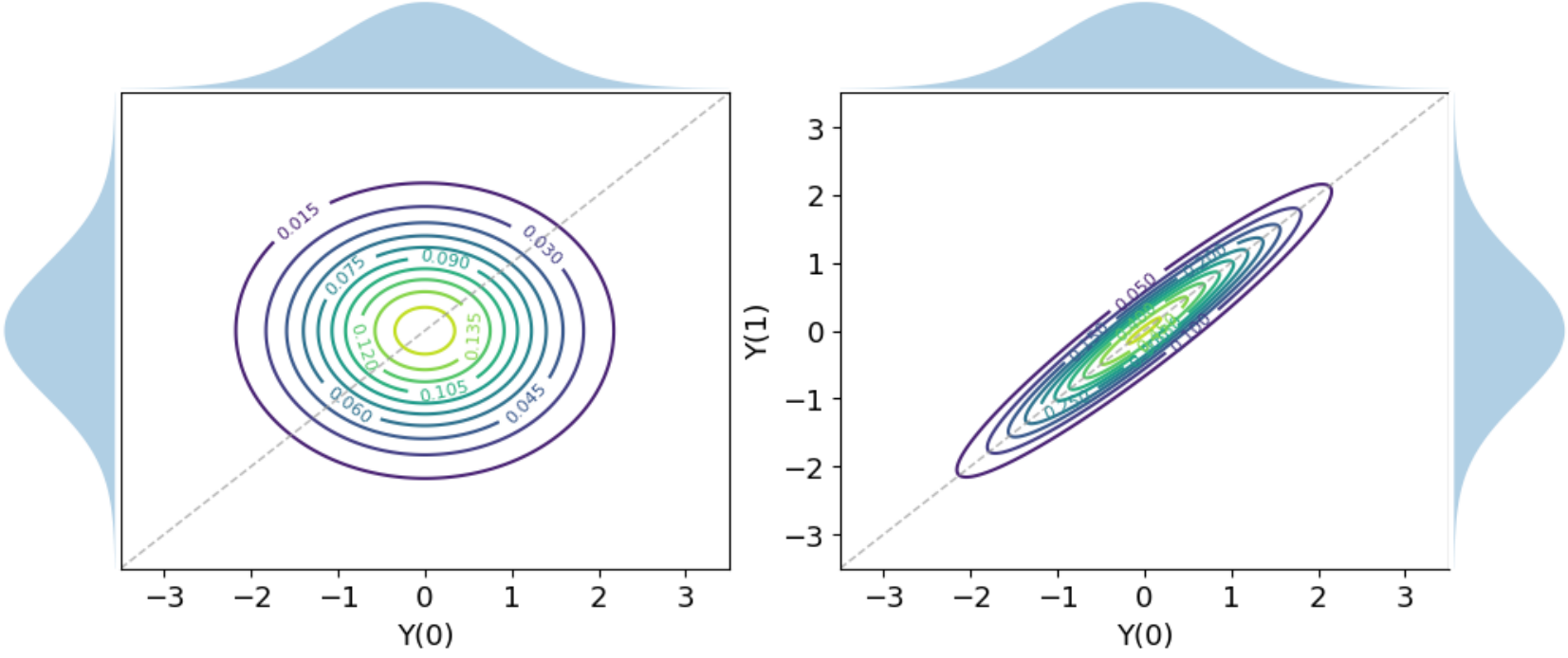
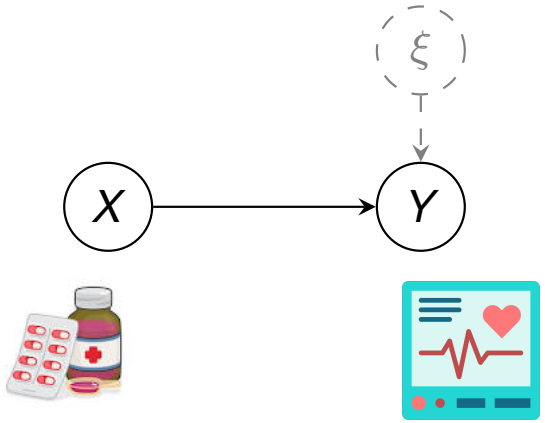


Existing Approaches

- Structural Causal Models (SCMs)
- Optimal Transport Methods (OT)

Limitations of Existing Methods

Structural Causal Models[7]



Structural Causal Model (SCM): $Y = f(X, \xi), \quad \xi \sim \mathbb{P}_\xi, \quad \xi \perp\!\!\!\perp X$

Counterfactuals: $Y(x) = f(x, \xi) \implies$ induced coupling: $(Y(1), Y(0)) = (f_1(\xi), f_0(\xi))$

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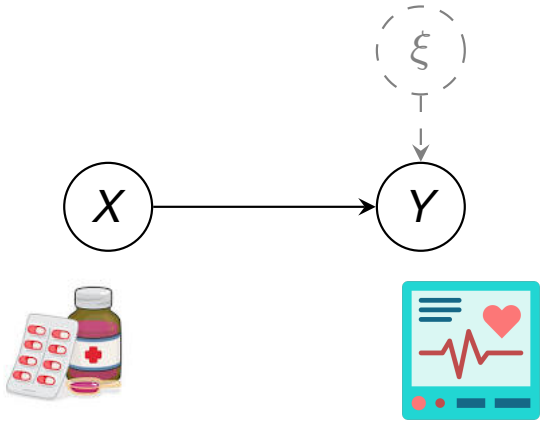

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. . . how to identify $(f, \mathbb{P}_\xi)$ from data?

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Structural Causal Model Non-Identifiability

Transport Problem : find $(f, \mathbb{P}_\xi)$ such that $(f_x)_\# : \mathbb{P}_\xi \mapsto \mathbb{P}_{Y|X=x}$ (i.e. $f_x(\xi) \sim \mathbb{P}_{Y|X=x}$)

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Issue: Can find $f^{(1)}$, $f^{(2)}$ such that $f_x^{(1)}(\xi) =_d f_x^{(2)}(\xi) \sim \mathbb{P}_{Y|X=x}$ for each x but:

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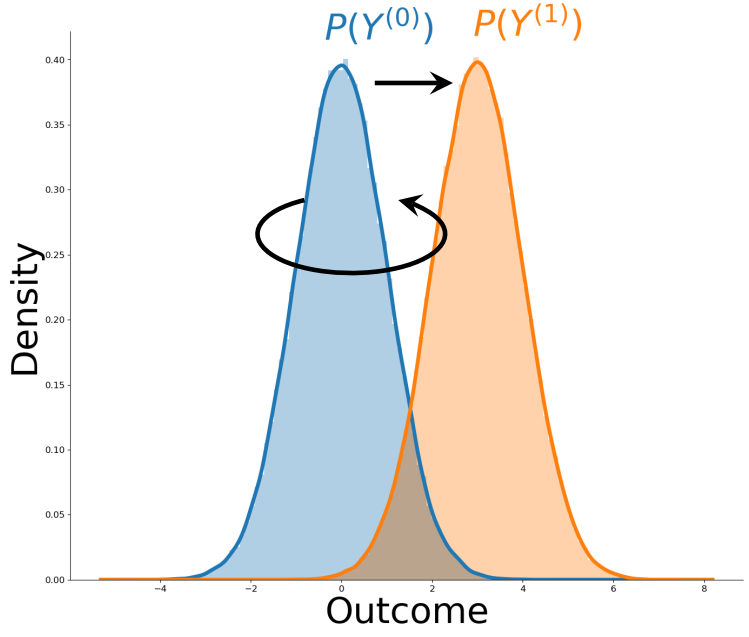
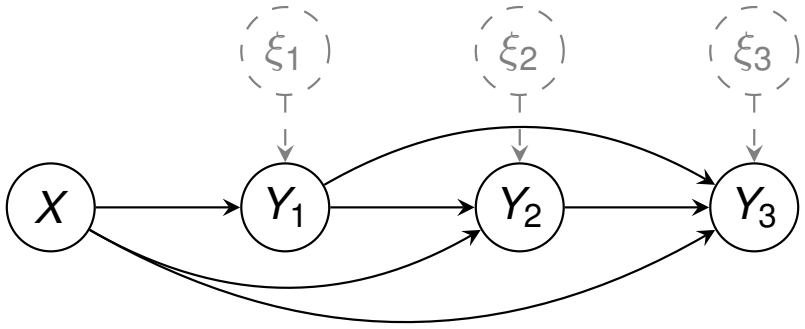
Example:

$$\xi \sim \mathcal{N}(0,1)$$
$$f^{(1)}(x,\xi) = \beta x + \xi$$
$$f^{(2)}(x,\xi) = \beta x + (2x-1)\xi$$



Couplings don't agree! $(\xi, 1+\xi) \neq_d (\xi, 1-\xi)$

Identifiability via Bijective Causal Models (BCMs)



Causal Ordering: $Y_1 \prec Y_2 \prec \cdots \prec Y_p \quad \Longrightarrow \quad$ **Acyclic-SCM:** $Y_j = f_j(X, Y_{<j}, \xi_j) \quad \forall j$

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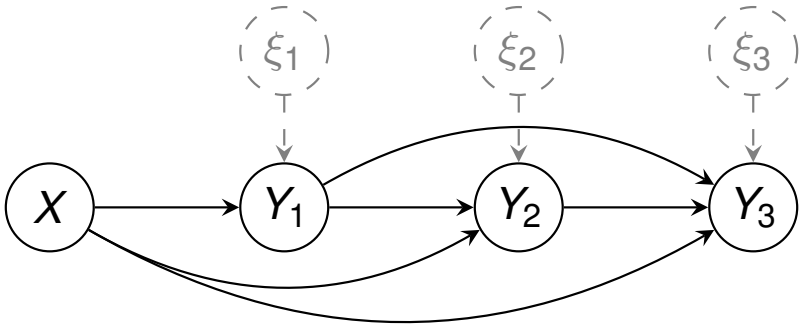

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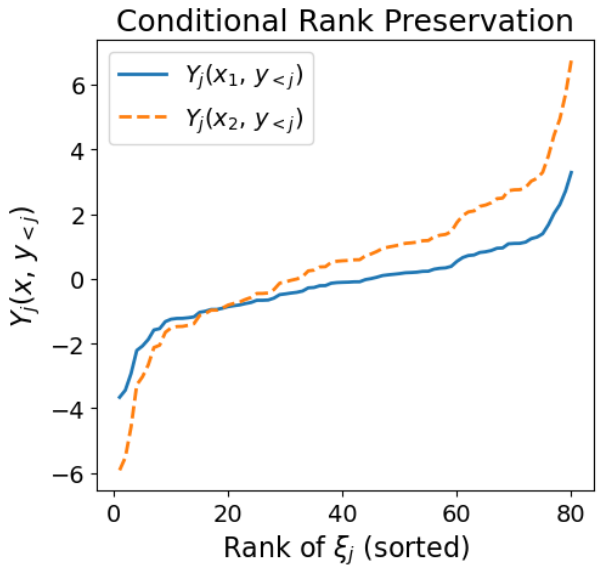
Conditions for Identifiability[8]

- Each f_j is bijective on ξ_j
- $\mathbb{P}_{Y|X=x}$ and $\mathbb{P}_{\xi}$ are abs. continuous on $\mathbb{R}^d$

$\Rightarrow f_x : \mathcal{E} \to \mathbb{Y}$ is *triangular, monotone, increasing*



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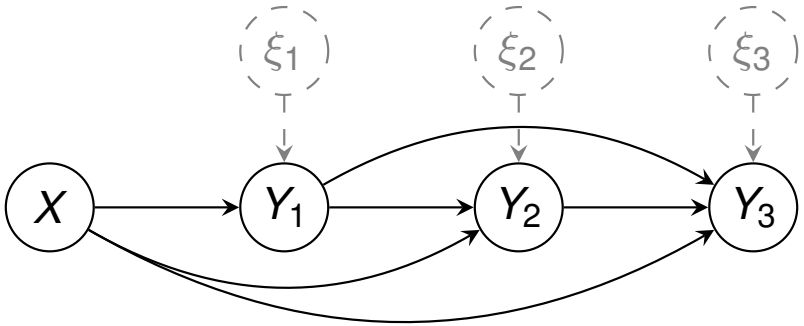

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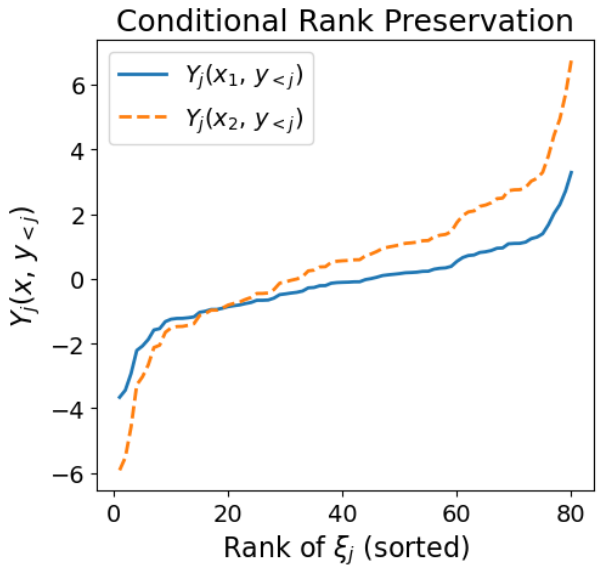

Can augment model with measured causes Z (age, gender, gene expression...)

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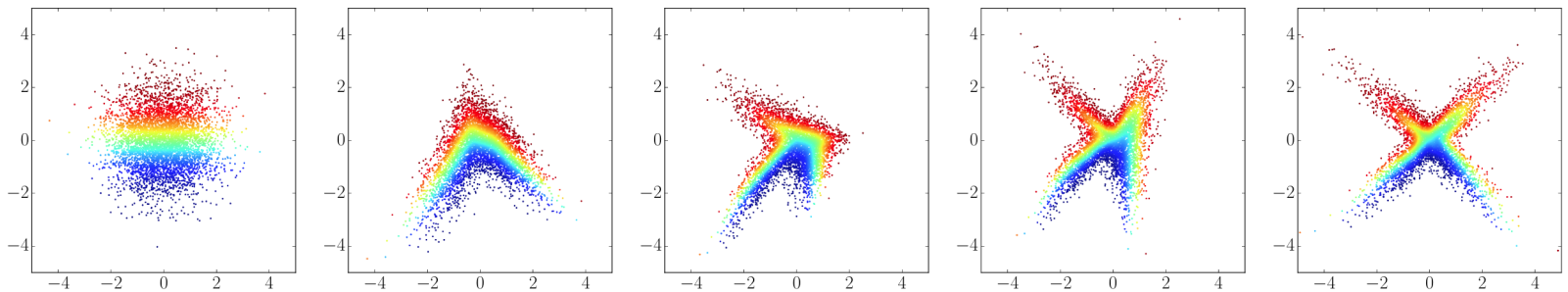
How to model BCMs?

Popular Approach[9]: Fix 'base' distribution $\mathbb{P}_\xi$ and learn diffeomorphisms $(f_x)_{x\in\mathbb{X}}$

$$y(x) = f_x^{(L)} \circ f_x^{(L-1)} \circ \cdots \circ f_x^{(1)}(\xi) \implies \log p(y|x) = \log p_\xi(f_x^{-1}(y)) + \log|\nabla_y f_x^{-1}(y)|$$



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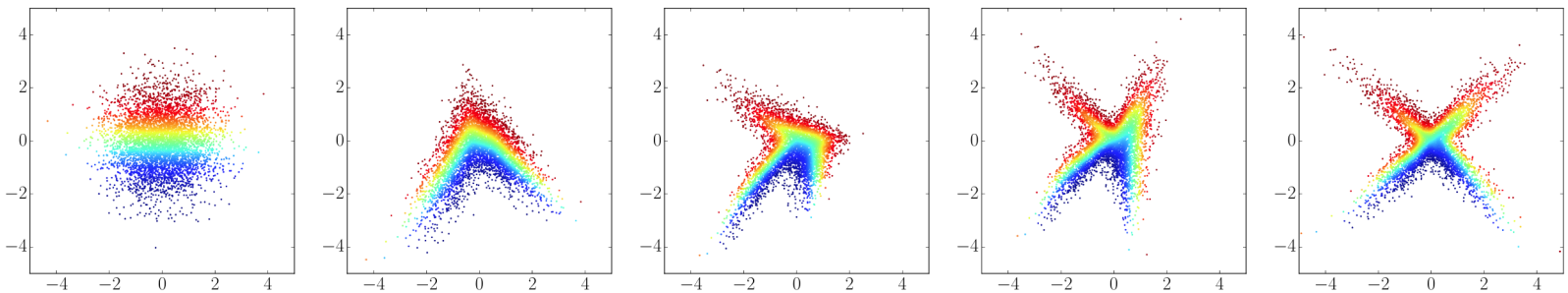
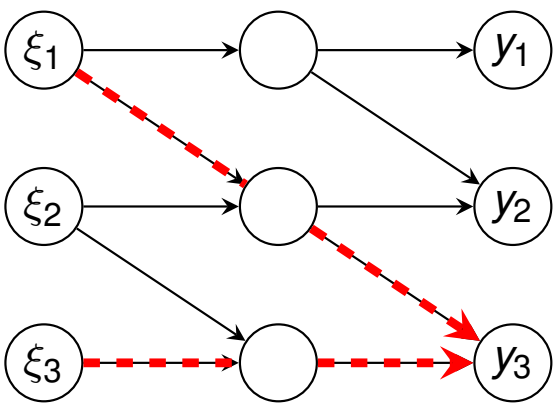


Autoregressive Normalizing Flows: Respect causal ordering when stacked!



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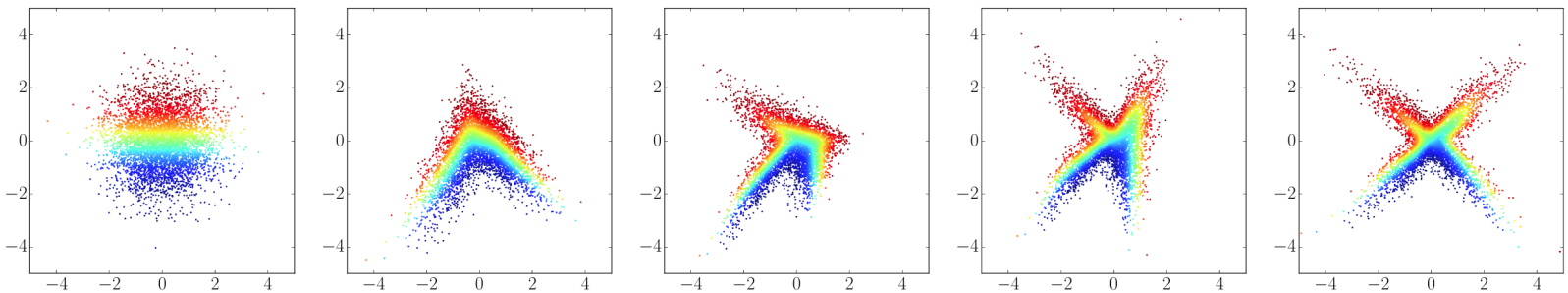

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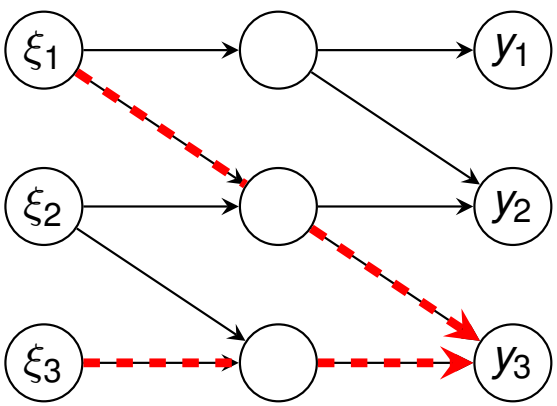

Model	**Autoregressive transform** $f_j(v_{<j}, \xi_j)$
NICE (Additve)	$\xi_j + \mu_j(v_{<j})$
MAF (Affine)	$\xi_j \mapsto \exp\big(\lambda_j(v_{<j})\big)\,\xi_j + \mu_j(v_{<j})$
NAF (INN)	$\xi_j \mapsto \sigma^{-1}(w(v_{<j}) \cdot \sigma(\sigma_j(v_{<j})\xi_j + \mu_j(v_{<j})))$
NSF (Spline)	$\xi_j \mapsto v_j 1_{v_j\notin[-B,B]} + M_j(\xi_j; v_{<j}) 1_{v_j\in[-B,B]}$

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Tail Mis-Specification Problems

- If tail decay of $\mathbb{P}_\xi$ doesn't match $\mathbb{P}_{Y|X=x}$, no bi-lipschitz transport f_x exists![10]
- Heavy tailed $\mathbb{P}_{Y|X=x}$, Gaussian $\hat{\mathbb{P}}_\xi$ = undefined likelihood:

$$|\mathbb{E} \log \hat{p}(Y(x))| \succeq \mathbb{E}\|f_x^{-1}(Y(x))\|^2 = \infty$$

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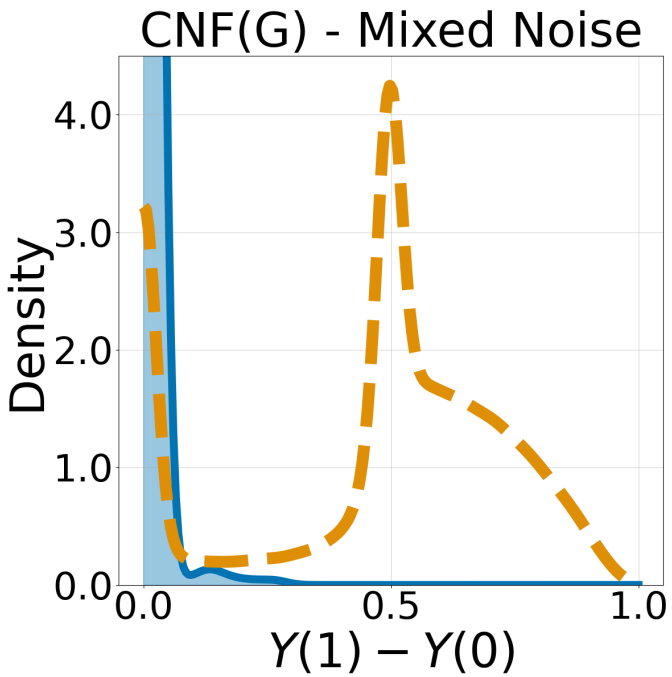
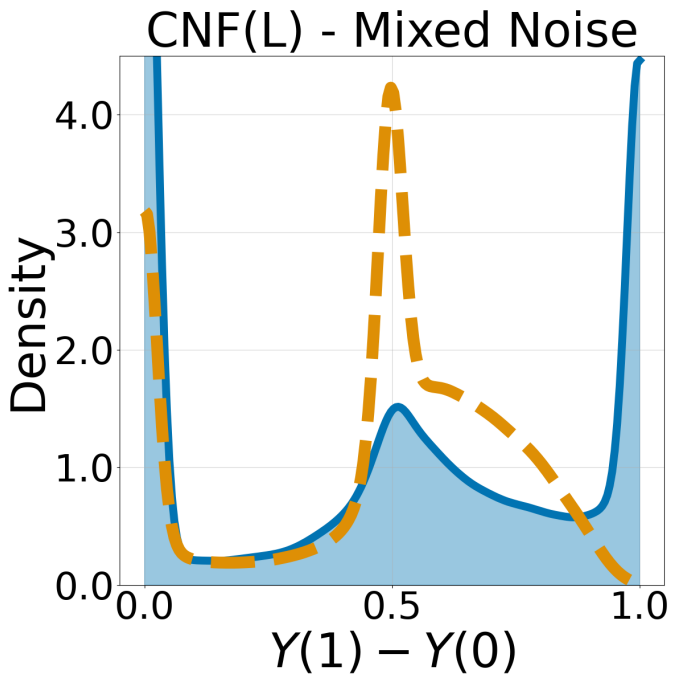
Example : $Y = (X+1)\xi\,, \quad X \sim Bern(1/2), \quad \xi \sim \frac{1}{2}|\mathcal{N}(0,1)| - \frac{1}{2}|NBP(0.1, 0.1)$





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Support Mis-Specification Problems

- Need diffeomorphic $\text{supp}(\hat{\mathbb{P}}_\xi)$ and $\text{supp}(\mathbb{P}_{Y|X=x})$ for existence of $f_x \in \mathcal{F}$
- Likelihood non-identifiability if $\text{supp}\big((f_x^{-1})_\#(\mathbb{P}_{Y|X=x})\big) \not\supset \text{supp}(\hat{\mathbb{P}}_\xi)$:

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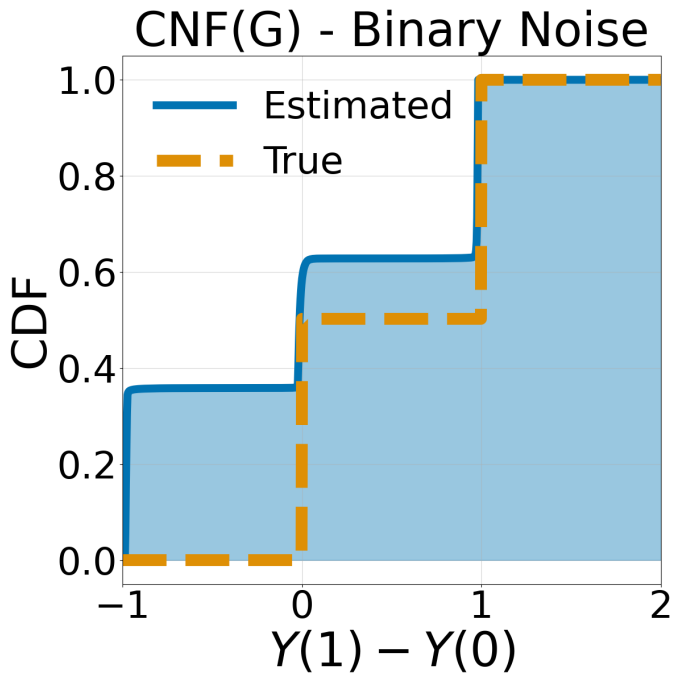
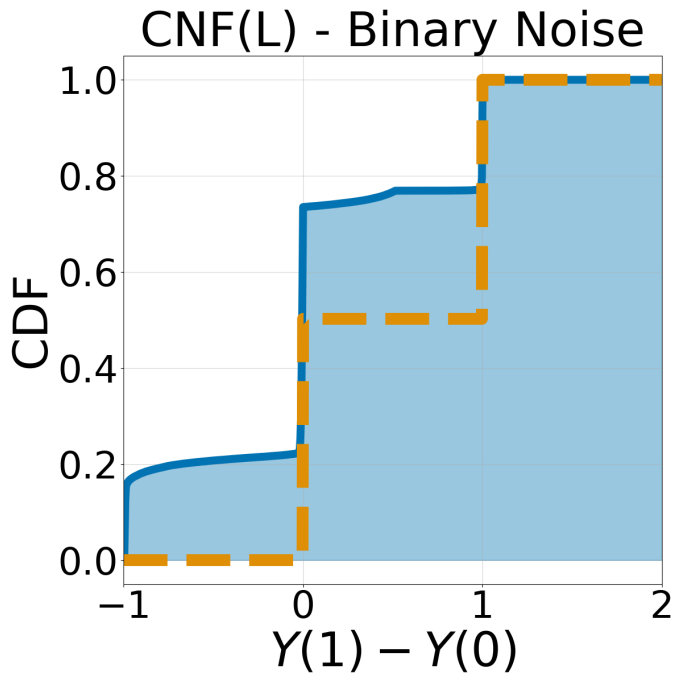




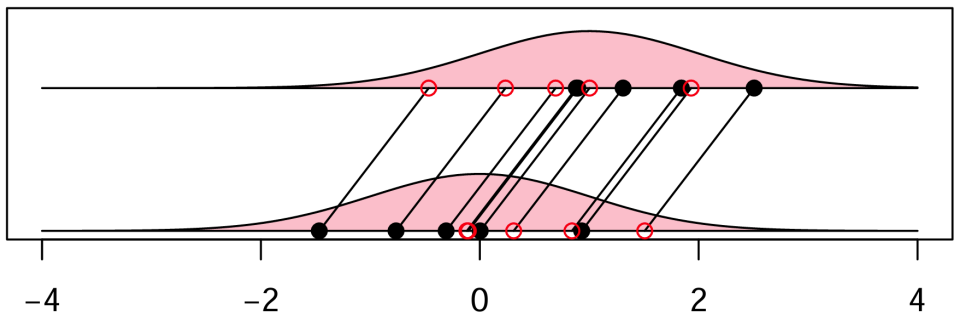
Optimal Transport Methods: An Alternative

Idea: Choose coupling between $Y(1), Y(0)$ using *optimal-transport*:

$$\pi^* = \arg \min_{\pi \in \Pi(\mathbb{P}_{Y(1)}, \mathbb{P}_{Y(0)})} \iint c(y(1), y(0)) d\pi(y(1), y(0))$$

Motivations:

- Conservativism[1]
- Counterfactual Similarity[2]
- Optimal Matching[3]



[1] Balakrishnan et al. (2025) "Conservative inference for counterfactuals." Journal of Causal Inference.

[2] De Lara et al. (2024) "Transport-based Counterfactual Models" JMLR.

[3] Charpentier et al (2023) "Optimal transport for counterfactual estimation: A method for causal inference.", Optimal transport statistics for economics and related topics.

Optimal Transport Methods: An Alternative

Idea: Choose coupling between $Y(1), Y(0)$ using *optimal-transport*:

$$\pi^* = \arg \min_{\pi \in \Pi(\mathbb{P}_{Y(1)}, \mathbb{P}_{Y(0)})} \iint c(y(1), y(0)) d\pi(y(1), y(0))$$

Motivations:

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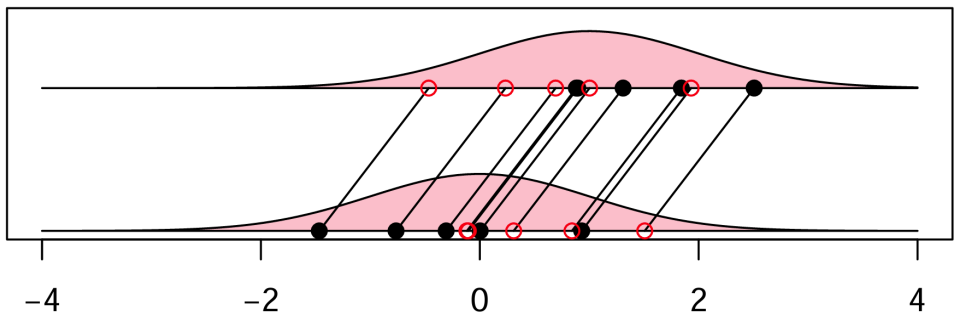

Deterministic coupling restriction: $Y(1) = T_{1,0}(Y(0))$

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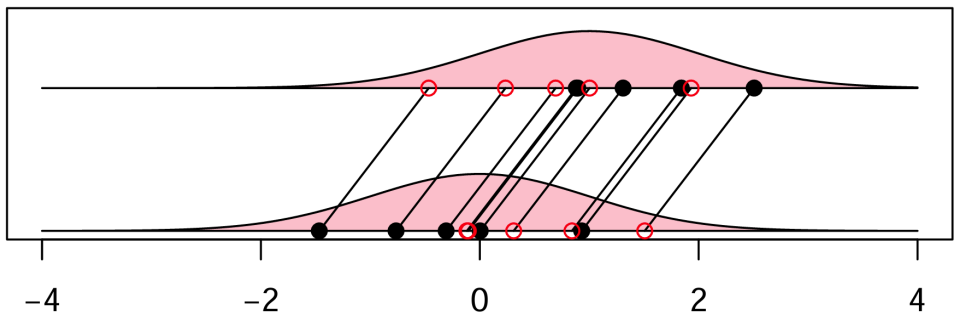

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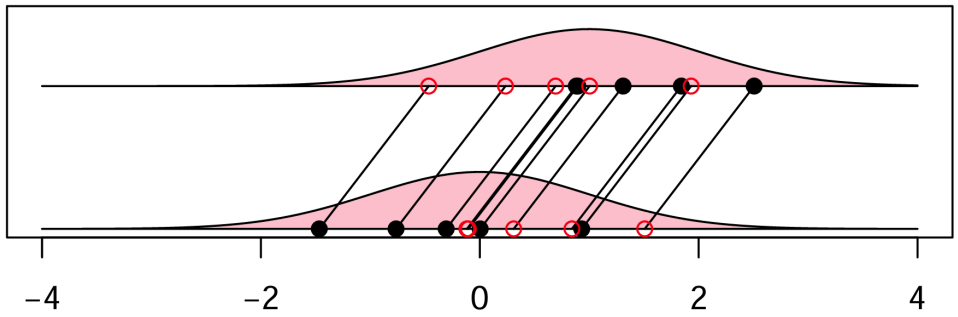

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Guarantees identifiability of $T_{1,0}$ between abs. continuous distributions!

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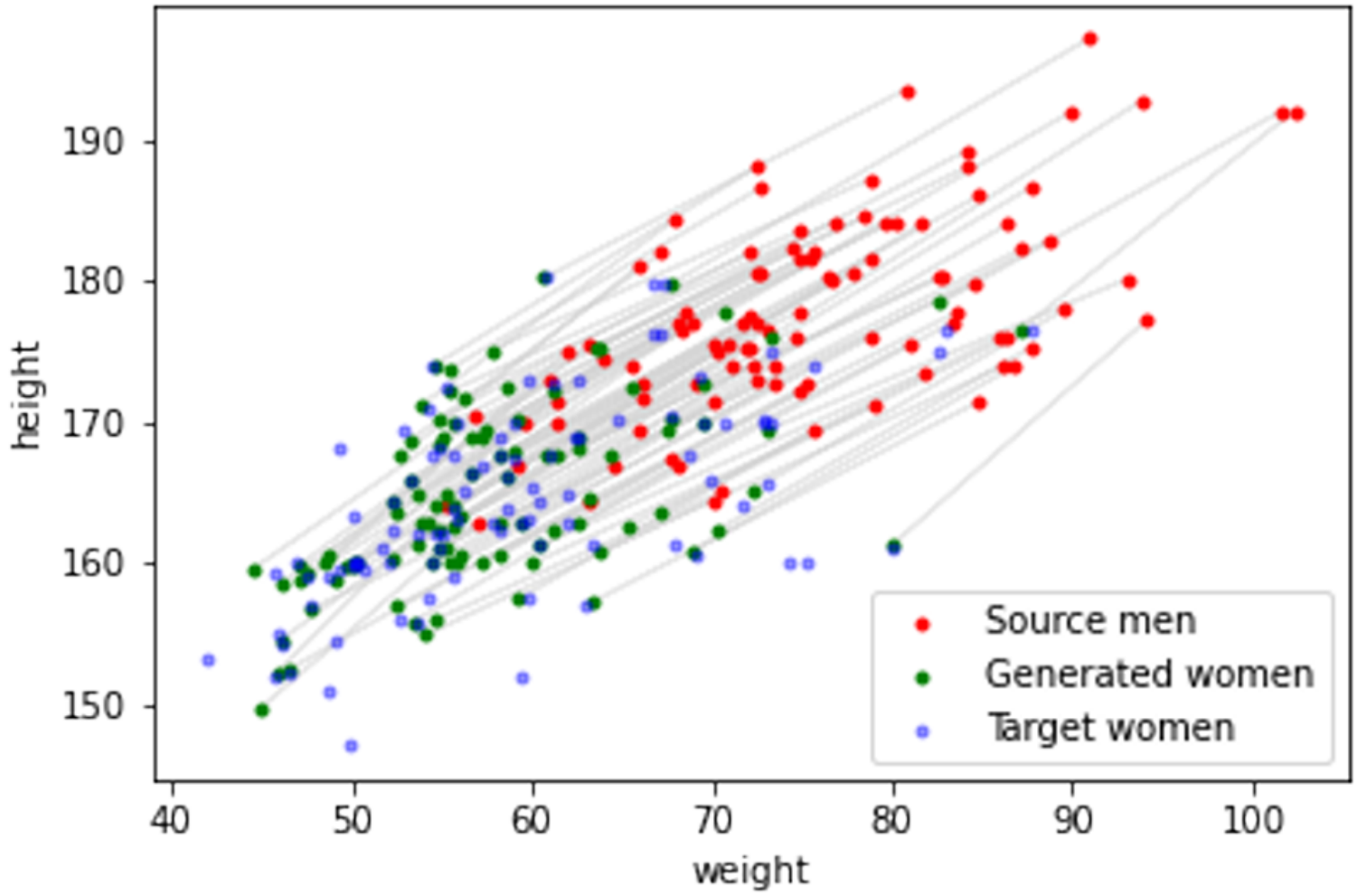
Example:[11]



[10] De Lara, L., Gonzales-Sans,A., Asher,N., Risser, L., Loubes, J.M. (2024) "Transport-based Counterfactual Models" JMLR.

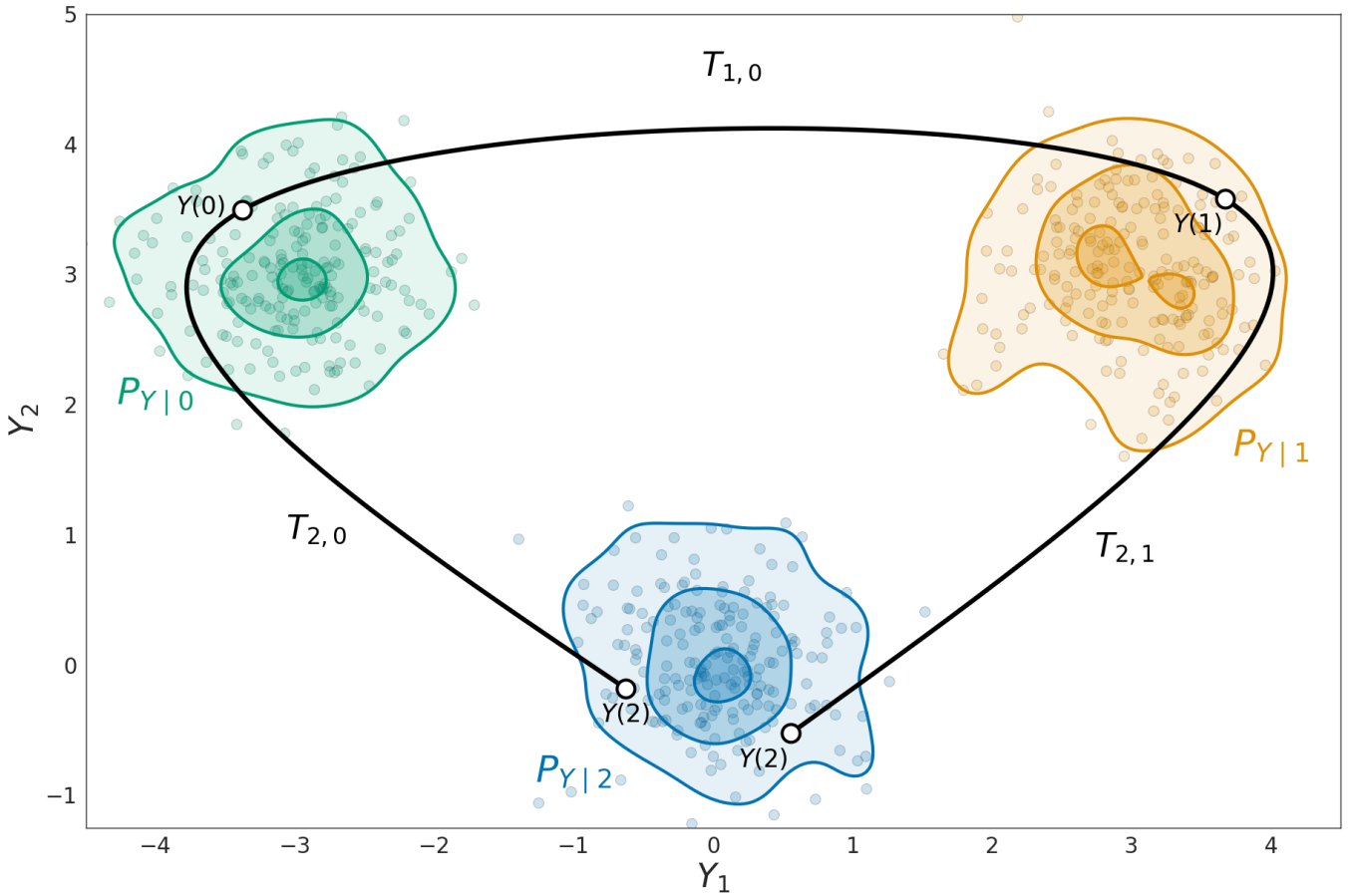
Incoherence of Transports Under Multiple treatments

Issue: If $x \in \{0, 1, 2\}$ and Y multivariate, OT maps not closed under composition!

$$T_{2,1} \circ T_{1,0} \neq T_{2,0}$$

Logical Impossibility:

$$Y(2) = T_{2,1} \circ T_{1,0}(Y(0)) \neq T_{2,0}(Y(0)) = T_{2,0} \circ T_{0,2}(Y(2)) = Y(2)$$



Example: Gaussian Transport

Three Multivariate Gaussians:

$$\mathbb{P}_0 = \mathcal{N}(\mu_0, \Sigma_0), \quad \mathbb{P}_1 = \mathcal{N}(\mu_1, \Sigma_1), \quad \mathbb{P}_2 = \mathcal{N}(\mu_2, \Sigma_2)$$

Brenier (OT) Map:

$$T_{x,x'}(y) = \mu_{x'} + \Sigma_x^{-1/2}\left(\Sigma_x^{1/2}\Sigma_{x'}\Sigma_x^{1/2}\right)^{1/2}\Sigma_x^{-1/2}(y - \mu_x)$$

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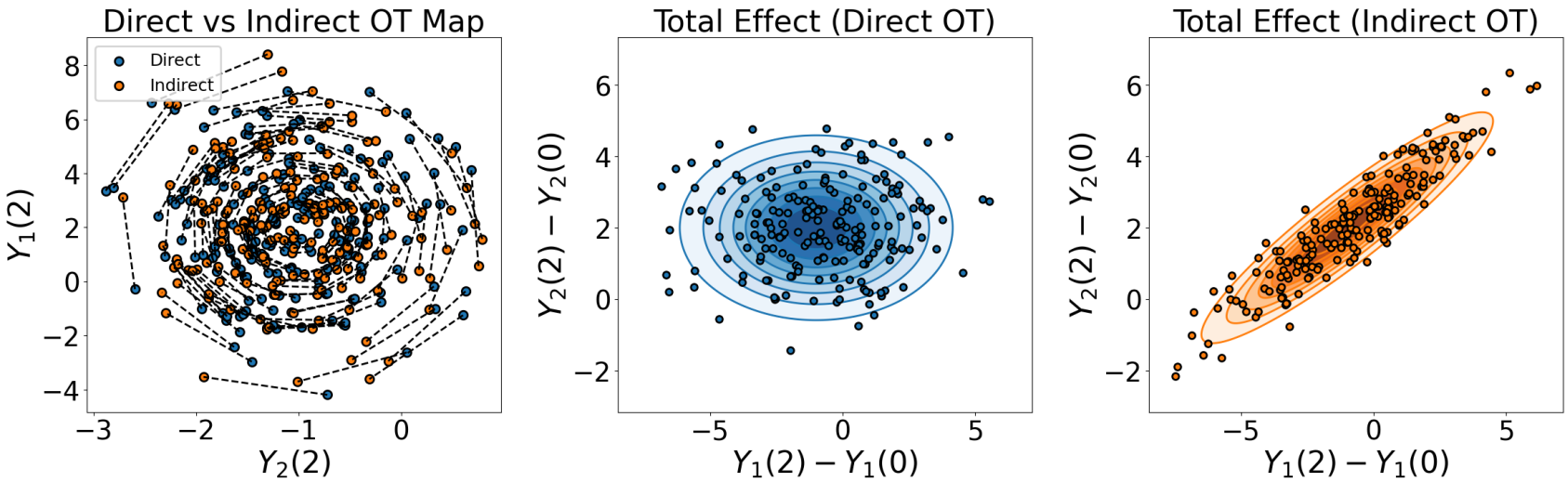
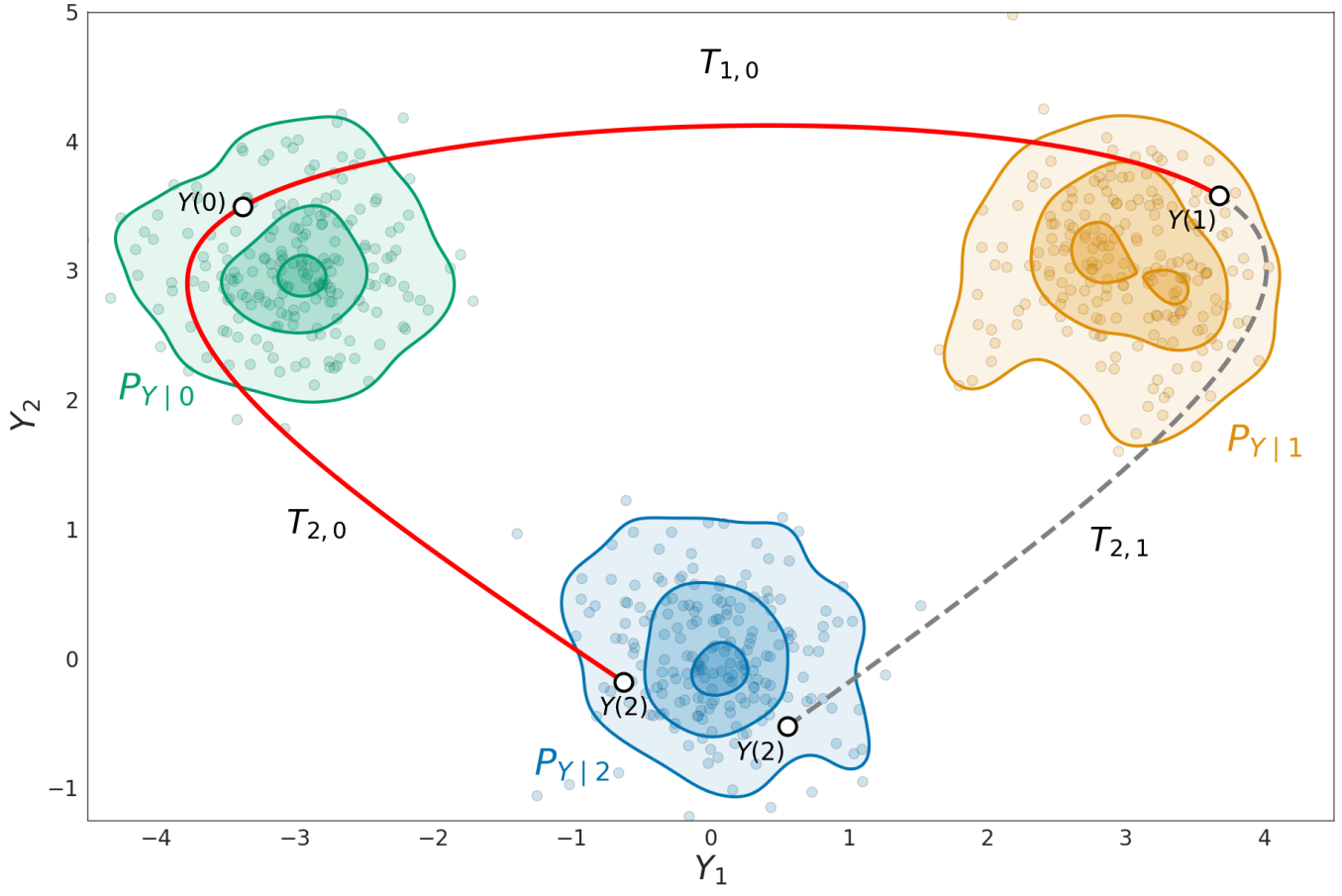
Illustration: Draw $Y(0) \sim \mathbb{P}_0$ and impute $Y(1)$, $Y(2)$

- **Direct:** $Y(1) = T_{1,0}(Y(0))\,, \quad Y(2) = T_{2,0}(Y(0))$
- **Indirect:** $Y(1) = T_{1,0}(Y(0))\,, \quad Y(2) = T_{2,1} \circ T_{1,0}(Y(0))$



Selecting Transport Subsets Induces Coupling Non-Identifiability



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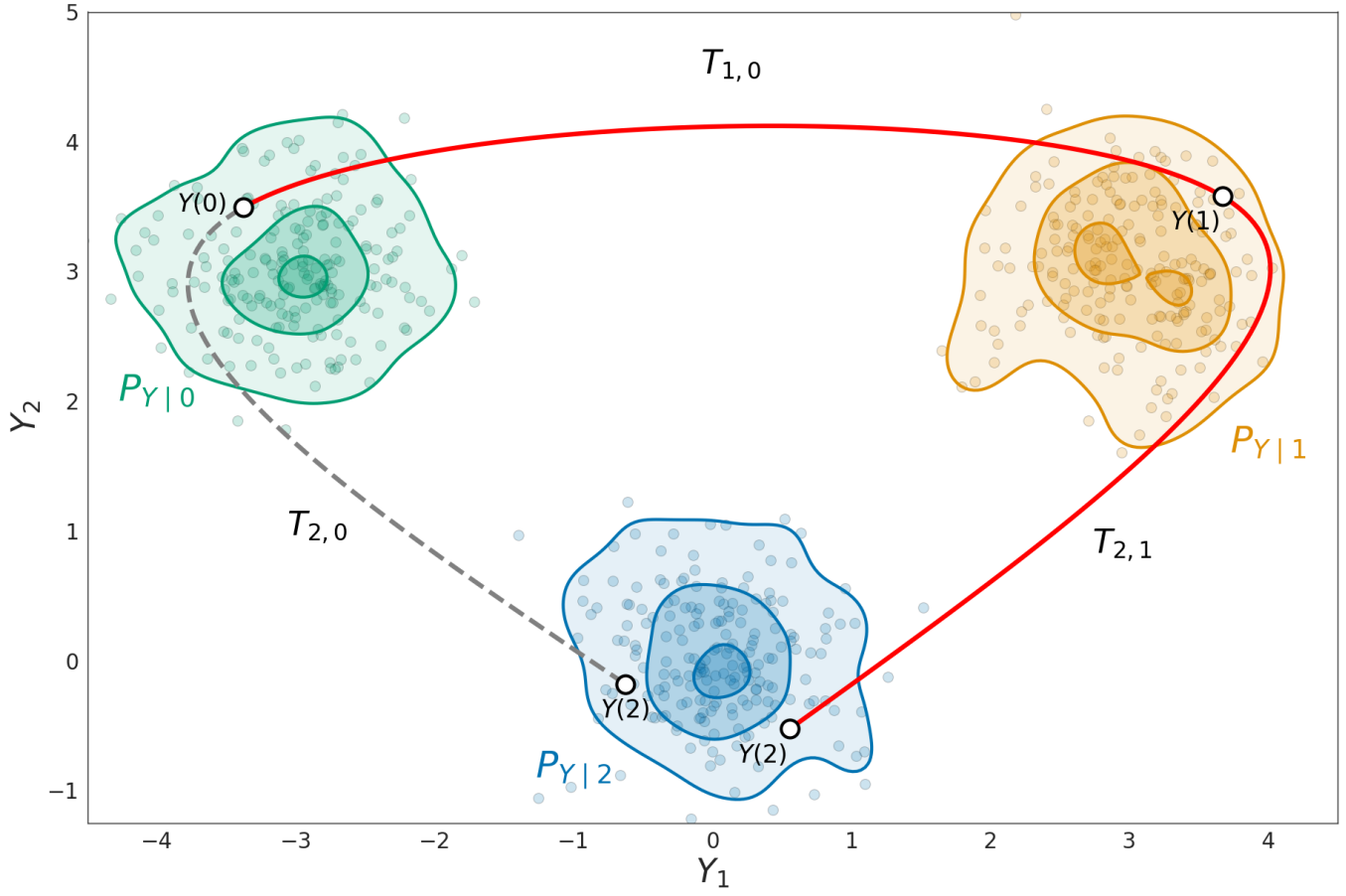


Transport-based Models with Cocycles

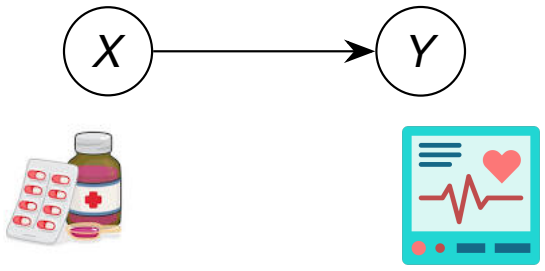
Goals

Modeling and Estimation Framework for counterfactual couplings that:

- Guarantees Coherence
- Avoids Latent Noise Assumptions

Formal Set-up

Treatment $X \in \mathbb{R}$, Outcomes $Y := (Y_1, \ldots, Y_p) \in \mathbb{R}^p$



Counterfactuals: There exist 'potential outcomes' $\{Y(x)\}_{x \in \mathbb{X}}$ satisfying

- Consistency: $X = x \implies Y(x) = Y$
- Exchangeability: $Y(x) \perp\!\!\!\perp X$

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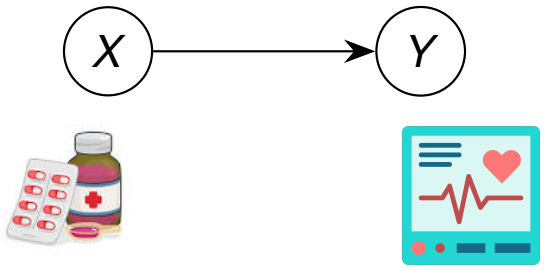

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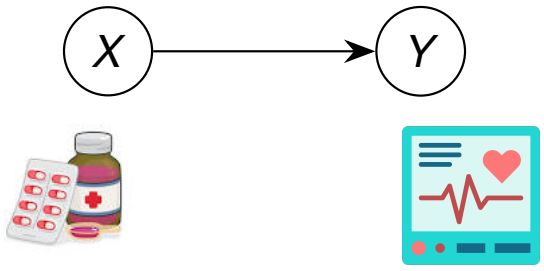

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Transport-based model:

$$Y(x) = T_{x,x'}(Y(x')), \quad \forall x, x' \in \mathbb{X} \tag{CC}$$

Necessary Algebraic Properties

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1. **Distribution Adaptedness**: For each $x, x' \in \mathbb{X}$,

$$(T_{x',x})_{\#}\mathbb{P}_{Y|X=x} = \mathbb{P}_{Y|X=x'} \tag{DA}$$

2. **Identity**: For each $x \in \mathbb{X}$:

$$T_{x,x}(y) = y, \quad \forall y \in \mathbb{Y}_x \tag{ID}$$

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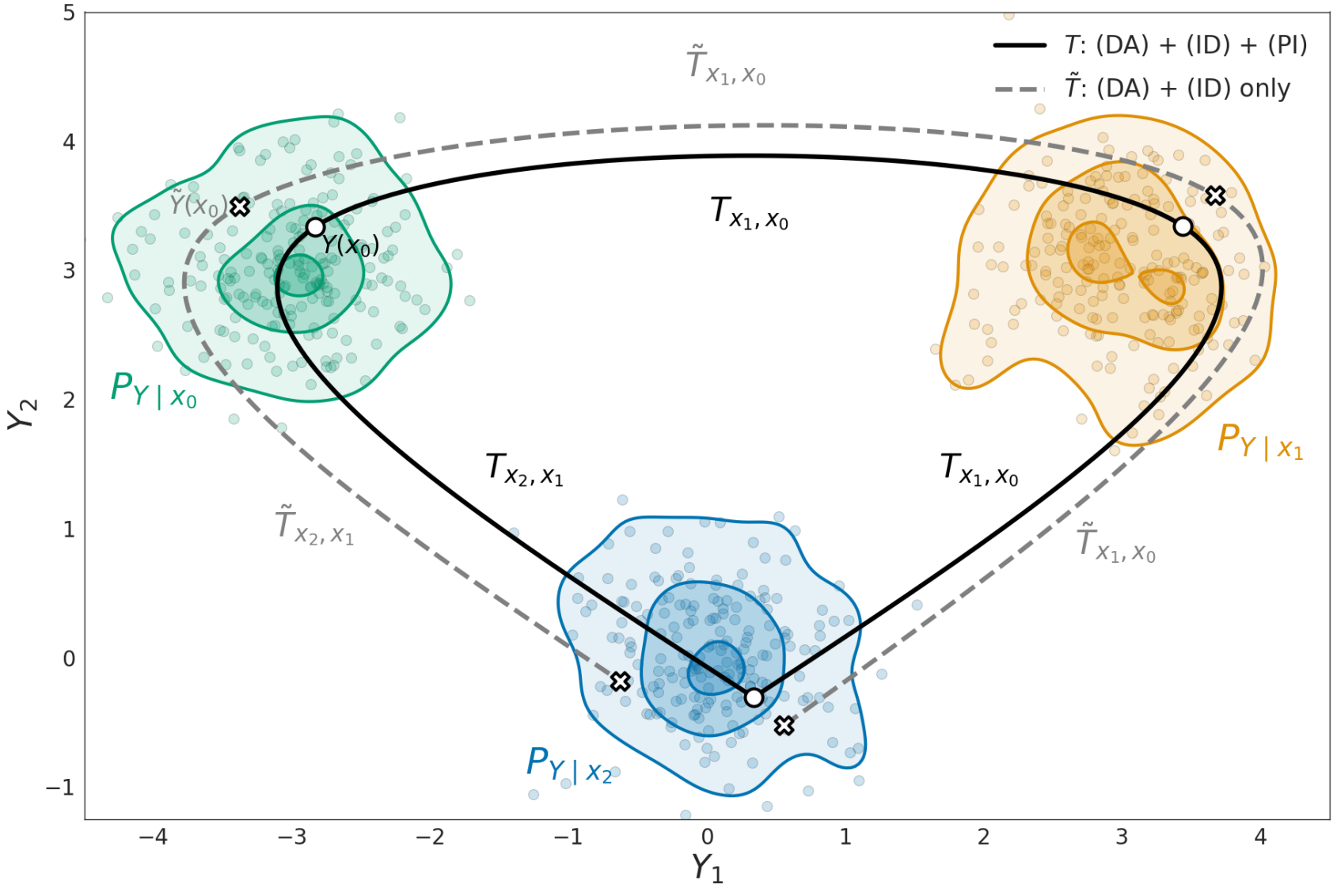
ID + PI = properties of a cocycle!

Importance of Path Independence



Sufficiency of Cocycle Properties for Admissible Transports

Are (DA) + (ID) + (PI) *sufficient* to enforce $Y(x) = T_{x,x'}(Y(x'))$? not quite!

But, they do guarantee the existence of *some* counterfactuals $\{\tilde{Y}(x)\}_{x\in\mathbb{X}}$:

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...how to enforce (ID) + (PI) + (DA) uniquely?

Structure of Counterfactual Cocycles

Theorem 1 (Cocycle Factorization)

Every cocycle T satisfying (ID), (PI), *and* (DA) *w.r.t.* $\mathbb{P}_{Y|X}$ *can be represented as:*

$$T_{x,x'} = f_x \circ f_{x'}^{+}, \quad \mathbb{P}_{Y|X=x'}\text{-a.s.}$$

Where $f_x : \mathbb{Y}_0 \to \mathbb{Y}$ *is injective with left-inverse* f_x^{+}

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Implication: Can construct classes of cocycles via parameterized bijections!

$$\mathcal{F} \subseteq \left\{ f : \mathbb{X} \times \mathbb{Y} \to \mathbb{Y} \;\middle|\; f_x := f(x, \bullet) \text{ bijective } \forall x \in \mathbb{X} \right\}$$

Examples: Normalizing flows, invertible NNs...

Can we use OT maps to construct a cocycle?

- Set $f_x := T^{(OT)}_{x,x_0}$ and $f^+_x := T^{(OT)}_{x_0,x}$
- Since OT maps are invertible: $f^+_x \circ f_x = \mathrm{id} \implies$ **Left inverse!**

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Since OT maps already satisfy (DA) + (NI) wrt. $P_{Y|X}$...

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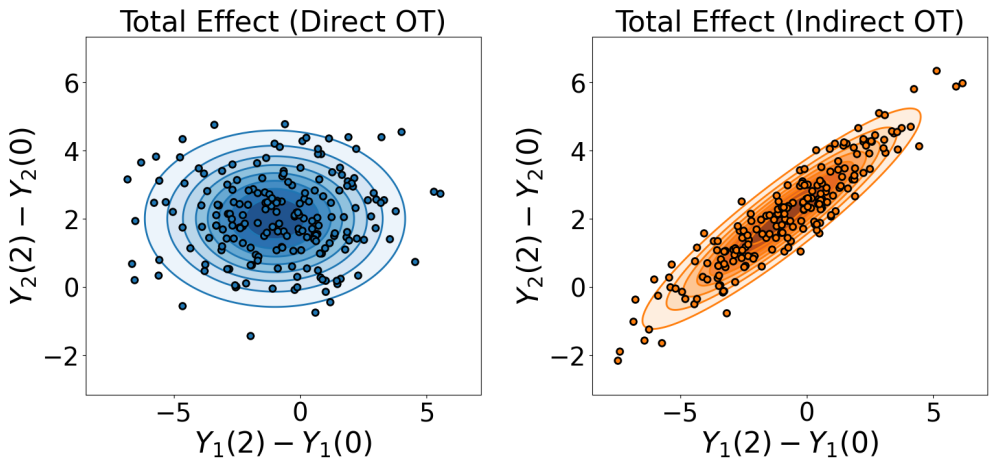
Problem: Construction depends on x_0!

- Direct: $x_0 = 0$

$$T_{x,x'} = T^{(OT)}_{x,0} \circ T^{(OT)}_{0,x'}$$

- Indirect: $x_0 = 1$

$$T_{x,x'} = T^{(OT)}_{x,1} \circ T^{(OT)}_{1,x'}$$



Identifiability of Counterfactual Cocycles

Some Preliminaries

- If $f_x : \mathbb{Y} \to \mathbb{Y}$ is exactly invertible, $f_x \in \mathbb{G}$ (transformation group on $\mathbb{Y}$)

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Theorem 2 (Identifiability of Counterfactual Cocycle)

Fix $x_0 \in \mathbb{X}$, and let T be a $\mathbb{P}_{Y|X}$-adapted, $\mathbb{G}$-valued cocycle with coboundary map f.

$$T \text{ is identifiable in } \mathcal{F}_{\mathbb{G}} \Leftrightarrow (\mathbb{P}_{Y|X=x_0})|_{\mathbb{G}} \subseteq [id]_{\mathbb{P}_{Y|X=x_0}}$$

Smaller $\mathbb{G} \implies$ better for identifiability, worse for flexibility...

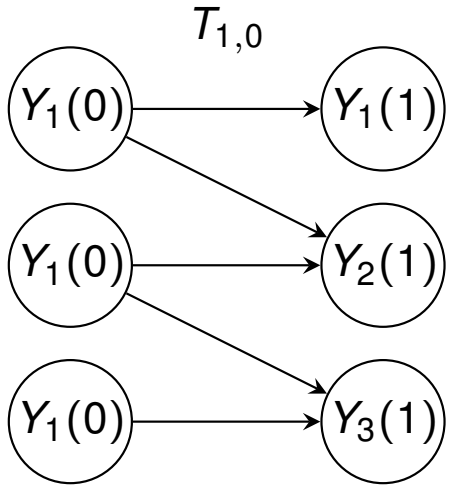
Practical Identifiability of Counterfactual Cocycles

Under known *causal ordering* of outcomes

$$Y_1 \prec Y_2 \prec \cdots \prec Y_p$$

...natural to constrain $T_{x,x'}$ to be *lower triangular*:

$$f_x(y) = \big(f_{x,1}(y_1), \ldots, f_{x,p}(y_1, \ldots, y_p)\big)$$



Practical Identifiability of Counterfactual Cocycles

Under known *causal ordering* of outcomes

$$Y_1 \prec Y_2 \prec \cdots \prec Y_p$$

...natural to constrain $T_{x,x'}$ to be *lower triangular*:

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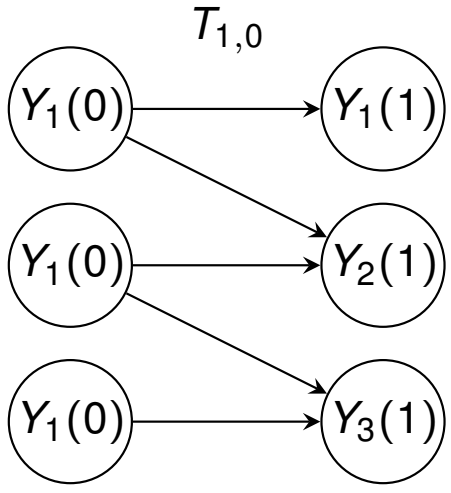

Enforcing conditional rank preservation leads to $f_x \in \mathbb{G}_{\text{TMI}}$!

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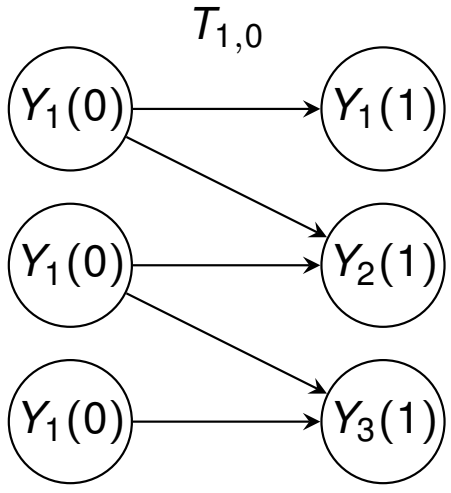

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- Can use autoregressive flows!
- Wait...isn't this just a flow-based BCM?

Model	**Autoregressive transform** $f_j(v_{<j}, \xi_j)$
NICE (Additve)	$\xi_j + \mu_j(v_{<j})$
MAF (Affine)	$\xi_j \mapsto \exp\big(\lambda_j(v_{<j})\big)\, \xi_j + \mu_j(v_{<j})$
NAF (INN)	$\xi_j \mapsto \sigma^{-1}(w(v_{<j}) \cdot \sigma(\sigma_j(v_{<j})\xi_j + \mu_j(v_{<j})))$
NSF (Spline)	$\xi_j \mapsto v_j 1_{v_j \notin [-B,B]} + M_j(\xi_j; v_{<j}) 1_{v_j \in [-B,B]}$

Connection to SCMs

Theorem 4 (Cocycle Equivalence to Structural Model)

$\{Y(x)\}_{x\in\mathbb{X}}$ *satisfies Exchangeability, Consistency and*

$$Y(x) = T_{x,x'}(Y(x')) \quad \forall x, x' \in \mathbb{X}$$

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Under TMI cocycle restriction, we recover Acyclic BCM $Y_j = f_j(Y_{<j}, X, \xi_j)$ again!

Our Idea: Center everything around the cocycle

Aim: Do all estimation and inference without ever referencing or specifying $\mathbb{P}_\xi$

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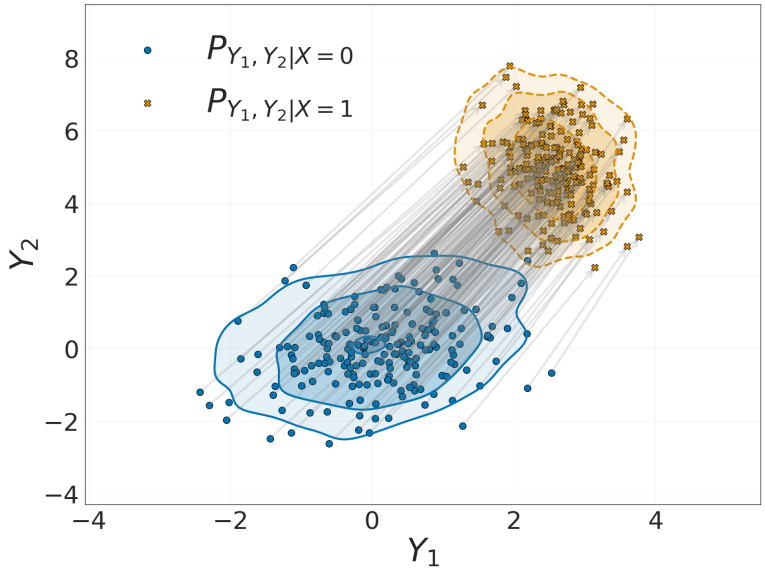
1. Directly target $T_{x,x'}$ between conditionals:

$$\ell(T) = \mathbb{E}_{x,x'} D(\mathbb{P}_{Y|X=x}, (T_{x,x'})_{\#}\mathbb{P}_{Y|X=x'})^2$$

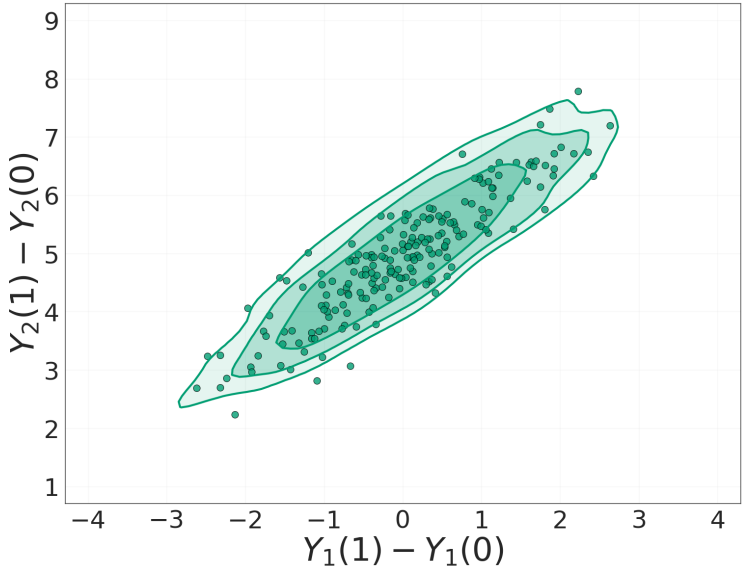


2. Use T to impute counterfactuals:

$$Y^{(i)}(x) = T_{x,X^{(i)}}(Y^{(i)})$$

... and empirically estimate quantities:

$$\widehat{THR} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}(Y^{(i)}(1) \prec Y^{(i)}(0))$$



Benefits of Counterfactual Cocycle Modelling

Noise Invariance and Model Mis-Specification

$$(\hat{f}_x)_{\#} : \hat{\mathbb{P}}_{\xi} \mapsto \mathbb{P}_{Y|X=x}, \qquad (T_{x,x'})_{\#} = (f_x \circ f_{x'}^{+})_{\#} : \mathbb{P}_{Y|X=x'} \mapsto \mathbb{P}_{Y|X=x}$$

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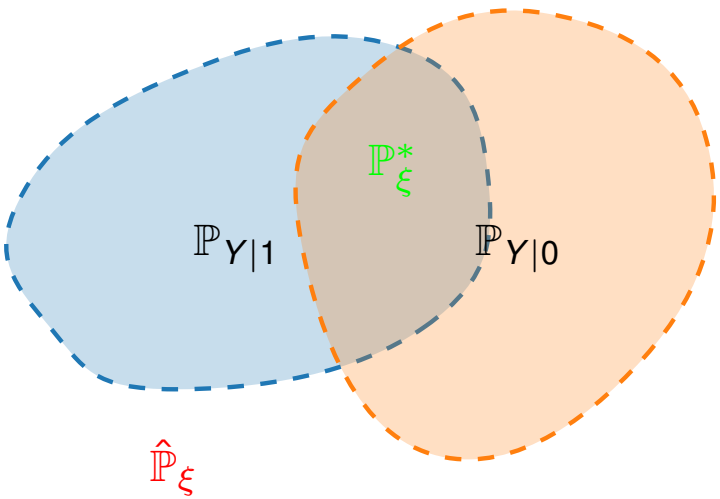
RCT case: $x \in \{0, 1\}$

- Consider class of functions $\mathcal{F}$ for $(f_x)_{\in\{0,1\}}$
- Let $\mathcal{P}_1(\mathcal{F}), \mathcal{P}_0(\mathcal{F})$ = distributions reachable by pushing $\mathbb{P}_{Y|1}, \mathbb{P}_{Y|0}$ through each $f^+ \in \mathcal{F}^+$



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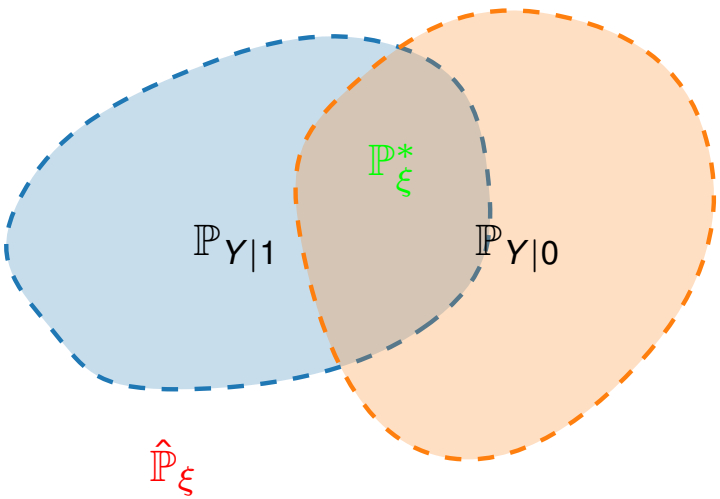

- $(\mathcal{F}, \hat{\mathbb{P}}_\xi)$ well-specified for $(f, \mathbb{P}_\xi)$ if

$$\hat{\mathbb{P}}_\xi \in \mathcal{P}_1(\mathcal{F}) \cap \mathcal{P}_0(\mathcal{F})$$

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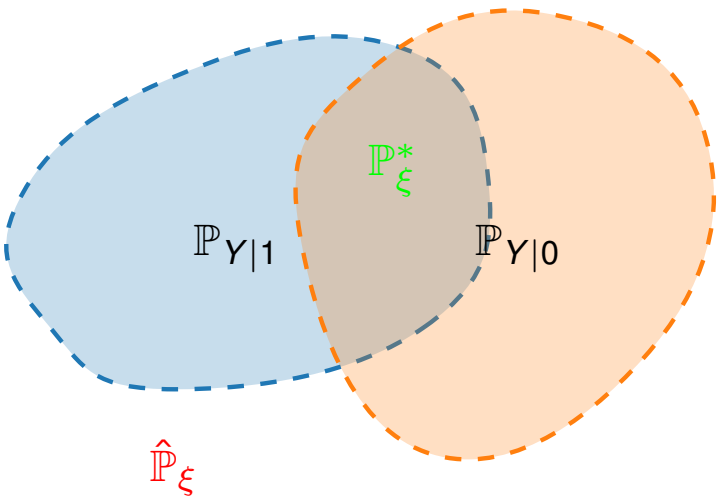

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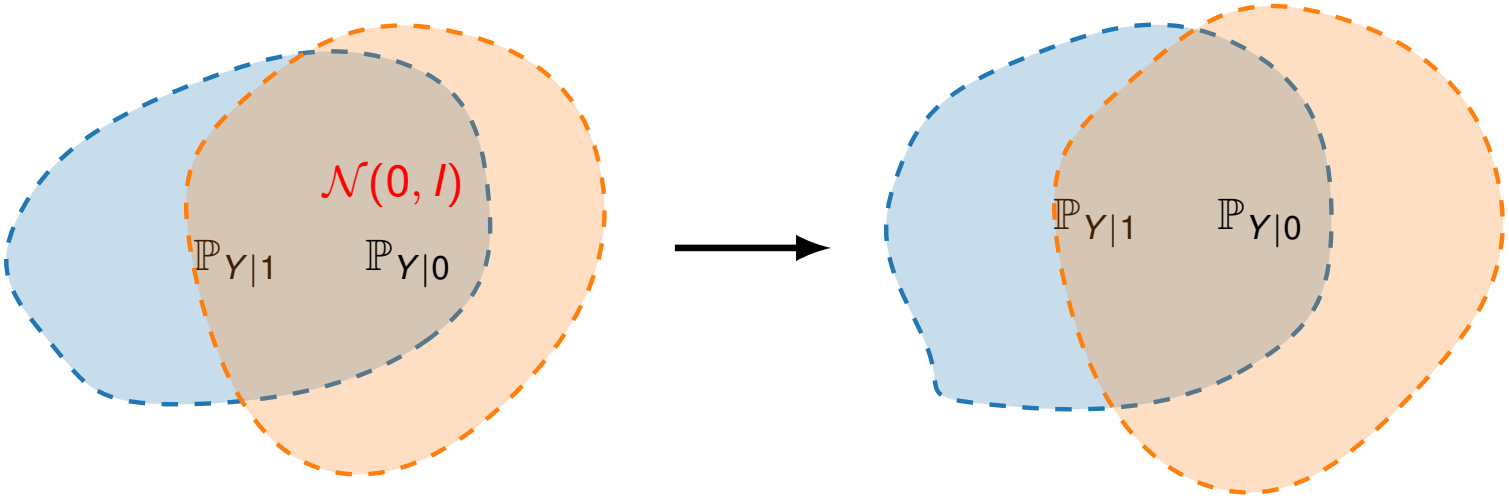
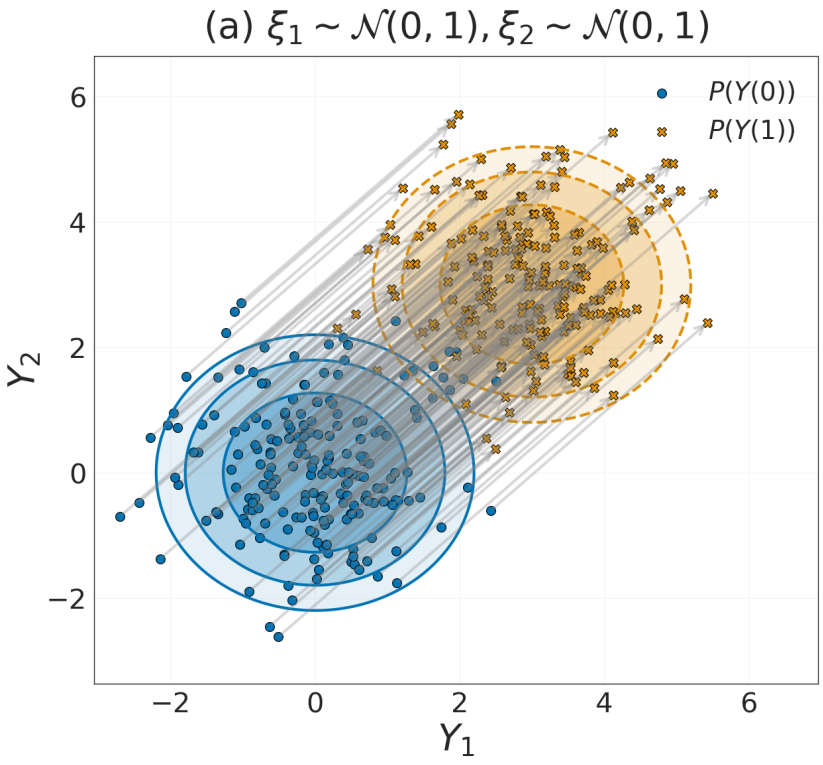
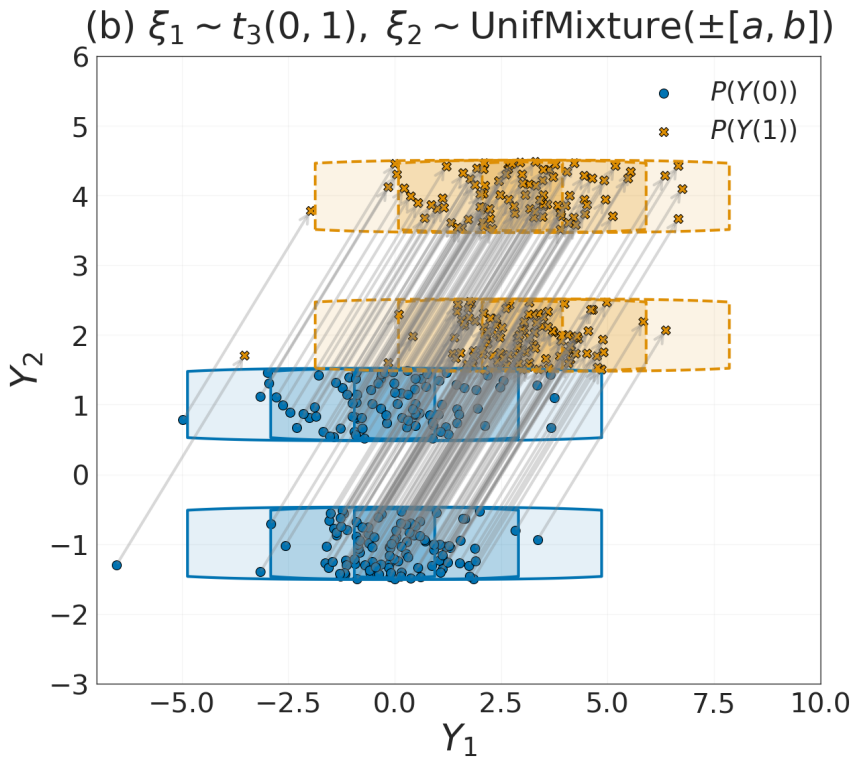
Invariance: Changing true $\mathbb{P}_\xi$ doesn't change $\mathcal{P}_1(\mathcal{F}) \cap \mathcal{P}_0(\mathcal{F}) \neq \emptyset$!

$$\tilde{Y}(x) = f_x(\tilde{\xi}) \implies \tilde{Y}(x) = f_x \circ f_{x'}^{+}(\tilde{Y}(x'))$$

Invariance Example







Noise Invariance and Minimal Complexity

Can reparameterize SCM using any bijection $g \in \mathrm{Aut}(\mathcal{E})$:

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$$\implies \text{can choose} \quad f^\star \in \arg\min_f \text{Complexity}(f) \quad \text{s.t.} \quad f \in (f^{(g)})_{g \in \mathrm{Aut}(\mathcal{E})}$$

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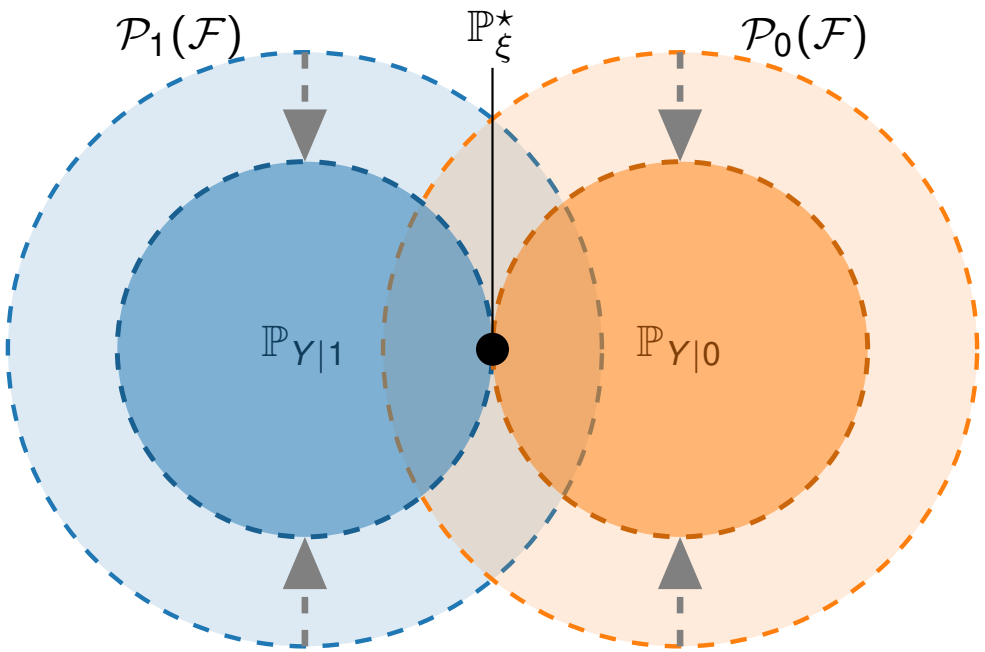

What is the optimal base distribution?

Recall $f_0, f_1 \in \mathbb{G} \implies T$ is $\mathbb{G}$-valued cocycle

Define smallest transformation group containing (f_0, f_1) : $\mathbb{G}_f := \langle f_0, f_1 \rangle$

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Theorem 5 (Minimal Complexity Cocycle)

Take $(f_1^\star, f_0^\star) = (T_{1,0}, id)$*. Then:*

(i) $\mathbb{G}_{f^\star} \subseteq \mathbb{G}_{f^\star \circ g}$ *and (ii)* $\mathbb{G}_{f^\star} \not\supseteq \mathbb{G}_{f^\star \circ g}$ *whenever* $g \notin \mathbb{G}_{f^\star}$

$\implies P_{Y|0}$ is an optimal base distribution!

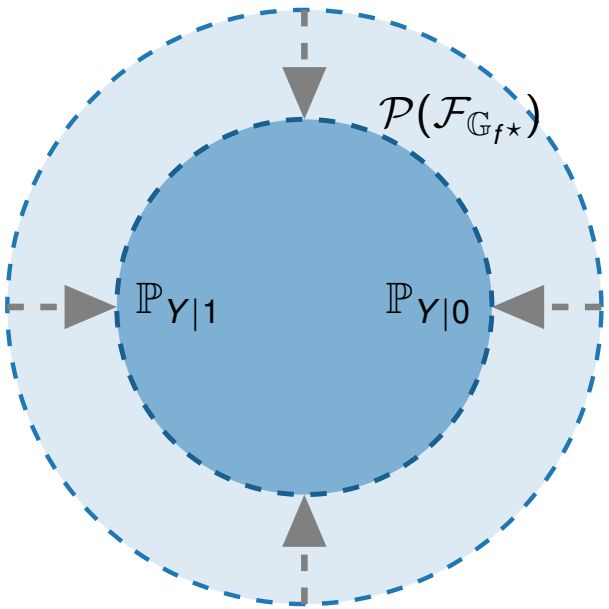
Example: $Y(x) = f_x(\xi) = x + \xi$

- Since $\mathbb{P}_\xi = \mathbb{P}_{Y|0}$:

$$f_x^\star = f_x \in \mathbb{G} = (\mathbb{R}, +)$$

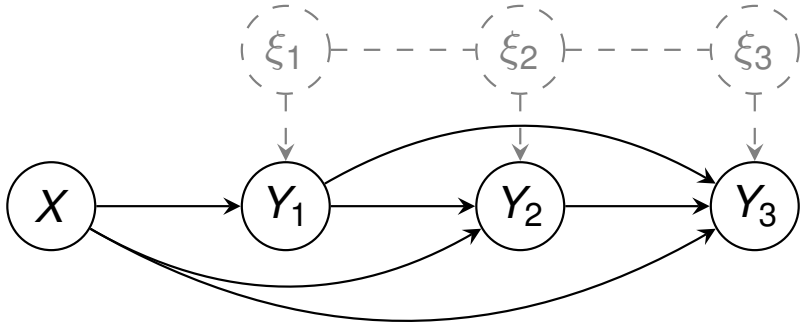
- Any $\hat{\mathbb{P}}_\xi$ not a shift of $\mathbb{P}_{Y|0}$ will need

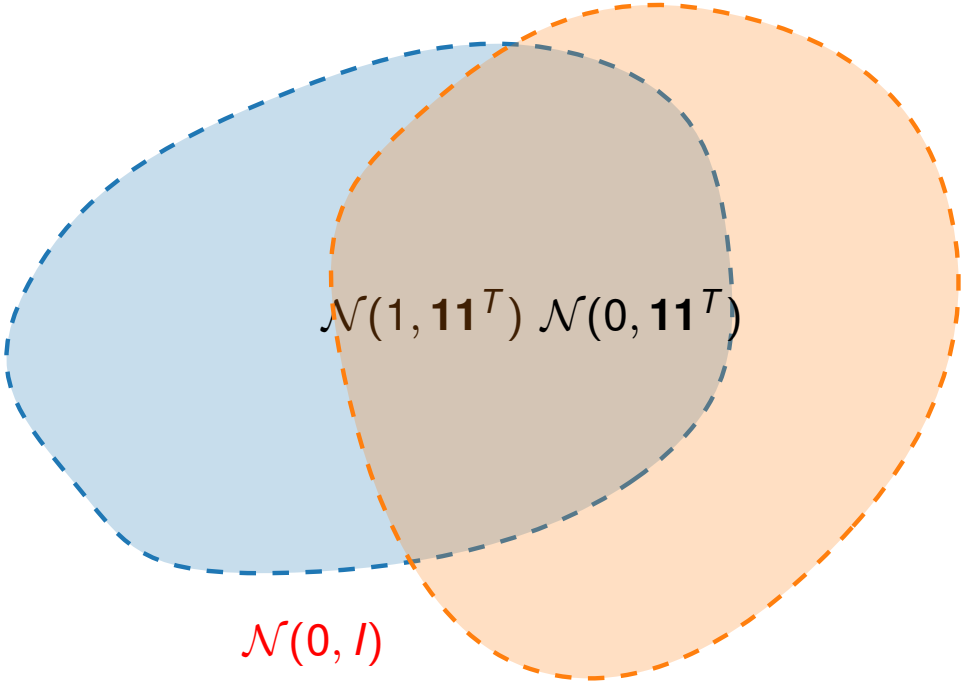
$$\hat{f}_x \in \hat{\mathbb{G}} \not\subseteq (\mathbb{R}, +)$$



Robustness to Error Dependence

Counterfactual cocycles do *not* assume independent errors!





Example: Single latent cause

- $Y = \mathbf{1}X + \xi, \quad \xi \sim \mathcal{N}(0, \mathbf{1}\mathbf{1}^T)$
- If choosing $\hat{\mathbb{P}}_\xi = \mathcal{N}(0, I)$, then even

$$\mathcal{F} = \{f : \mathbb{Y} \to \mathbb{Y} \text{ is bijective}\}$$

... is mis-specified for f_0, f_1...

Cocycle Estimation

Estimating cocycles by minimising a distributional distance

Disrecpancy in (DA):

$$\tilde{\ell}(T) = \mathbb{E}_{X,X' \sim P_X} D(\mathbb{P}_{Y|X=X}, (T_{X,X'})_{\#}\mathbb{P}_{Y|X=X'})^2$$

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Issues:

1. Can't generally compute D in closed form since $\mathbb{P}_{Y|X}$ is unknown
2. No obvious empirical analogue $\tilde{\ell}_n(T) \to_p \tilde{\ell}(T)$.

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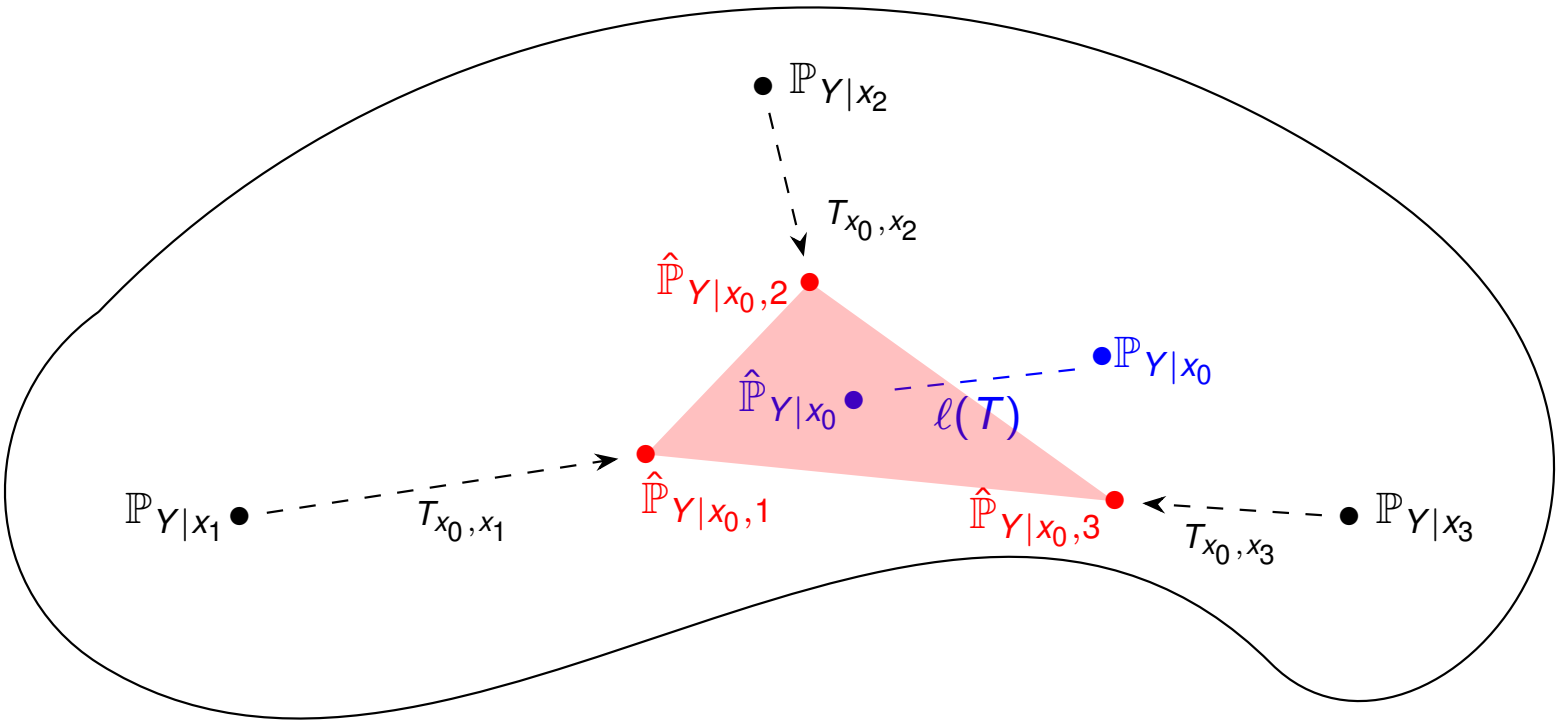
MMD Example: $\tilde{\ell}(T) = \mathbb{E}\|\mathbb{E}[\psi(Y)|X] - \mathbb{E}[\psi(T_{X,X}(Y')|X, X']\|^2_{\mathcal{H}_k}$

... would need to learn conditional expectations $\mathbb{E}[\psi(Y)|X]$, $\mathbb{E}[\psi(T_{X,X}(Y')|X, X']$...

A second attempt at the estimation objective

Idea: move expectation over X' inside the metric

$$\ell(T) = \mathbb{E}_{X \sim P_X} D(\mathbb{P}_{Y|X=X}, \mathbb{E}_{X' \sim P_X}[(T_{X,X'})_{\#}\mathbb{P}_{Y|X=X'}])^2$$



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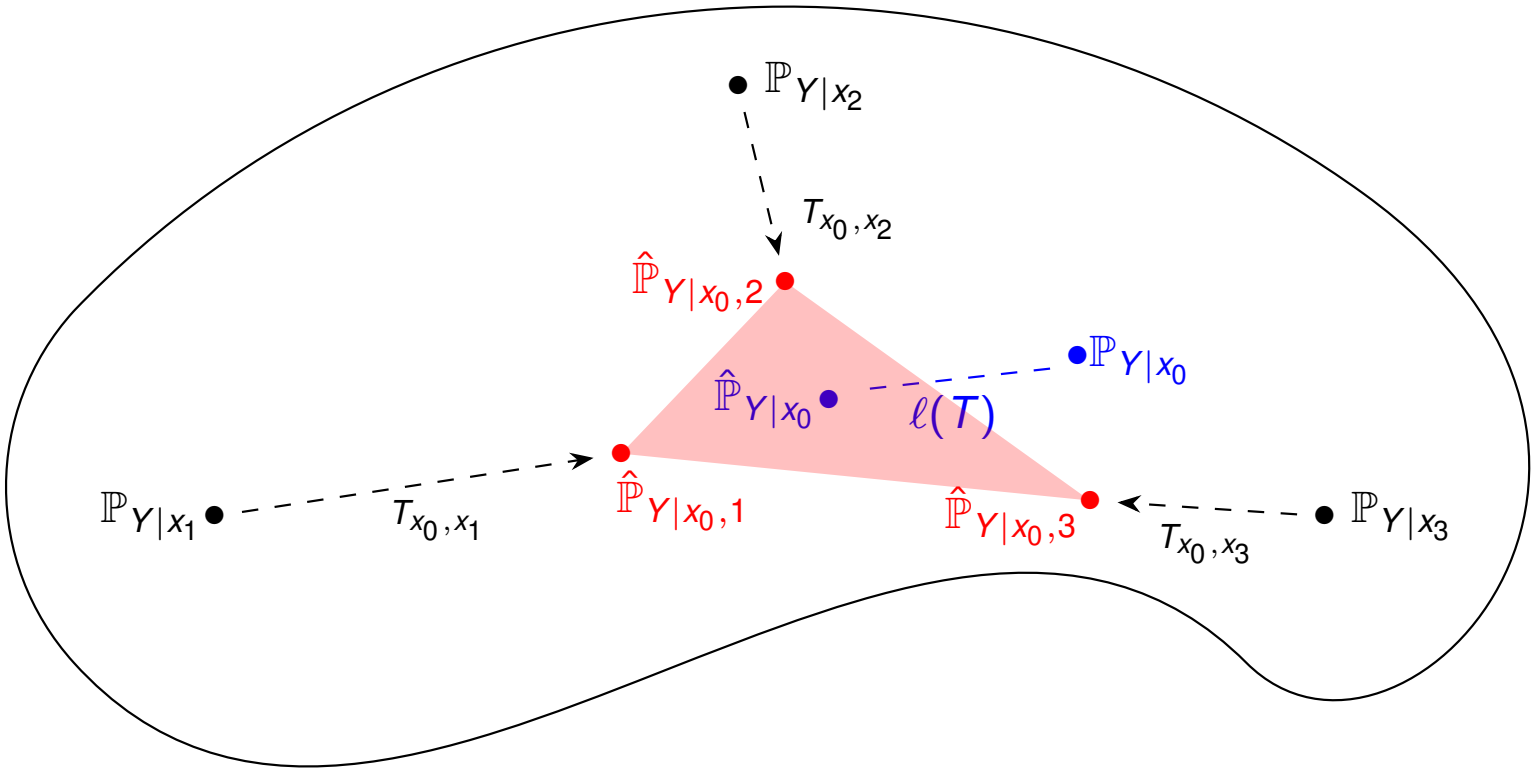

- We prove $\arg\min_T \ell(T) = \arg\min_T \tilde{\ell}(T)$ in the well-specified setting!
- $\ell(T)$ can be estimated with simple empirical averages when $D = \text{MMD}$!

Cocycle Conditional Maximum Mean Discrepancy (CMMD)

CMMD: Take $D =$ as Maximum Mean Discrepancy:

$$\ell(T) = \mathbb{E} \left\| \psi(Y) - \mathbb{E}[\psi(T_{X,X'}(Y')|X] \right\|^2_{\mathcal{H}} + \text{constant}$$

Empirical analogue V-statistic :

$$\ell_n(T) = \frac{1}{n} \sum_i^n \left\| \psi(Y^{(i)}) - \frac{1}{n} \sum_j^n \psi(T_{X^{(i)},X^{(j)}}(Y^{(j)})) \right\|^2_{\mathcal{H}}$$

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Theoretical properties

1. Under bounded, characteristic kernel k: $\ell_n(T) \to_{a.s.} \ell(T)$
2. Under continuous+compact+identifiable T: $\hat{T}_n \to_{a.s.} T$
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In context of BCM $Y = f(X, \xi)$, consistency of $\hat{T}$ does not depend on properties of ξ!

Extension to Larger Systems and Confounding

Current RCT setting implies:

$$Y = f(X, \xi), \quad X \perp\!\!\!\perp \xi, \quad f(X, \bullet) \text{ injective}$$

Limitations

- Injectivity will break if too many independent causes $\xi_1, \ldots, \xi_m$
- Independence will break under confounding

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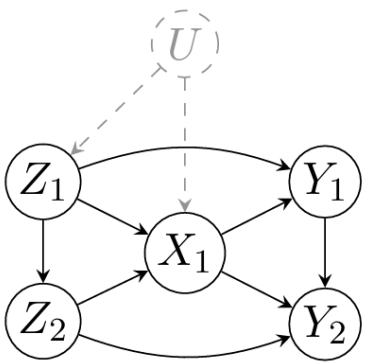
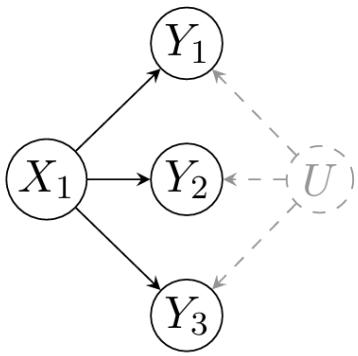
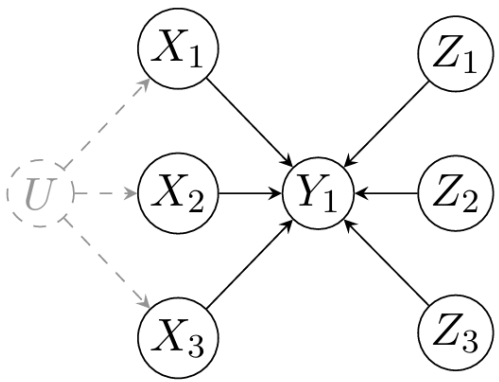
$$Z \prec X \prec Y$$







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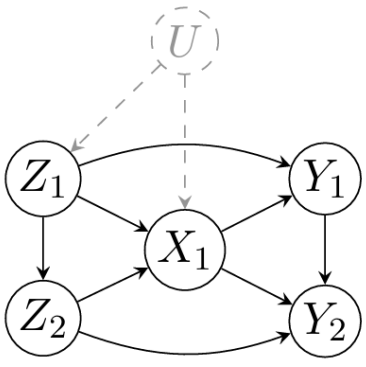
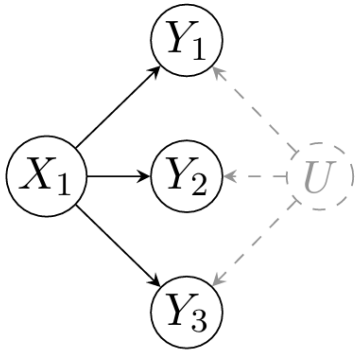
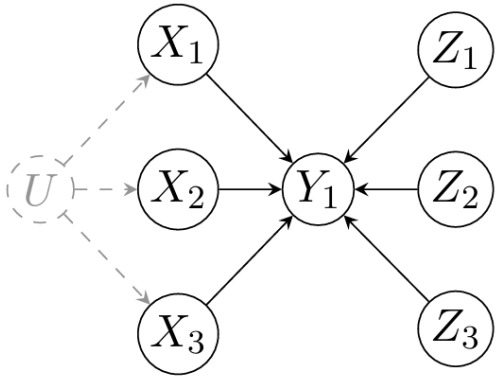




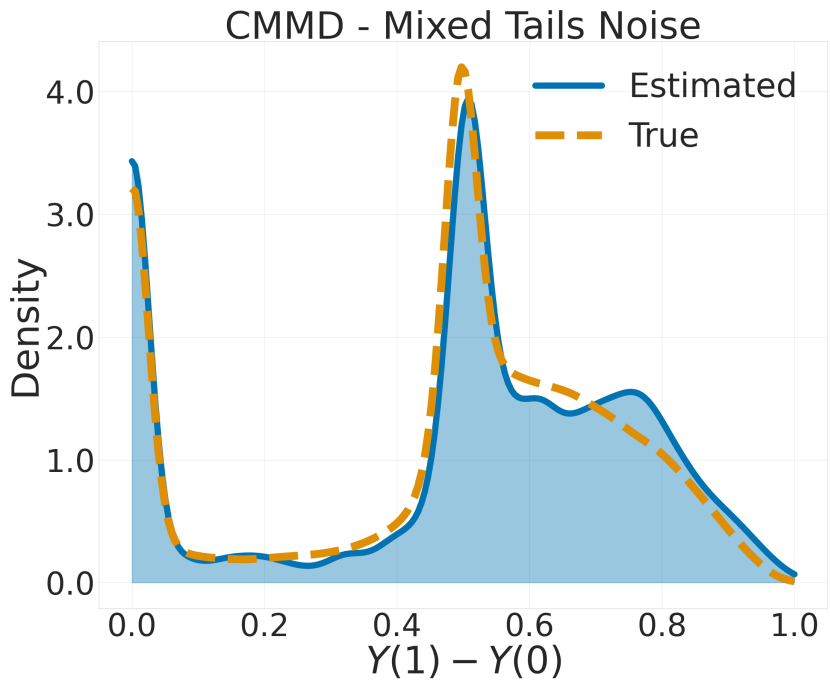


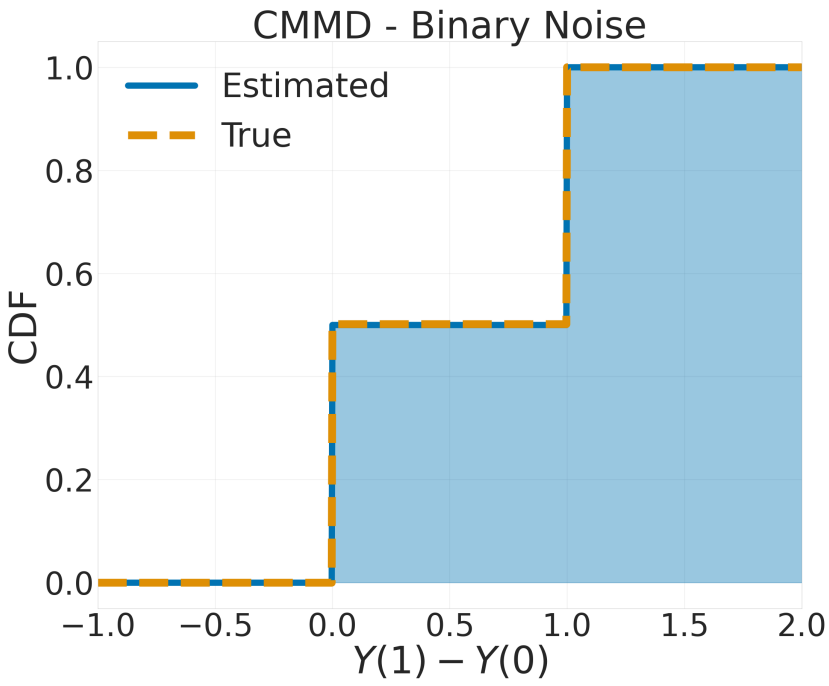
Idea: Do everything on counterfactuals $\{Y(x, z)\}_{(x,z)\in\mathbb{X}\times\mathbb{Z}}$ that relate to $Y(x)$ via nested consistency property: $Y(x) := Y(x, Z)$.

$$Y(x) = T_{(x,Z),(x',Z)}(Y(x'))$$

Experiments

Demonstration on the Toy Example





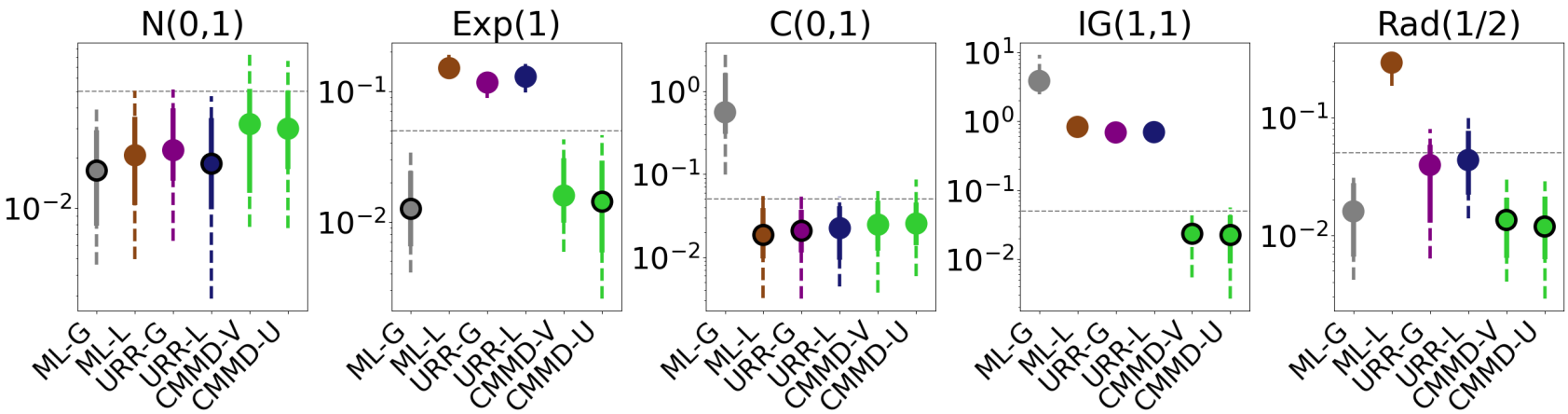
Noise Ablation vs flow-based SCMs

$$Y = X + \xi$$

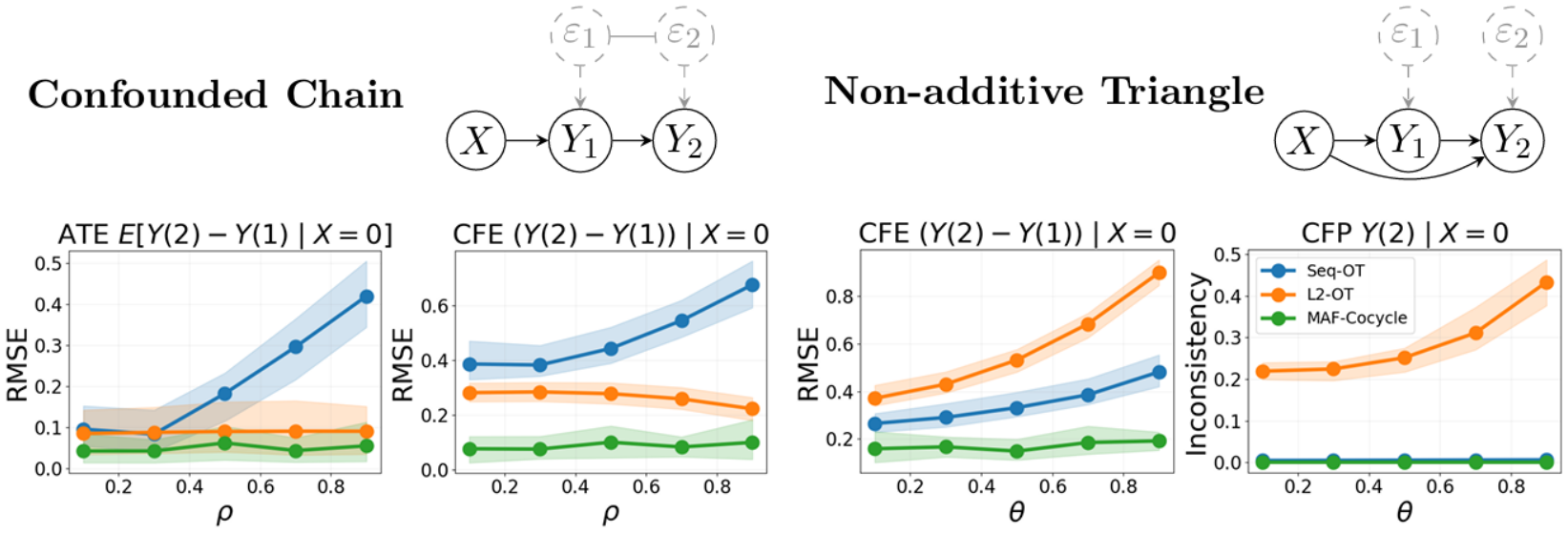
Method	$\mathbb{P}_\xi = \mathsf{N}(0,1)$	$\mathbb{P}_\xi = \mathsf{Ga}(1,1)$	$\mathbb{P}_\xi = \mathsf{t}_1(0,1)$	$\mathbb{P}_\xi = \mathsf{IG}(1,1)$	$\mathbb{P}_\xi = \mathsf{Rad}(1/2)$
Interventional KS					
ML-G	$\mathbf{0.015 \pm 0.007}$	0.081 ± 0.041	0.121 ± 0.079	0.208 ± 0.162	0.405 ± 0.069
ML-L	0.055 ± 0.010	0.074 ± 0.036	0.110 ± 0.069	0.120 ± 0.090	0.415 ± 0.067
ML-T	0.018 ± 0.008	0.079 ± 0.040	0.029 ± 0.007	0.075 ± 0.031	0.412 ± 0.062
CMMD-V	0.028 ± 0.009	$\mathbf{0.027 \pm 0.008}$	$\mathbf{0.027 \pm 0.009}$	$\mathbf{0.027 \pm 0.008}$	$\mathbf{0.271 \pm 0.031}$
CMMD-U	$\mathbf{0.010 \pm 0.004}$	$\mathbf{0.012 \pm 0.005}$	$\mathbf{0.008 \pm 0.003}$	$\mathbf{0.009 \pm 0.004}$	$\mathbf{0.268 \pm 0.008}$
Counterfactual RMSE					
ML-G	$\mathbf{0.035 \pm 0.035}$	0.277 ± 0.118	113.667 ± 341.875	114.946 ± 147.841	0.326 ± 0.258
ML-L	0.036 ± 0.028	0.258 ± 0.073	97.745 ± 351.815	112.300 ± 165.014	0.480 ± 0.294
ML-T	$\mathbf{0.033 \pm 0.031}$	0.270 ± 0.097	0.044 ± 0.053	29.872 ± 41.628	0.391 ± 0.307
CMMD-V	$\mathbf{0.035 \pm 0.026}$	$\mathbf{0.020 \pm 0.015}$	$\mathbf{0.040 \pm 0.031}$	$\mathbf{0.028 \pm 0.024}$	$\mathbf{0.017 \pm 0.019}$
CMMD-U	0.040 ± 0.027	$\mathbf{0.022 \pm 0.016}$	$\mathbf{0.033 \pm 0.027}$	$\mathbf{0.027 \pm 0.023}$	$\mathbf{0.014 \pm 0.011}$
True Architecture Selection %					
ML-G	96%	14%	0%	2%	2%
ML-L	**100%**	2%	4%	0%	0%
ML-T	98%	8%	94%	0%	0%
CMMD-V	**100%**	**100%**	**100%**	**100%**	**98%**
CMMD-U	**100%**	**100%**	**100%**	**100%**	**100%**

Noise Ablation vs flow-based SCMs

$$Y = X + \xi$$



Confounding + Non-Additivity Ablation vs OT



Performance on SCM Benchmarks

Table 4: Mean ± SD of KS_{int} and KS_{CF} on the *linear* SCMs.

Method	2var (lin)		triangle (lin)		fork (lin)		5chain (lin)	
	KS_{int}	KS_{CF}	KS_{int}	KS_{CF}	KS_{int}	KS_{CF}	KS_{int}	KS_{CF}
BGM	0.13 ± 0.07	0.19 ± 0.12	0.37 ± 0.05	0.06 ± 0.01	0.05 ± 0.07	0.61 ± 0.07	0.14 ± 0.05	0.06 ± 0.01
CausalNF	0.31 ± 0.11	0.24 ± 0.10	0.44 ± 0.05	0.06 ± 0.02	0.04 ± 0.02	0.66 ± 0.09	0.14 ± 0.02	0.06 ± 0.01
CAREFL	0.40 ± 0.04	0.15 ± 0.14	0.43 ± 0.05	0.06 ± 0.01	0.19 ± 0.01	0.58 ± 0.10	0.13 ± 0.02	0.06 ± 0.01
CocycleNF	$\mathbf{0.03 \pm 0.02}$	$\mathbf{0.04 \pm 0.04}$	$\mathbf{0.23 \pm 0.19}$	$\mathbf{0.02 \pm 0.01}$	$\mathbf{0.02 \pm 0.01}$	$\mathbf{0.19 \pm 0.23}$	$\mathbf{0.02 \pm 0.01}$	$\mathbf{0.03 \pm 0.01}$

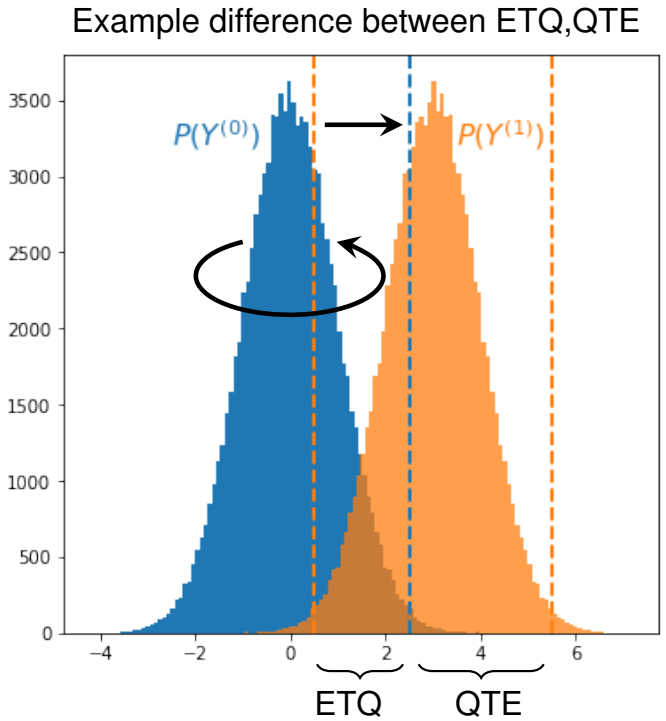
Table 5: Mean ± SD of KS_{int} and KS_{CF} on the *nonlinear* SCMs.

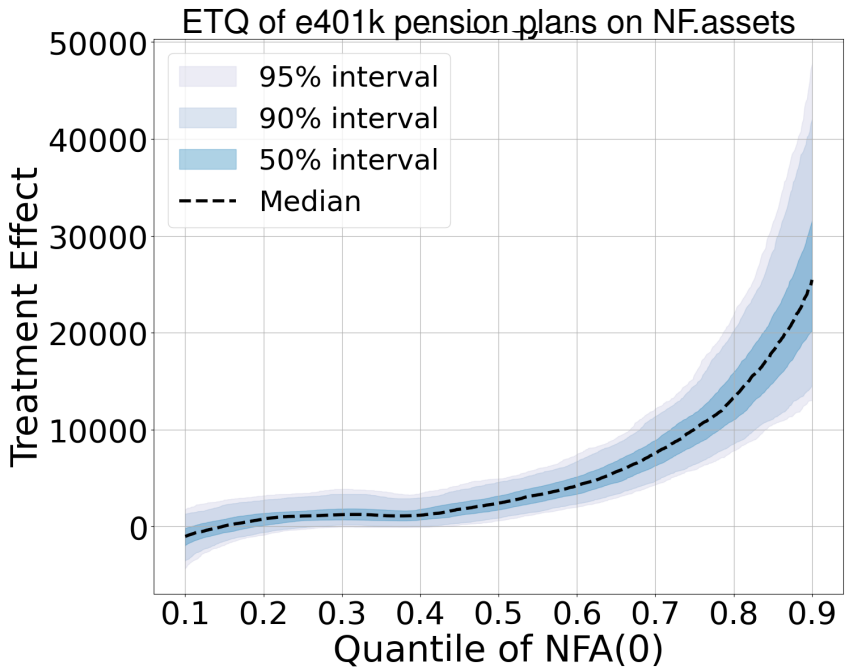
Method	2var (nonlin)		triangle (nonlin)		fork (nonlin)		5chain (nonlin)	
	KS_{int}	KS_{CF}	KS_{int}	KS_{CF}	KS_{int}	KS_{CF}	KS_{int}	KS_{CF}
BGM	0.12 ± 0.07	0.27 ± 0.13	0.41 ± 0.07	$\mathbf{0.09 \pm 0.05}$	$\mathbf{0.04 \pm 0.01}$	0.59 ± 0.08	0.07 ± 0.03	0.41 ± 0.12
CausalNF	0.30 ± 0.11	0.26 ± 0.08	0.47 ± 0.04	0.23 ± 0.08	0.07 ± 0.06	0.61 ± 0.09	0.06 ± 0.06	0.24 ± 0.16
CAREFL	0.44 ± 0.04	0.22 ± 0.15	0.47 ± 0.06	0.22 ± 0.09	0.19 ± 0.01	0.51 ± 0.21	0.17 ± 0.04	0.60 ± 0.25
CocycleNF	$\mathbf{0.04 \pm 0.02}$	$\mathbf{0.13 \pm 0.05}$	$\mathbf{0.28 \pm 0.13}$	0.20 ± 0.16	0.08 ± 0.05	$\mathbf{0.20 \pm 0.24}$	$\mathbf{0.05 \pm 0.02}$	$\mathbf{0.20 \pm 0.09}$

Counterfactual quantile effects on a real dataset

Quantile treatment effect: $\mathrm{QTE}(\tau) = Q_{Y(1)}(\tau) - Q_{Y(0)}(\tau)$

Effect of Treatment on Quantile: $\mathrm{ETQ}(\tau) = \mathbb{E}[Y^{(1)} - Y^{(0)} | Y^{(0)} = Q_{Y(0)}(\tau)]$





Summary

1. Counterfactual Cocycles as framework for Admissible counterfactual transports
2. Every counterfactual cocycle can be represented via left-invertible functions
3. Equivalent to injective SCMs, but cocycle is noise invariant + minimally complex
4. Robust cocycle estimator with consistency guarantees independent of true noise
5. Flexible parameterizations using flow-based toolkit
6. State-of-the-art performance on various benchmarks

Future Directions

1. ~~Causal discovery?~~[12]
2. More general forms of confounding?
3. Non-iid settings?
4. Stochastic cocycles?
5. Efficiency theory?

[12] Xi, J., Dance, H., Orbanz, P. & Bloem-Reddy, B. *'Distinguishing Cause From Effect with Causal Velocity Models'* (ICML25).

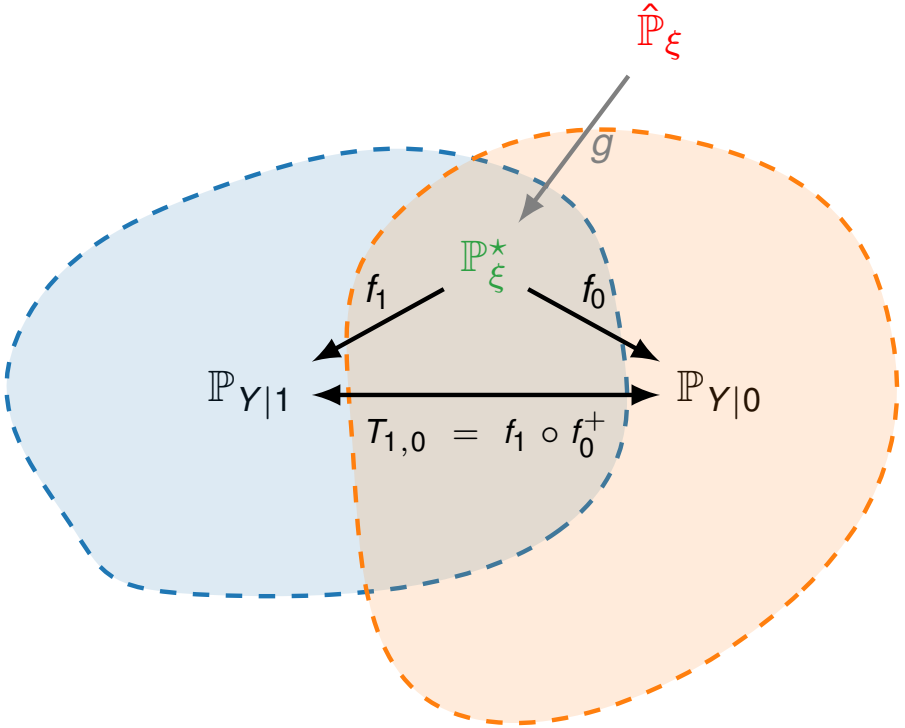
Thank you!

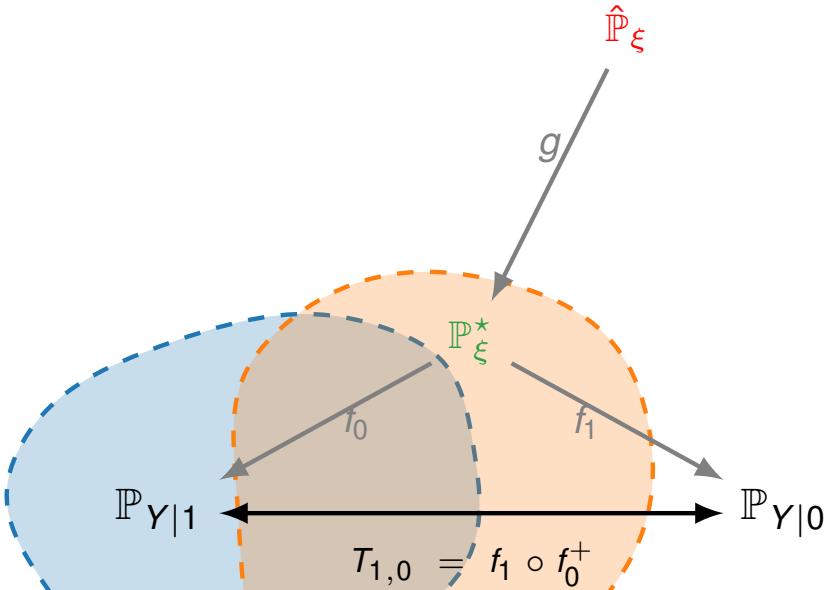
Paper Link: This Version (soon to be on arXiv)

Github Repo: hwdance/Cocycles

To contact: hugh.dance.15@ucl.ac.uk, benbr@stat.ubc.ca

Appendix


$\hat{\mathbb{P}}_\xi$
g
$\mathbb{P}^\star_\xi$
f_1
f_0
$\mathbb{P}_{Y|1}$
$\mathbb{P}_{Y|0}$
$T_{1,0} = f_1 \circ f_0^+$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