

From structural to optimal transport counterfactuals

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Institut de Mathématiques de Toulouse Artificial and Natural Intelligence Toulouse Institute 1. Introduction to counterfactual reasoning

- 2. Structural counterfactuals, revisited
- 3. Optimal transport counterfactuals
- 4. Conclusion

Introduction to counterfactual reasoning

Counterfactual statement: Had Bob been a woman, she would have been 176cm tall

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Definition

A *counterfactual* is a statement of the form "Had event A occurred then event B would have occurred". It relates an intervention on the state-of-things to its consequences.

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We need a model to deduce the counterfactual value(s)

Application in explicability

 $X \in \mathbb{R}^d$ Features $S \in \mathbb{R}$ Sensitive $h(X,S) \in \mathbb{R}$ Predictor

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Procedure:

- 1. Compute $x' \ the \ {\rm counterfactual} \ {\rm value} \ {\rm of} \ x \ {\rm for} \ {\rm a} \ {\rm change} \ s \mapsto s'$
- 2. If $h(x,s) \neq h(x',s')$, then ||x' x|| furnishes an explanation of the disparate treatment underlining the influence of S

1st way: Nearest counterfactual instance

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$$(x,s)\mapsto (x,s')$$

(Simplicity/Feasibility) Assumption free and easy to compute (Unfaithful) Implies that gender and height are independent (Useless) Non explanatory if *h* is unaware of *S*. Deduce the consequences through Pearl's causal modelling

Deduce the consequences through Pearl's causal modelling

 U_0, U_1, U_2 Random seeds Gender $S=G_0(U_0)$ Height $X_1=G_1(S, U_1)$ Hired $X_2=G_2(X_1, S, U_2)$



Figure 1: Example of causal graph

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(Faithful) Respect structural relationships beyond correlations (Unfeasible) The causal model is unknown in practice

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Counterfactuals must be:

- 1. Distribution-aware
- 2. Computationally feasible and assumption-light

3rd way: Optimally preserving distributions [Black et al., 2020]



Figure 2: Distribution of female and male height

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Trading-off causality for correlations

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Trading-off causality for correlations

(Faithful) Fits intuition

(Feasible) No assumption on the data-generation process

Structural counterfactuals, revisited

Pearl's causal framework [Pearl, 2009]

Exogenous $U = (U_1, U_2, \ldots)$

Immutable, prior knowledge

Endogenous $V = (X_1, X_2, \dots, X_d, S)$

Defined as $V_i = G_i(V_{ ext{Endo}(i)}, U_{ ext{Exo}(i)})$

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Figure 3: Principle of an SCM

Solvability: There exists a solution map Γ such that $V = \Gamma(U)$

In particular $X = F(S, U_X)$

Do-intervention

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Forces the sensitive variable to take the fixed value s' while keeping the rest of the causal equations untouched.

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Figure 4: Graph of \mathcal{M}



Figure 5: Graph of $\mathcal{M}_{S=s'}$

Counterfactual distribution:

Had S been equal to s' instead of $s,\,X$ would have follow $\mathcal{L}(X_{S=s'}|S=s)$

Generated by estimating and sampling $\mathcal{L}(U_X|S=s)$

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Counterfactuals of a single instance *x*:

Had S been equal to s' instead of s, X would have follow $\mathcal{L}(X_{S=s'}|X=x,S=s)$ instead of δ_x

Generated by estimating and sampling $\mathcal{L}(U_X|X=x,S=s)$

The effect of do(S = s' | S = s) is fully characterized by the coupling

$$\pi^*_{\langle s' | s \rangle} := \mathcal{L}\left((X, X_{S=s'}) | S=s \right).$$

It assigns a probability to all the pairs (x, x') between an observable value x and a counterfactual counterpart x'.

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Remark:

This coupling admits $\mu_s := \mathcal{L}(X|S = s)$ as first marginal and $\mu_{\langle s'|s \rangle} := \mathcal{L}(X_{S=s'}|S = s)$ as second marginal.
Assumption (RE):

The intervened variable *S* can be considered a root node of the graph:

 $S \perp U_X$



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Consequence: $\pi^*_{\langle s' | s \rangle} \in \Pi(\mu_s, \mu_{s'}).$

The deterministic case

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The function $f_s := F(s, \cdot)$ is injective

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 is injective

Proposition

If (SW) holds, then each instance $x \sim \mu_s$ admits a unique counterfactual counterpart $x' = T^*_{\langle s' \mid s \rangle}(x)$ where

$$T^*_{\langle s'|s\rangle} := f_{s'} \circ f_s^{-1}|_{\mathcal{X}_s}.$$

In such a scenario, U is unnecessary to compute counterfactuals

An example

Linear additive SCM:

$$S = \dots$$
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Consequently,

$$T^*_{\langle s'|s\rangle}(x) := x + (I - M)^{-1}w(s' - s).$$

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- \cdot Under (RE), the target distribution is observable
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$$\begin{array}{c|c} & \neg(\mathsf{RE}) & (\mathsf{RE}) \\ \hline \neg(\mathsf{SW}) & \pi^*_{\langle s'|s \rangle} \in \Pi(\mu_s, \mu_{\langle s'|s \rangle}) & \pi^*_{\langle s'|s \rangle} \in \Pi(\mu_s, \mu_{s'}) \\ \hline (\mathsf{SW}) & T^*_{\langle s'|s \rangle_{\sharp}} \mu_s = \mu_{\langle s'|s \rangle} & T^*_{\langle s'|s \rangle_{\sharp}} \mu_s = \mu_{s'} \end{array}$$

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- A causal-based pipeline would lack efficiency (unrealistic large-scale deployment)
- Causal modeling is intrinsically uncertain
- Causal counterfactuals may not exist [Bongers et al., 2021]

Optimal transport counterfactuals

Optimal transport

- P, Q probability distributions of \mathbb{R}^d
- · $c: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_+$ cost function, typically $\left\|\cdot \cdot\right\|^2$

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An optimal transport plan $\pi_{P,Q}$ between P and Q w.r.t. cost c is a solution to

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Provides a natural way to create a coupling between two distributions when no canonical choice is available

Under (RE), we know that $\pi^*_{\langle s'|s \rangle} \in \Pi(\mu_s, \mu_{s'})$... Why not replacing $\pi^*_{\langle s'|s \rangle}$ by an optimal transport plan $\pi_{\langle s'|s \rangle}$ between μ_s and $\mu_{s'}$?

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Causal counterfactual fairness [Kusner et al., 2017]: h(x,s) = h(x',s') for any s,s' and (x,x') supported by $\pi^*_{\langle s'|s \rangle}$ Under (RE), we know that $\pi^*_{\langle s'|s \rangle} \in \Pi(\mu_s, \mu_{s'})$... Why not replacing $\pi^*_{\langle s'|s \rangle}$ by an optimal transport plan $\pi_{\langle s'|s \rangle}$ between μ_s and $\mu_{s'}$?

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OT counterfactual fairness:

h(x,s) = h(x',s') for any s,s' and (x,x') supported by $\pi_{\langle s'|s \rangle}$

- Distributions: μ_s and $\mu_{s'}$ admit densities and have finite second-order moments
- Causal model: Both (RE) and (SW) hold
- Transportation cost: $c(x, x') = ||x x'||^2$

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The critical assumptions hold for any linear additive model. Recall the example:

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$$f_{s'} \circ f_s^{-1} = x + (I - M)^{-1} w(s' - s).$$

We don't know μ_s and $\mu_{s'}$ but have access to independent samples. The OT plan $\pi_{\langle s'|s\rangle}$ must be estimated from data. We don't know μ_s and $\mu_{s'}$ but have access to independent samples. The OT plan $\pi_{\langle s'|s \rangle}$ must be estimated from data.

Exact solver between an *n*-sample and an *m*-sample:

- $O((n + m)nm \log(n + m))$ operations
- \cdot solution stored as an n imes m matrix

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Growing literature on out-of-samples generalization: plugin estimators, stochastic methods, entropic regularization, generative neural networks...

Dataset: Body measurements of 247 men and 260 women.

$$\begin{split} X &= (\textit{Weight},\textit{Height}) \\ S &= \textit{Gender} \end{split}$$



Figure 7: OT intervention

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Bob is a 80kg and 190cm man.

Had he been a woman, she would have been 59kg and 177cm.

Remarks

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Optimal transport counterfactuals and structural counterfactuals can be written in a common formalism, making them natural surrogate Conclusion
Take-away messages

Counterfactual reasoning

Room for sound correlation-based counterfactuals, between mere translation and causality

Not bound to be either unfaithful or unfeasible

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Fairness

Room for individual fairness notions between group fairness and causal fairness

Had my presentation been better, the audience would have asked questions...

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More on the equivalence between SCM and OT counterfactuals

Positive example:

$$X_1 = \alpha(S)U_1 + \beta_1(S)$$

$$X_2 = -\alpha(S)\ln^2\left(\frac{X_1 - \beta_1(S)}{\alpha(S)}\right)U_2 + \beta_2(S)$$

$$S = U_S \perp (U_1, U_2)$$

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$$S = U_S \perp (U_1, U_2)$$

Negative example:

$$\begin{split} X_1 &= U_1 \\ X_2 &= SX_1^2 + U_2 \\ S &= U_S \perp (U_1, U_2) \end{split}$$

$$\mathcal{R}(\theta) := \mathbb{E}[\ell(h_{\theta}(X, S), Y)] \\ + \lambda \sum_{s \in S} \mathbb{P}(S = s) \sum_{s' \neq s} \mathbb{E}_{\pi_{\langle s' \mid s \rangle}} \left[\left| h_{\theta}(X, s) - h_{\theta}(X', s') \right|^2 \right]$$

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Theorem

Under some assumptions (compactness, density, linearity),

$$\mathcal{R}(\theta_n) - \min_{\theta \in \Theta} \mathcal{R}(\theta) \xrightarrow[n \to +\infty]{a.s.} 0.$$

Counterfactually fair learning



Figure 8: Acc, CFR and DI of the baseline predictors and regularized predictors.