A Framework for Generalization and Transportation of Causal Estimates under Covariate Shift

Apoorva Lal, Wenjing Zheng, Simon Ejdemyr

February 15, 2023

### Introduction

- Scientists, policy-makers, and practitioners care about different kinds of study validity
  - ▶ Internal validity: findings are informative about the *population under study* 
    - estimand: Sample Average Treatment Effect (SATE)
  - **External** validity: findings are informative about the *population of interest* 
    - estimand: Target Average Treatment Effect (TATE); Population ATE (PATE)
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  - Limited feasibility in regime with many concurrent experiments
- This project: Framework and package for model-based solutions to bridging (generalizing or transporting) causal estimates to new populations



### Developmental Psychology n = 1.342Social Psychology n = 1.63274% Cognitive Psychology n = 2.340**Clinical Psychology** n = 876**Organizational Psychology** n = 992 Personality Psychology n = 587

Replication score

Perspective Published: 22 July 2021

# Behavioural science is unlikely to change the world without a heterogeneity revolution

Christopher J. Bryan 🖂, Elizabeth Tipton 🖂 & David S. Yeager 🖂

Nature Human Behaviour 5, 980–989 (2021) | Cite this article 6138 Accesses | 60 Citations | 240 Altmetric | Metrics

#### Abstract

In the past decade, behavioural science has gained influence in policymaking but suffered a crisis of confidence in the replicability of its findings. Here, we describe a nascent heterogeneity revolution that we believe these twin historical trends have triggered. This revolution will be defined by the recognition that most treatment effects are heterogeneous, so the variation in effect estimates across studies that defines the replication crisis is to be expected as long as heterogeneous effects are studied without a systematic approach to sampling and moderation. When studied

### **Data and Estimands**

### **>** Data: $\mathcal{D}_i = (\mathbf{X}_i, S_i, S_iA_i, S_iY_i)_{i=1}^N$ where

- $\blacktriangleright$  covariates  $\mathbf{X}_i \in \mathbb{R}^p$ ,
- treatment  $A_i \in \mathcal{A} := \{0, \dots, K\}$ ,
- outcome  $Y_i \in \mathbb{R}$ ,
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- The *overall* sample is  $S := S_1 \cup S_0$ .
- Two kinds of missing data

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### Estimands Generalizability

 $\mathbb{E}\left[Y^{a,S=1}\right]$ 

### Transportability

 $\mathbb{E}\left[Y^a|S=0\right]$ 

Lets us construct causal contrasts for any pair  $a, a' \in \mathcal{A}$ 

### Reasoning about extrapolation bias

• Let  $\mathcal{X}_b, p_b(\mathbf{x}), b \in \{s, t\}$  denote Support and Distribution of covariates in study and target. Bias from naive extrapolation is

$$\begin{aligned} \mathsf{TATE} - \mathsf{SATE} &= \sum_{x \in \mathcal{X}_t} p_t(\mathbf{x}) \tau_t(\mathbf{x}) - p_s(\mathbf{x}) \tau_s(\mathbf{x}) \\ &= \sum_{x \in \mathcal{X}_t} \left( p_t(\mathbf{x}) - p_s(\mathbf{x}) \right) \tau(\mathbf{x}) \\ &= \sum_{x \in \mathcal{X}_t} \underbrace{p_s(\mathbf{x})}_{\mathsf{Strata Size}} \underbrace{\left( \frac{p_t(\mathbf{x})}{p_s(\mathbf{x})} - 1 \right)}_{\mathsf{Imbalance}} \underbrace{\tau(\mathbf{x})}_{\mathsf{Heterogeneity}} \end{aligned}$$

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**Bias contributions** 

- Imbalance in effect-modifying strata x s.t. τ(x) > 0
- Failure of overlap:  $p_s(\mathbf{x}) = 0$  but  $p_s(\mathbf{x}) > 0$
- ► Heterogeneity model instability  $\tau_s(\mathbf{x}) \neq \tau_t(\mathbf{x})$ DRO problem (Sahoo, Lei, and Wager 2022; Jeong and Namkoong 2020)

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- 4. Selection
  - 4.1  $Y^0, \ldots, Y^a \perp \!\!\!\perp S | \mathbf{X} = \mathbf{x}$ . Ignorability of Selection.
  - 4.2  $\mathbb{E}[Y|A, \mathbf{X}, S = 1] = \mathbb{E}[Y|A, \mathbf{X}, S = 0]$ . The outcome model is stable across S strata.

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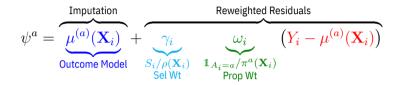
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Under A1,2,3,4.1, the generalization effect is identified. (Dahabreh, Robertson, Tchetgen, et al. 2019; Bia, Huber, and Lafférs 2020)

Under A1,2,3,4.2, the transportation effect is identified. (Dahabreh, Robertson, Steingrimsson, et al. 2020; Josey et al. 2021)

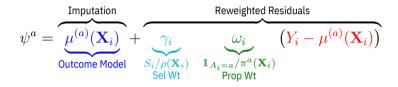
### **Estimator Structure**

#### Augmented Augmented IPW influence function (uncentered)



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- ▶ Difference between  $\psi^a$  and  $\psi^{a'}$  estimates causal contrasts (Robins et al 1994, Newey 1994, Hahn 1998, Cattaneo 2010)
- Estimation: put hats on Nuisance functions estimated by flexible nonparametric regression (L1/L2 reg, random forest, boosting) using cross-fitting
- Construct observation level influence function (=: doubly robust score)
- Average over target sample for point estimate, standard deviation for confidence interval

### **Estimators**

	Generalization	Transportation
	$\sum_{x} \mathbb{E}\left[Y A=a, S=1, \mathbf{X}\right] \mathbf{P}(\mathbf{X})$	$\sum_{x} \mathbb{E}\left[Y A=a, S=1, \mathbf{X}\right] P(\mathbf{X} S=0)$
ОМ	$rac{1}{n}\sum_i \widehat{\mu}^a(\mathbf{X}_i)$	$rac{1}{ \mathcal{S}_0 }\sum_i (1-S_i)\widehat{\mu}^a(\mathbf{X}_i)$
ISW	$\frac{1}{n}\sum_{i}\frac{S_{i}}{\widehat{\rho}(\mathbf{X}_{i})}\frac{\mathbb{1}_{A\equiv a}}{\widehat{\pi}^{a}(\mathbf{X}_{i})}Y_{i}$	$\frac{1}{n}\sum_{i}\frac{1}{\widehat{\mathbb{E}}[S_{i}=0]}\frac{S_{i}(1-\widehat{\rho}(\mathbf{X}_{i}))}{\widehat{\rho}(\mathbf{X}_{i})}\frac{1_{A\equiv a}}{\widehat{\pi}^{a}(\mathbf{X}_{i})}Y_{i}$
AISW	$\frac{1}{n}\sum_{i}\widehat{\mu}^{a}(\mathbf{X}_{i}) + \frac{S_{i}}{\widehat{\rho}(\mathbf{X}_{i})}\frac{\mathbb{1}_{A\equiv a}}{\widehat{\pi}^{a}(\mathbf{X}_{i})}(Y_{i} - \widehat{\mu}^{a}(\mathbf{X}_{i}))$	$\frac{1}{n}\sum_{i}\frac{1}{\widehat{\mathbb{E}}[S_{i}=0]}\left((1-S_{i})\widehat{\mu}^{a}(\mathbf{X}_{i})+\frac{S_{i}(1-\widehat{\rho}(\mathbf{X}_{i}))}{\widehat{\rho}(\mathbf{X}_{i})}\frac{1_{A\equiv a}}{\widehat{\pi}^{a}(\mathbf{X}_{i})}(Y_{i}-\widehat{\mu}^{a}(\mathbf{X}_{i}))\right)$

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- Outcome modelling (OM), Inverse Selection Weighting (ISW), and Augmented Inverse Selection Weighting (AISW)
- Target population
- Implemented in ateGT

- goal for selection weights: balance covariates across study and target
- Inverse propensity weighting is indirect: fit
   Pr (S = 1|X), then invert
  - This inversion dramatically inflates errors when selection weights are small
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$$\begin{split} \min_{\gamma} &= \sum_{i \in \mathcal{S}_1} f(\gamma_i) \; \text{ s.t.} \\ \text{Balance} &\sum_{i \in \mathcal{S}_1} \gamma_i c_{ij}(X_{ij}) = \sum_{i \in \text{target}} c_{ij}(X_{ij}) \\ \text{Simplex} &\sum_{i \in \mathcal{S}_1} \gamma_i = 1 \text{ and } \gamma_i \geq 0 \; \forall \left\{ i : i \in \mathcal{S}_1 \right\} \end{split}$$

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Dual is easy to solve for certain fs (L2, entropy) as regularized propensity score (Wang and Zubizarreta 2019). Implemented in ateCAL

### **Incorporating Surrogate Outcomes**

- Suppose further that we observe a short-run outcome Z<sub>i</sub> for both S<sub>1</sub>, S<sub>0</sub>, but outcome of interest Y<sub>i</sub> only for S<sub>1</sub>
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 Under analogues of A1-4, Kallus and Mao (2022) derive an influence function for the generalization effect with surrogates

$$\psi = \mu^{(a)}(\mathbf{X}_{i}) + \underbrace{\gamma_{i}}_{S_{i}/\rho(\mathbf{X}_{i})} \underbrace{\omega_{i}}_{\mathbb{1}_{A_{i}=a}/\pi^{a}(\mathbf{X}_{i})} \left(Y_{i} - \mu^{(a)}(\mathbf{X}_{i})\right) + \\\omega_{i} \left(\nu^{(a)}(Z_{i}, \mathbf{X}_{i}) - \mu^{(a)}(\mathbf{X}_{i})\right) - \tau$$

 Second residual is information gained from incorporating surrogate outcome in prediction of Y

### Characterizing Sensitivity via OVB

- Identification hinges on A4.1 (selection ignorability).
- Motivates our estimation strategy via reweighting  $\gamma_i$
- Suppose there is an omitted variable U that makes A4.1 hold.
- True  $(\mu, (\pi, \gamma) =: \alpha)$  and feasible  $(\mu_s, (\pi, \gamma_s) =: \alpha_s)$  nuisance functions (Chernozhukov et al. 2022) where former includes U as covariate

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$$\alpha_s(\mathcal{D}) = \frac{S_i}{\rho(\mathbf{X}_i)} \left( \frac{\mathbbm{1}_{A=a}}{\pi^a(\mathbf{X}_i)} - \frac{\mathbbm{1}_{A=a'}}{\pi^{a'}(\mathbf{X}_i)} \right)$$
$$\alpha(\mathcal{D}, U) = \frac{S_i}{\rho(\mathbf{X}_i, U_i)} \left( \frac{\mathbbm{1}_{A=a}}{\pi^a(\mathbf{X}_i)} - \frac{\mathbbm{1}_{A=a'}}{\pi^{a'}(\mathbf{X}_i)} \right)$$

Squared Bias can be bounded as  $B^2 = S^2 C_Y^2 C_A^2$  where

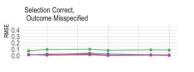
• 
$$S^2 := \mathbb{E}(Y - \mu_s)^2 \mathbb{E} \alpha_s^2$$
 (identifiable)

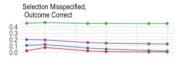
- ►  $C_Y^2 = R_{Y-\mu_s \sim \mu-\mu_s}^2$ : conjectured proportion of residual variance in outcome explained by confounders
- $C_A^2 = (1 R_{\alpha \sim \alpha_s}^2)/R_{\alpha \sim \alpha_s}^2$ : conjectured proportion of residual variance in long RR explained by confounders

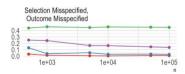
## Simulation Study

- **Covariates**  $X_1, ..., X_10 \sim U[-1, 1]$
- **Data Generating Process** 
  - $\blacktriangleright$   $A_i \sim \text{Bernoulli}(0.5)$
  - $Y_i^* = Y^0(\mathbf{X}_i) + A_i \tau(\mathbf{X}_i)$   $Y_i = Y_i^*$  w.p.  $\rho(\mathbf{X})$ , else missing
    - - For non-trivial functions  $\rho(\mathbf{X})$ , there is selection bias and SATE is biased for  $\mathbb{E}\left[\tau(\mathbf{X})\right]$
- Vary functional form of
  - $\blacktriangleright$   $Y^0(\mathbf{X})$  (Outcome Model)
  - $\triangleright \rho(\mathbf{X})$  (Selection Model)

#### **Root Mean Squared Error**

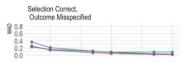


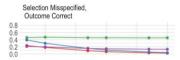


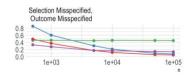


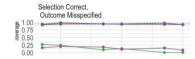
#### Bias

🔸 aisw 🔶 isw 🔶 naive 🔶 om

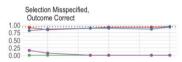


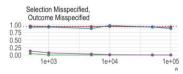






Coverage





### Implementation in causalTransportR

- Main function: ateGT (ATE Generalization or Transportation)
- Input vectors y, a, s of outcome, treatment, and selection where y, a are missing for s = 0
- Matrix of X of covariates (no missings)
- Additional arguments for nuisance function estimation

```
ateGT(
 у,
 a,
 Х.
 s = NULL.
 treatProb = NULL,
 Z = NULL,
 nuisMod = c("rlm", "rf"),
 target = c("generalize", "transport", "insample"),
 estimator = c("AISW", "ISW", "OM", "CW", "ACW"),
 hajekize = FALSE,
  separateMus = TRUE,
 glmnet_lamchoice = "lambda.min",
 glmnet alpha = 1.
 glmnet_rho_family = "binomial",
 glmnet_pi_family = "binomial",
 glmnet_mu_family = "gaussian",
 qlmnet_parl = FALSE,
 arf tuneRf = "none".
 noi = FALSE
```

### Conclusion

- Proposes a multi-treatment framework for causal generalization and transportation
- provide a performant computational implementation for it in causalTransportR::ateGT
  - calibrated generalization for when only summary statistics are available for target (ateCAL)
  - poststratification weights using fast fixed effects regressions (ateGTreg)
- Future work: more work on sensitivity analyses
  - Partial identification for generalization using marginal sensitivity model (Nie, Imbens, and Wager 2021) or Proportion with confounding (Kennedy and Bonvini 2021)
  - Estimate how different the population needs to be from the experimental sample to explain away the effect (Devaux and Egami 2022)

# Thanks!

software: https://github.com/apoorvalal/causalTransportR
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