



Causal Inference with Instrumental Variables

Kun Kuang

Zhejiang University

<https://kunkuang.github.io/>

An example of decision making

- Does predictive models guide decision making?
- When should the System change algorithm from A to B?
- Is the new algorithm B better?
- Say algorithm that provides promotion or discount link to a different customers



Algorithm A



Algorithm B

An example of decision making

- Measure success rate (SR)

Old Algorithm (A)	New Algorithm (B)
50/1000 (5%)	54/1000 (5.4%)



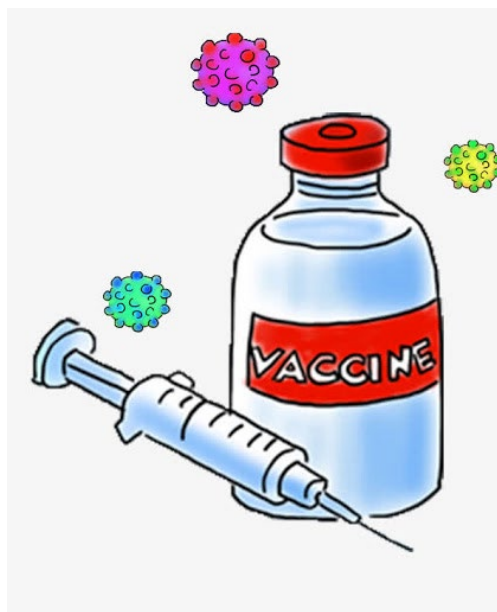
New algorithm increases overall success rate, so it is better?

	Old Algorithm (A)	New Algorithm (B)
Low-income Users	10/400 (2.5%)	4/200 (2%)
High-income Users	40/600 (6.6%)	50/800 (6.2%)
Overall	50/1000 (5%)	54/1000 (5.4%)

Which is better?

Decision Making with Causality

- **Causal Effect Estimation** is necessary for decision making!



Causal effect estimation plays an important role on decision making!

A practical definition

Definition: T causes Y if and only if
changing T leads to a change in Y,
keep everything else constant.

Causal effect is defined as the magnitude by which Y is changed by a unit change in T.

Two key points: changing T, keeping everything else constant

Treatment Effect Estimation

- Treatment Variable: $T = 1$ or $T = 0$
- Potential Outcome: $Y(T = 1)$ and $Y(T = 0)$
- Individual Treatment Effect (ITE)

$$ITE(i) = Y_i(T_i = 1) - Y_i(T_i = 0)$$

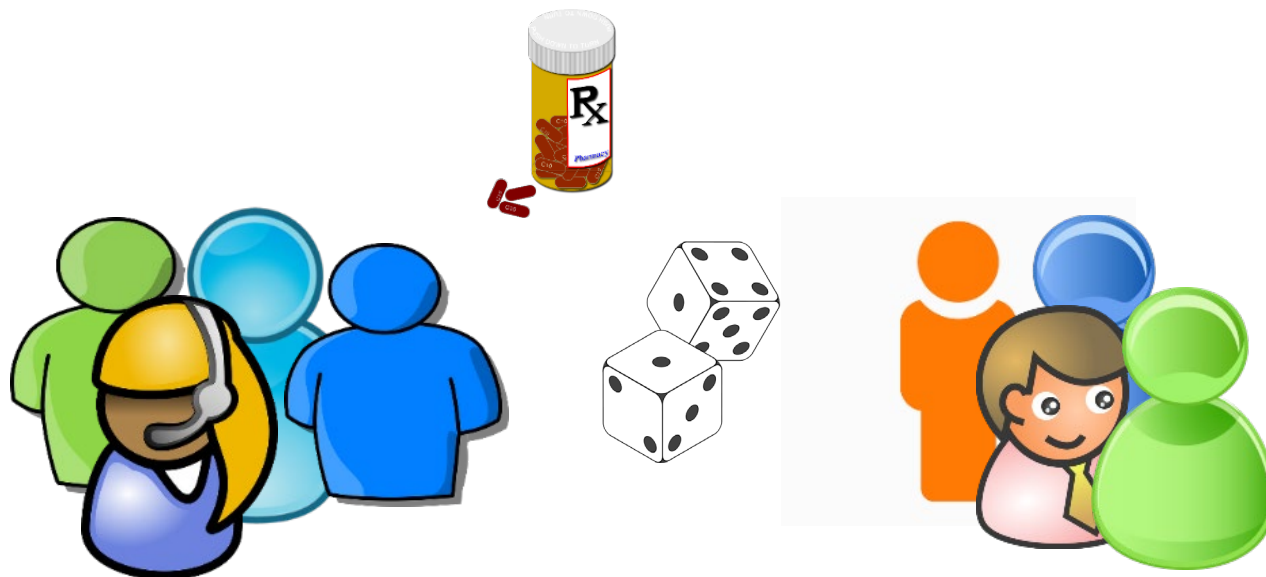
- Average Treatment Effect (ATE):

$$ATE = E[Y(T = 1) - Y(T = 0)]$$

Counterfactual problem: $Y(T = 1)$ or $Y(T = 0)$



Randomized Experiments are the “Gold Standard”



- Drawbacks of randomized experiments:
 - Cost
 - Unethical

Two key points: changing T, keeping everything else constant

Causal Inference with Observational Data

- Definition of ATE: $ATE = E[Y(T = 1) - Y(T = 0)]$
- In observational data, we have units with different T:

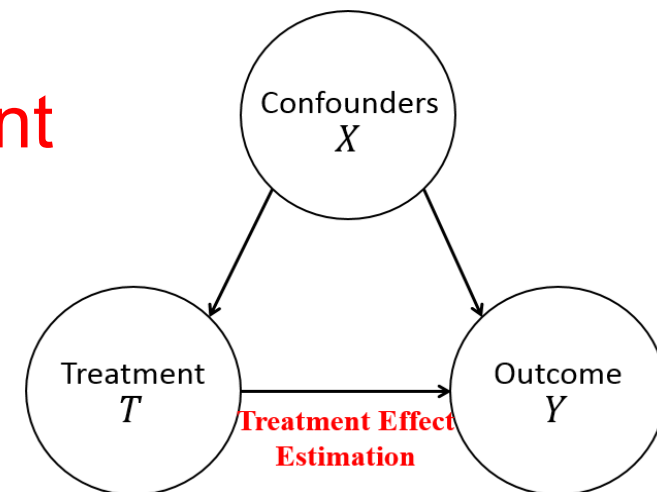
$$E[Y(T = 1)] \text{ or } E[Y(T = 0)]$$

- Can we estimate ATE by directly comparing the average outcome between groups with T=1 and T=0?

- **No, because confounders X might not be constant**

- Two key points:

- Changing T (T=1 and T=0)
- Keeping everything else (Confounder X) constant



Causal Inference with Observational Data

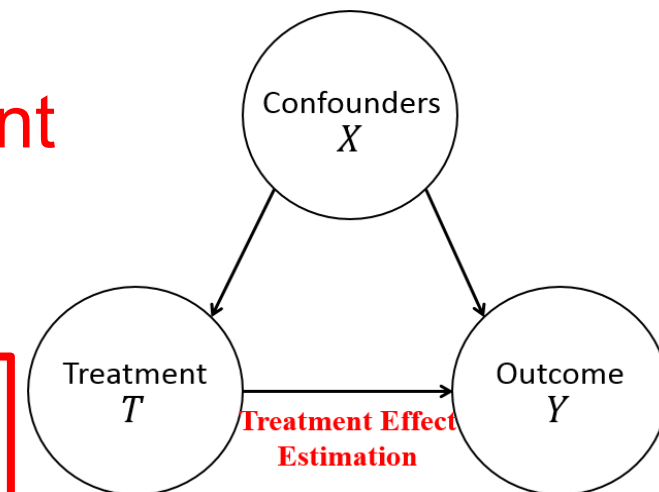
- Counterfactual problem: $Y(T = 1)$ or $Y(T = 0)$
- In observational data, we have units with different T :

$$E[Y(T = 1)] \text{ or } E[Y(T = 0)]$$

- Can we estimate ATE by directly comparing the average outcome between groups with $T=1$ and $T=0$?
 - **No, because confounders X might not be constant**

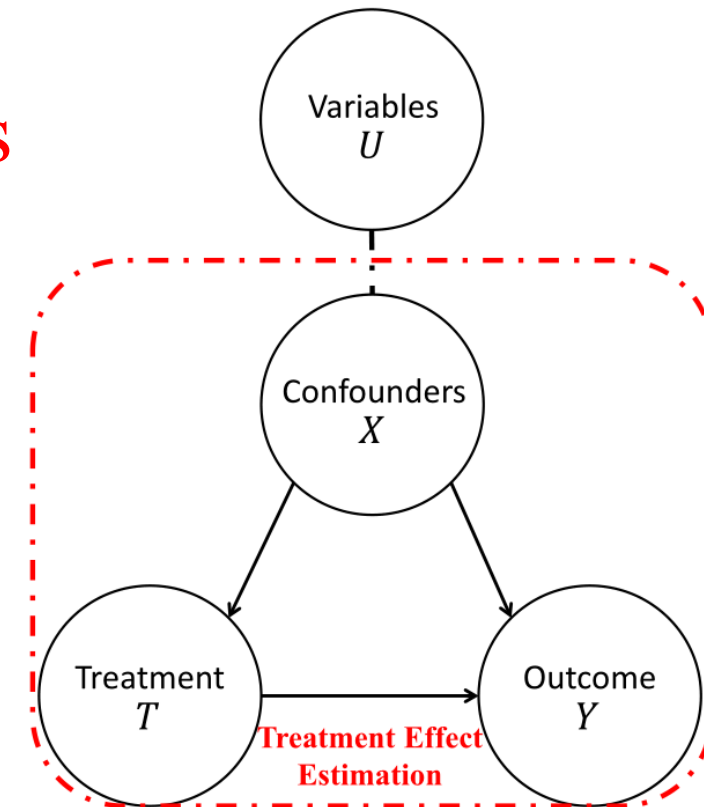
- Two key points:

Balancing Confounders' Distribution



Related Work

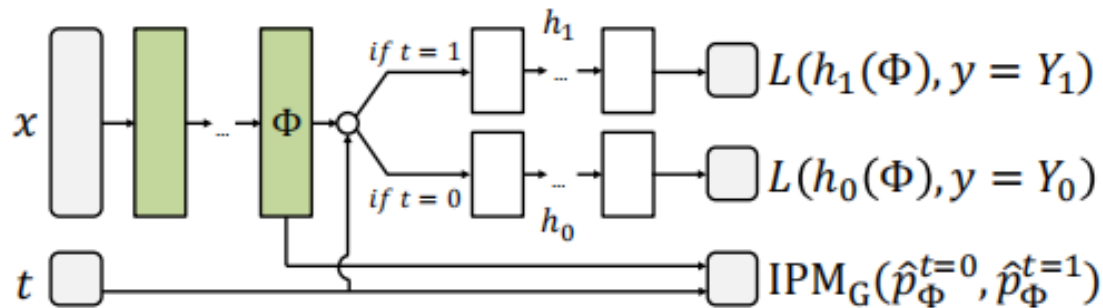
- Matching Methods
 - *Exactly Matching, Coarse Matching*
 - **Poor performance in high dimensional settings**
- Propensity Score based Methods
 - Propensity score $e(\mathbf{X}) = p(T = 1|\mathbf{X})$
 - *Matching, Weighting, Doubly Robust*
 - **Treat all observed variables as confounders, and ignore the non-confounders**
 - **Mainly designed for binary treatment**



(a) Previous Causal Framework.

Related Work

- Representation Learning based Methods
 - Similar representation between treatment groups.
 - Accurate prediction on factual/counterfactual outcome



$$\min_{\substack{h, \Phi \\ \|\Phi\|=1}} \frac{1}{n} \sum_{i=1}^n w_i \cdot L(h(\Phi(x_i), t_i), y_i) + \lambda \cdot \mathfrak{R}(h) \\ + \alpha \cdot \text{IPM}_G(\{\Phi(x_i)\}_{i:t_i=0}, \{\Phi(x_i)\}_{i:t_i=1}),$$

with $w_i = \frac{t_i}{2u} + \frac{1-t_i}{2(1-u)}$, where $u = \frac{1}{n} \sum_{i=1}^n t_i$

and \mathfrak{R} is a model complexity term.

- **Confounder differentiation, binary treatment, might ignore confounders**

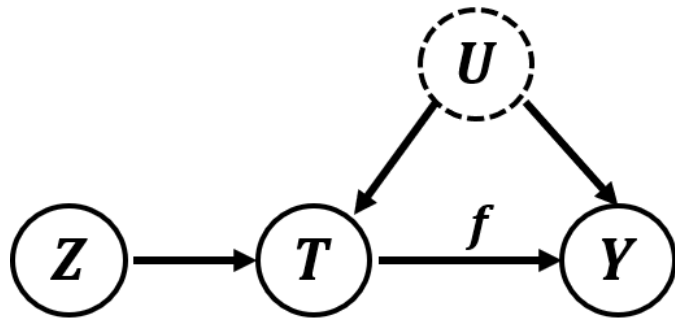
New challenges in Big Data era

- **Automatically separate confounders**
 - Not all observed variables are confounders
 - Data-Driven Variables Decomposition (D^2VD , DeR-CFR)
- **Remove unobserved confounding bias**
 - Not all confounders are observed
 - Automatic Instrumental Variable Decomposition (AutoIV, GIV)
- **Continuous/Complex treatment effect estimation**
 - Treatment variables are not always binary
 - Generative Adversarial De-confounding (GAD, CRNet)

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Instrumental Variable Regression



Conditions of IV (instrumental variable)

- Relevance: $P(T|Z) \neq P(T)$
- Exclusion: $P(Y|Z, T, U) \neq P(Y|T, U)$
- Unconfounded: $Z \perp U$



2SLS:

Stage 1: regressing T on Z

$$\hat{T} = \hat{g}(Z)$$

Stage 2: regressing Y on \hat{T}

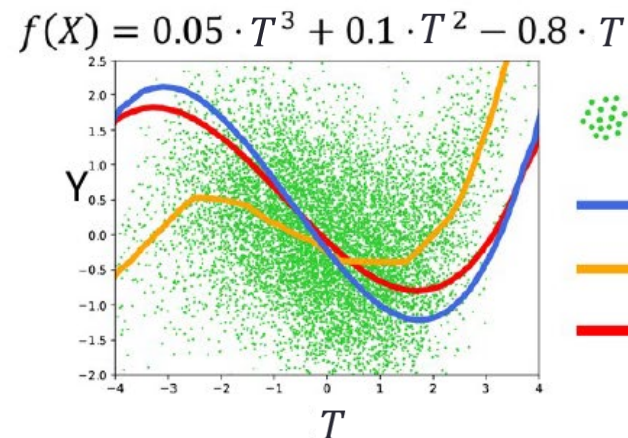
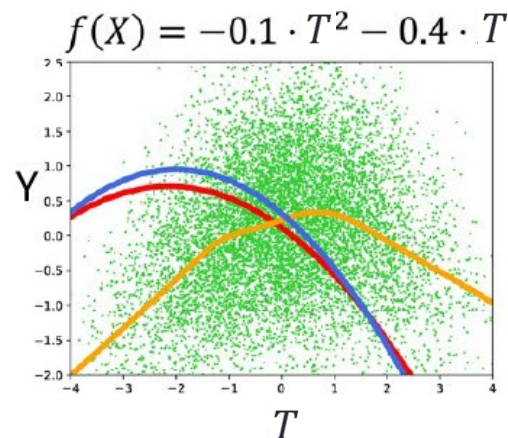
$$\hat{Y} = \hat{f}(\hat{T})$$

$$Z \sim \mathcal{N}(0,1)$$

$$U \sim \mathcal{N}(0,1)$$

$$T = Z + U$$

$$Y = f(T) + U$$



Data $P(T, Y)$

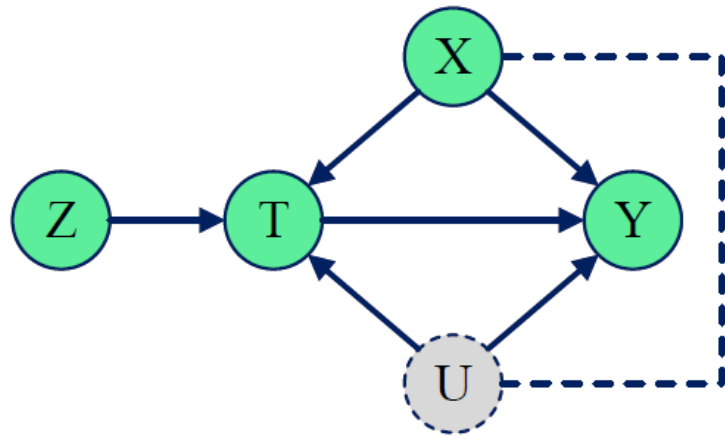
f

\hat{f}^{NN}

\hat{f}^{IV}

Assuming the additive separability of noise U and
and
Limited to linear setting

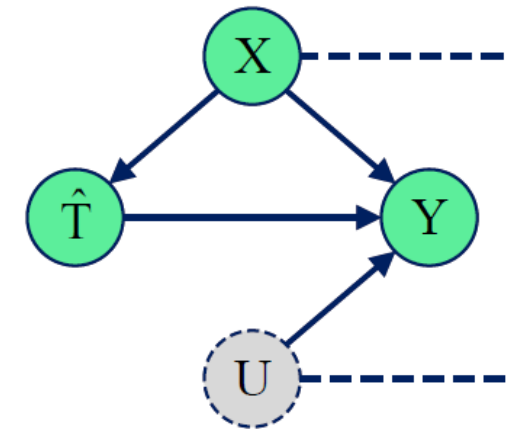
Non-linear Instrumental Variable Regression



Non-linear IV regression (DeepIV, KernelIV et.al)

Stage 1: regressing T on Z and X $\hat{T} = \hat{g}(Z, X)$

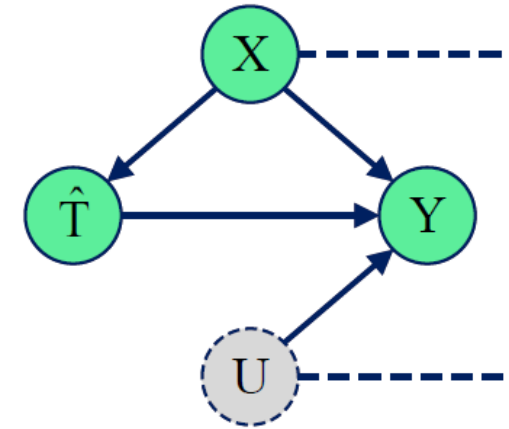
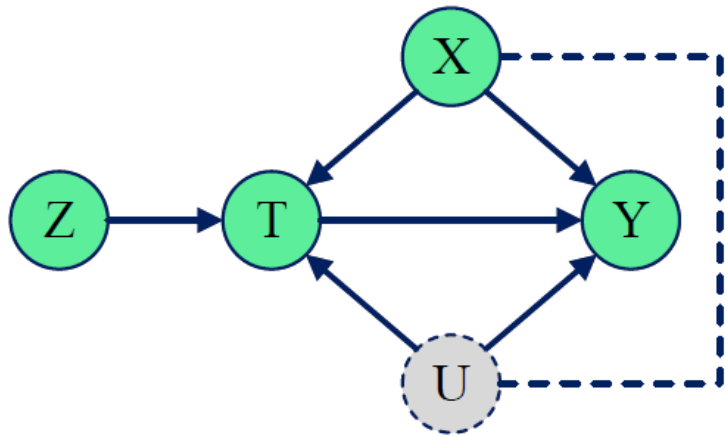
Stage 2: regressing Y on \hat{T} and X $\hat{Y} = \hat{f}(\hat{T}, X)$



Stage 1 regression brings
confounding bias in stage 2

Confounder Balancing + IV Regression

Confounder Balanced Instrumental Variable Regression



CB-IV (Confounder Balanced IV regression):

Stage 1 (Treatment regression): regressing T on Z and X $\hat{T} = \hat{g}(Z, X)$

Confounder balancing: learning a balanced confounder representation $\phi(X)$ such that $\hat{T} \perp \phi(X)$

Stage 2 (Outcome regression): regressing Y on \hat{T} and $\phi(X)$ $\hat{Y} = \hat{f}(\hat{T}, \phi(X))$

Confounder Balanced Instrumental Variable Regression

Table 2: The bias (mean \pm std) of ATE estimation on real-world data (Data- m_Z - m_X - m_U)

		Within-Sample			
Method		IHDP-2-6-0	IHDP-2-4-2	Twins-5-8-0	Twins-5-5-3
IV regression based methods	DeepIV-LOG	2.8736 \pm 0.0577	2.6227 \pm 0.0651	0.0135 \pm 0.0215	0.0237 \pm 0.0111
	DeepIV-GMM	3.7760 \pm 0.0316	3.7396 \pm 0.0402	0.0194 \pm 0.0047	0.0221 \pm 0.0041
	OneSIV	1.7249 \pm 0.3752	1.7411 \pm 0.3422	0.0083 \pm 0.0191	0.0080 \pm 0.0167
	DFIV	3.5543 \pm 0.0891	3.6218 \pm 0.1038	0.0268 \pm 0.0005	0.0265 \pm 0.0003
Confounder balancing based methods	DFL	3.2018 \pm 0.0496	3.1991 \pm 0.0374	0.0624 \pm 0.0586	0.0847 \pm 0.0049
	DirectRep	0.0675 \pm 0.0562	0.4600 \pm 0.0711	0.0167 \pm 0.0171	0.0193 \pm 0.0251
	CFR	0.0854 \pm 0.0579	0.4826 \pm 0.0642	0.0115 \pm 0.0167	0.0223 \pm 0.0176
	DRCFR	0.0553 \pm 0.0644	0.4336 \pm 0.0692	0.0114 \pm 0.0221	0.0118 \pm 0.0174
	CB-IV	0.0117 \pm 0.3882	0.1601 \pm 0.2499	0.0067 \pm 0.0271	0.0014 \pm 0.0249
		Out-of-Sample			
Method		IHDP-2-6-0	IHDP-2-4-2	Twins-5-8-0	Twins-5-5-3
	DeepIV-LOG	2.8760 \pm 0.0553	2.6226 \pm 0.0692	0.0140 \pm 0.0208	0.0238 \pm 0.0111
	DeepIV-GMM	3.7760 \pm 0.0316	3.7396 \pm 0.0402	0.0194 \pm 0.0047	0.0221 \pm 0.0041
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	DRCFR	0.0450 \pm 0.0953	0.4321 \pm 0.0673	0.0113 \pm 0.0219	0.0118 \pm 0.0174
	CB-IV	0.0150 \pm 0.3927	0.1578 \pm 0.2540	0.0065 \pm 0.0270	0.0015 \pm 0.0247

Require a well predefined valid IV

No-predefined IV: Confounded IVs

Confounded IVs:

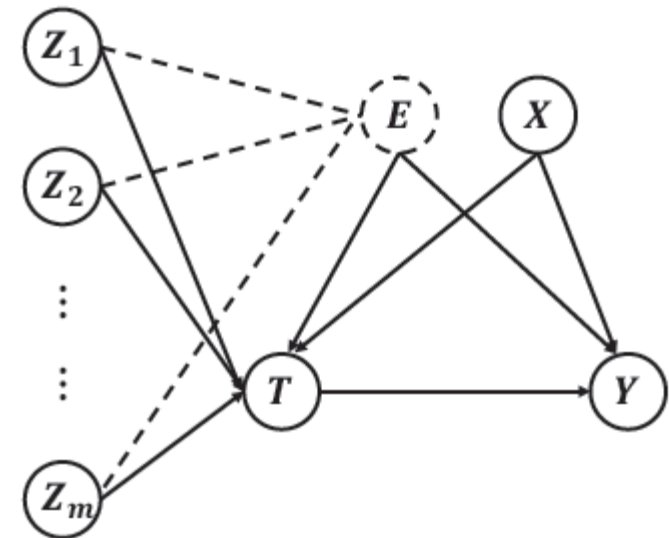
- Violation on Unconfounded Instrument: Z_i correlates to E conditioning on X
- Often happens in real cases and leads to failure of all IV methods.

Our setting:

- $\{Z_i\}_{i=1}^m$ represents candidates for IV
- A subset of $\{Z_i\}_{i=1}^m$ are valid, while others are confounded IVs

Our Goal:

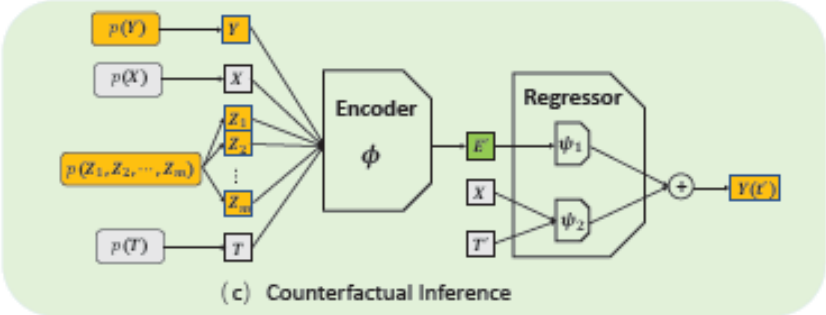
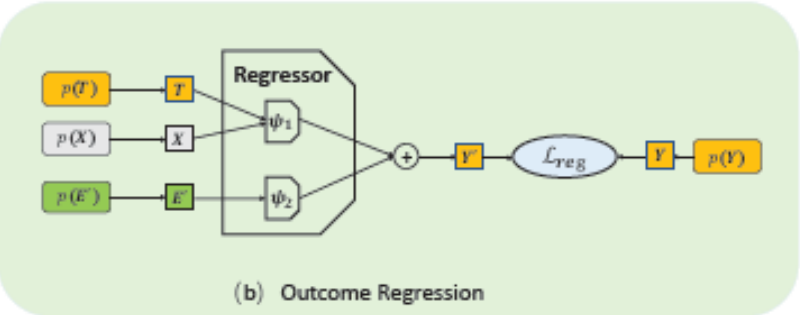
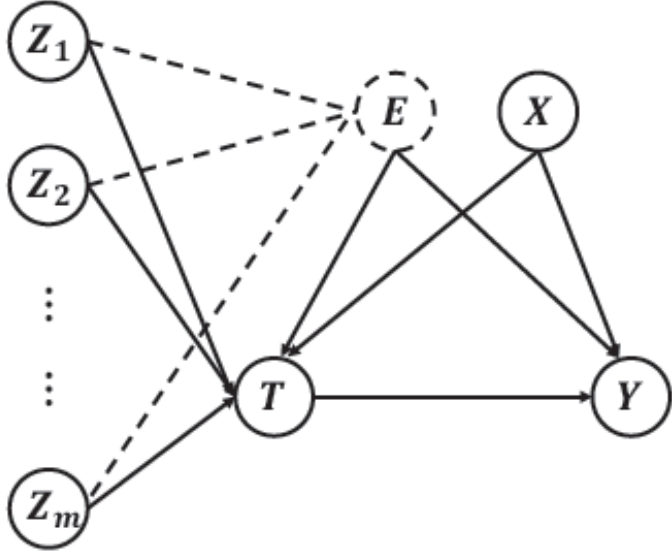
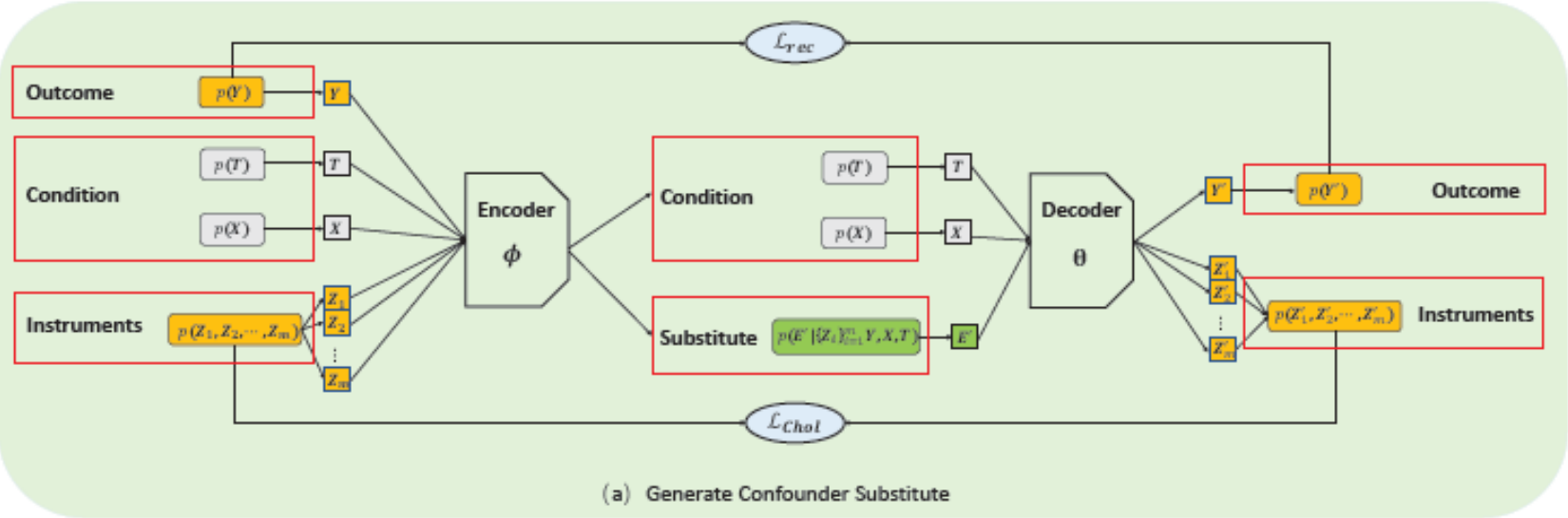
- Estimating Individual Causal Effect



CVAE-IV: Constructing substitute for unobserved confounders

Conditional Independence Criteria:

- Generating E' such that $Y \perp (Z_1, Z_2, \dots, Z_m) \mid E', T, X$
- E' captures the info of confounders from E rather than recovers E



CVAE-IV: Constructing substitute for confounders

- Conditional Independence Criteria:

- Generating E' such that $Y \perp (Z_1, Z_2, \dots, Z_m) \mid E', T, X$
- E' captures E rather than recovers E

- Constructing the conditional variational autoencoder model (CVAE)

- Variational inference:

$$\begin{aligned} & \log p(Y, \bar{Z} \mid T, X) \\ & \geq \mathbb{E}[\log p_\theta(Y, \bar{Z} \mid E', T, X)] - D_{KL}(q_\phi(E' \mid Y, \bar{Z}, X, T) \parallel p(E' \mid T, X)), \end{aligned}$$

- Separating construction of outcome from that of IVs:

$$\log p_\theta(Y, \bar{Z} \mid E', T, X) = \log p_\theta(Y \mid E', T, X) + \log p_\theta(\bar{Z} \mid E', T, X),$$

- Constructing the IVs using Cholesky approximation:

- Isotropic Gaussian eliminates the dependence among $\{Z_i\}_{i=1}^m$
- Estimating covariance matrix of $\{Z_i\}_{i=1}^m$ using Cholesky decomposition

$$\mathcal{L}_{Chol} = \log |\Sigma_{\bar{Z}}(E')| + (\bar{Z} - \mu(E'))^T \Sigma_{\bar{Z}}(E')^{-1} (\bar{Z} - \mu(E')),$$

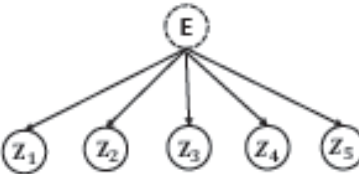
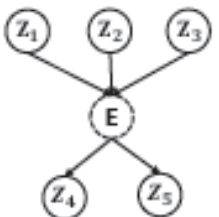
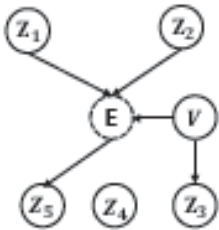
- Reconstruction of $\{Z_i\}_{i=1}^m$

$$\mathcal{L}_{Chol} = -2 \sum_{i=1}^m (\log L(E')_{ii}) + (\bar{Z} - \mu(E'))^T L(E') L(E')^T (\bar{Z} - \mu(E'))$$

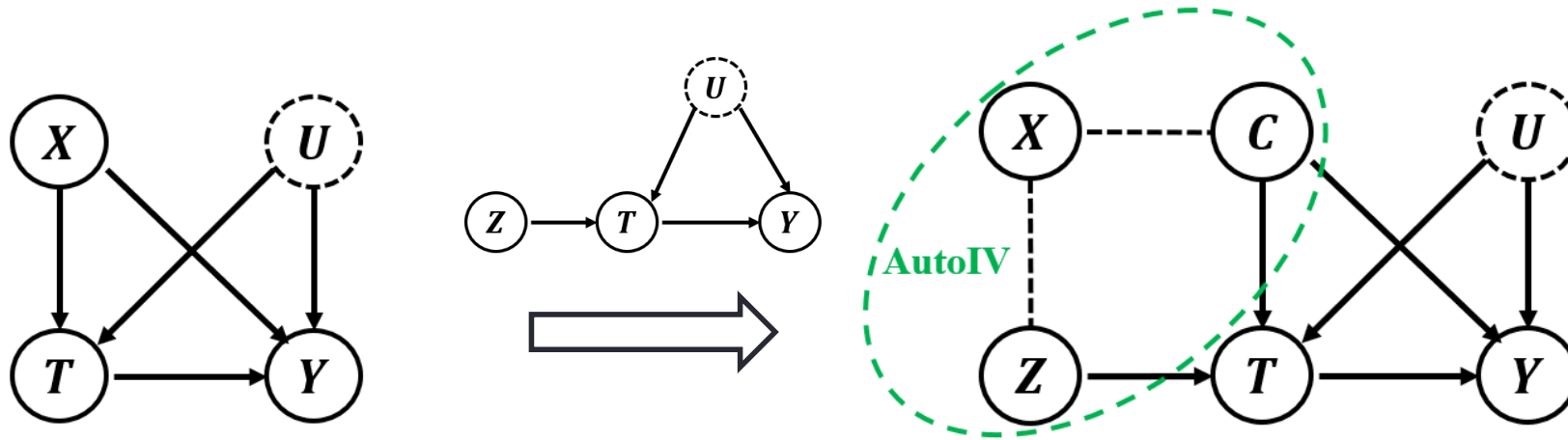
- Constructing the IVs using Cholesky approximation:

$$\mathcal{L}_{rec} = \log p_\theta(Y \mid E', T, X) \approx \frac{1}{\sigma_Y^2} \|Y - Y'(E', T, X)\|_2^2$$

No-predefined IV: Confounded IVs

Scenario	Function	Dim	DirectNN	2SLS-Ploy	KernelIV	DeepIV	CEVAE	ModeIV	Ours
S ₁ : 	Linear	Low	2.091	55.437	8.565	1.977	9.959	3.120	0.928
		High	2.069	56.476	9.220	2.261	10.283	4.426	0.858
	Abs	Low	1.874	44.144	6.893	2.426	8.481	1.988	0.697
		High	1.671	41.731	7.998	1.675	9.921	2.088	0.918
	Square	Low	1.414	52.872	8.521	1.163	6.569	2.423	0.490
		High	1.602	41.731	9.988	1.545	7.039	2.018	0.791
S ₂ : 	Linear	Low	1.788	45.287	8.922	1.910	7.621	3.314	0.706
		High	2.152	56.484	9.215	1.788	8.109	2.040	0.601
	Abs	Low	1.595	34.214	5.864	1.224	7.178	2.064	0.562
		High	0.836	42.181	4.030	0.835	8.015	2.134	0.301
	Square	Low	1.168	41.108	5.749	1.064	10.385	1.565	0.125
		High	1.650	51.129	6.030	1.568	9.015	2.031	0.257
S ₃ : 	Linear	Low	1.650	41.009	6.617	2.023	7.234	3.638	0.485
		High	1.821	41.374	7.656	1.729	7.203	4.134	0.608
	Abs	Low	2.095	44.471	4.867	1.148	9.789	1.916	0.689
		High	1.590	41.132	6.330	1.484	7.293	1.972	0.504
	Square	Low	1.111	41.199	7.826	1.019	8.362	1.580	0.516
		High	2.179	41.915	6.407	1.442	8.825	1.709	0.941

AutoIV: Counterfactual Learning with Unobserved Confounders via Automatically generating IVs



Conditions of IV

- Relevance: $P(T|Z) \neq P(T)$
- **Exclusion:** $P(Y|Z, T, C) \neq P(Y|T, C)$
- Unconfounded: $Z \perp C$



Mutual Information
Representation Learning

But exclusion might not be satisfied

AutoIV: Counterfactual Learning with Unobserved Confounders via Automatically generating IVs

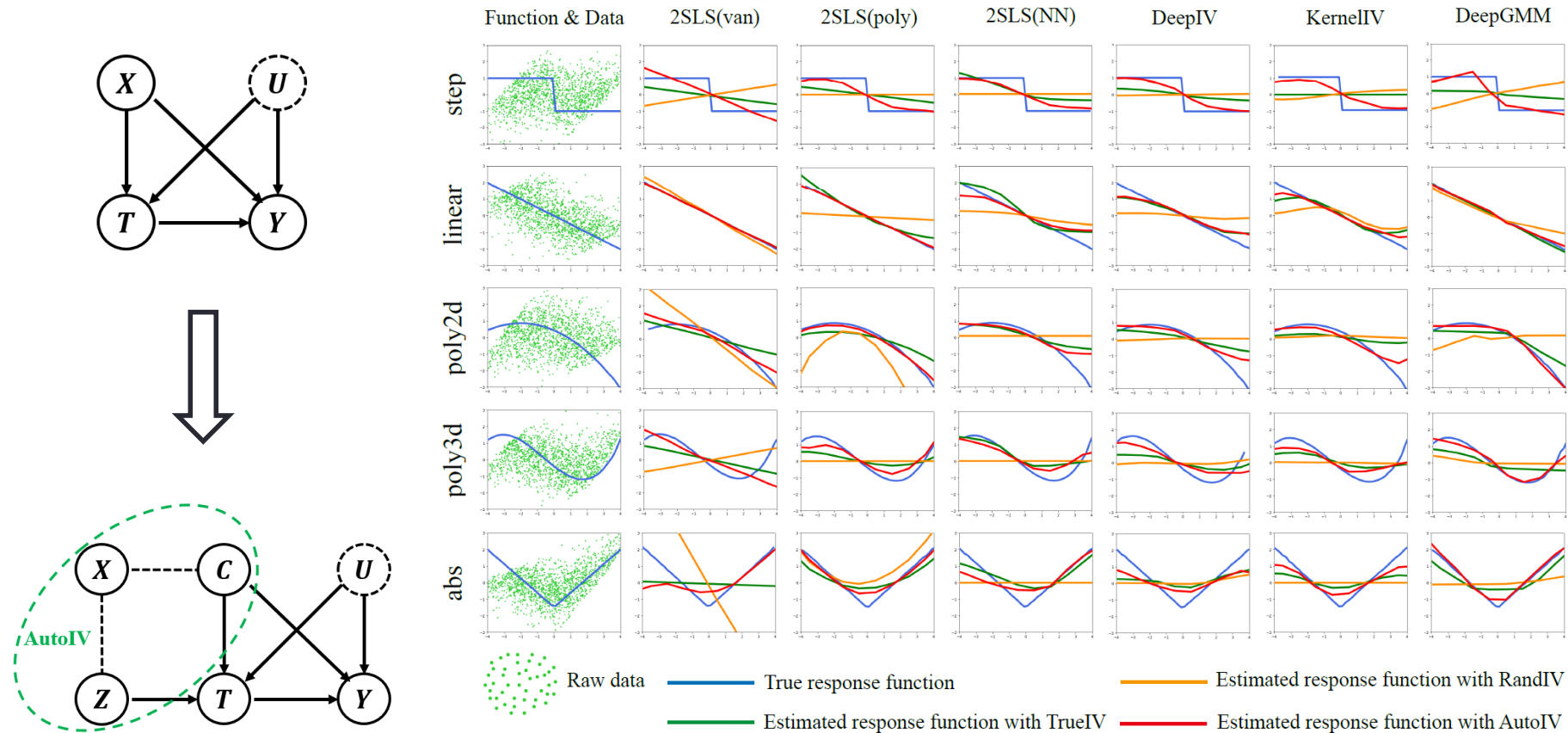


Figure 2: Response function prediction in low-dimensional scenarios.

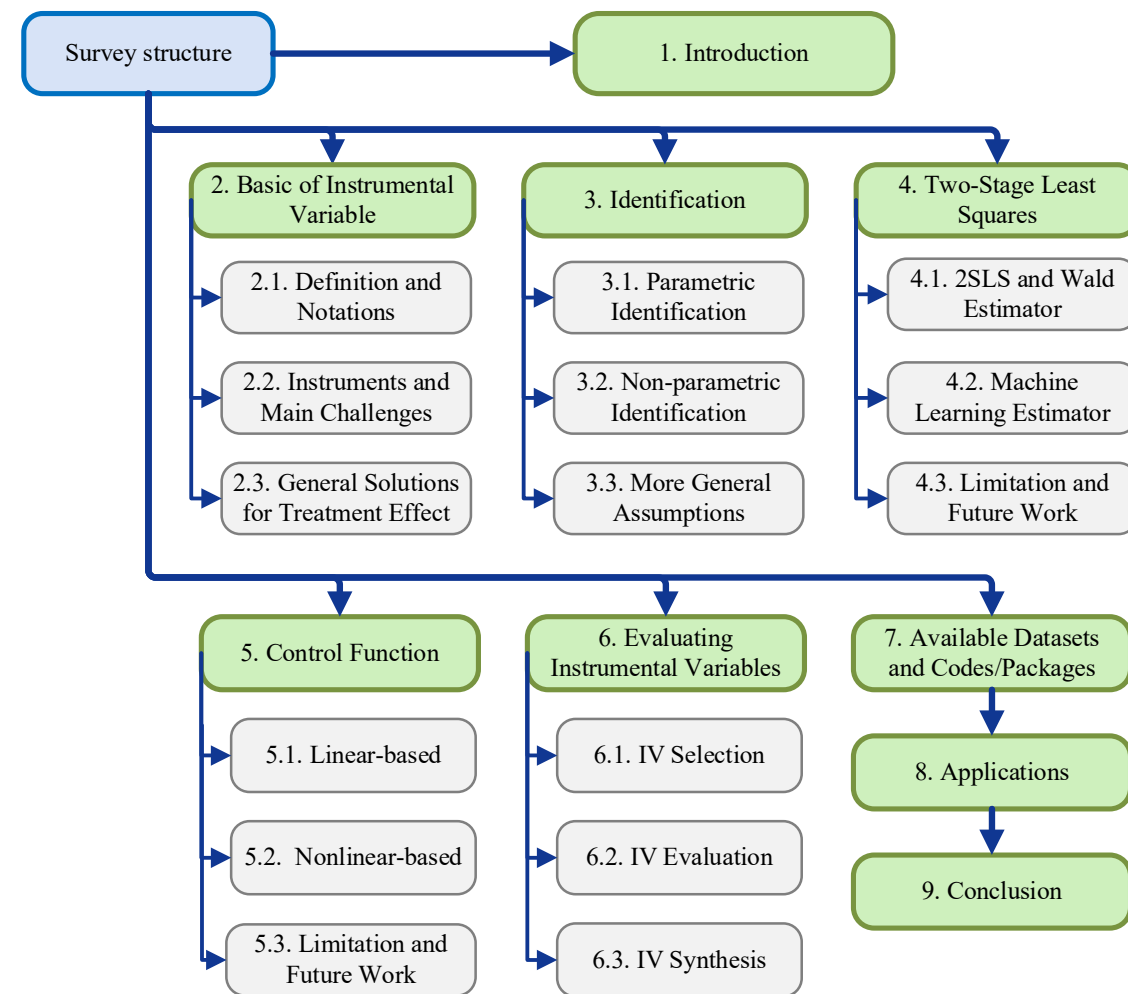
Yuan J, Wu A, Kuang K, et al. Auto IV: Counterfactual Prediction via Automatic Instrumental Variable Decomposition[J]. TKDD, 2022.

IVs in Causal Inference and Machine Learning

Instrumental Variables in Causal Inference and Machine Learning: A Survey

Anpeng Wu, Kun Kuang*, Ruoxuan Xiong, Fei Wu, *Senior Member, IEEE*

Abstract—Causal inference, which refers to the process of drawing a conclusion about a causal connection based on the conditions of the occurrence of an effect, is crucial for stable learning and decision making by understanding the mechanism underlying the data. How to precisely and unbiasedly estimate the treatment effect from observational data with unobserved confounders is becoming an appealing research direction in both causal inference and machine learning communities. Instrumental Variables (IV) plays a critical role to draw causal inference from the settings where the treatment of interest cannot be randomly assigned and even with unobserved confounders. In recent years, IV methods have attracted considerable attention in the literature of both causal inference and machine learning, and various IV-based methods have sprung up. This paper serves as the first effort to systematically and comprehensively introduce and discuss the IV methods and their applications in both causal inference and machine learning. Firstly, we provide the formal definition of IVs and discuss the identification problem of IV regression methods under different assumptions. Secondly, we categorize the existing work on IV methods into three groups according to the focus on the proposed method, including two-stage least squares based IV methods, control function based IV methods and evaluation on IVs. For each category, the main advances of both traditional statistical methods and machine learning enhanced methods are presented and discussed. Then, we introduce a variety of applications of IV methods in real world scenarios and summarize the available datasets and algorithms. Finally, we summarize the whole literature, discuss the open problems and suggest promising future research directions for IV method and its application. We also develop a toolkit of IVs methods reviewed in this survey at <https://github.com/causal-machine-learning-lab/mliv>.



Anpeng Wu, Kun Kuang, Ruoxuan Xiong, Fei Wu, Instrumental Variables in Causal Inference and Machine Learning, working paper.

IVs in Causal Inference and Machine Learning

mliv

```
from mliv.dataset.demand import gen_data
from mliv.utils import CausalDataset
gen_data()
data = CausalDataset('./Data/Demand/0.5_1.0_0.0_10000/1/')

from mliv.inference import Vanilla2SLS
from mliv.inference import Poly2SLS
from mliv.inference import NN2SLS
from mliv.inference import OneSIV
from mliv.inference import KernelIV
from mliv.inference import DualIV
from mliv.inference import DFL
from mliv.inference import AGMM
from mliv.inference import DeepGMM
from mliv.inference import DFIV
from mliv.inference import DeepIV          # Tensorflow & keras

for mod in [OneSIV,KernelIV,DualIV,DFL,AGMM,DeepGMM,DFIV,Vanilla2SLS,Poly2SLS,NN2SLS]:
    model = mod()
    model.config['num'] = 100
    model.config['epochs'] = 10
    model.fit(data)

print(mod)
```

Anpeng Wu, Kun Kuang, Ruoxuan Xiong, Fei Wu, Instrumental Variables in Causal Inference and Machine Learning, working paper.

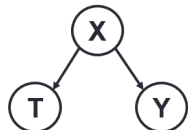
■ Sources of Correlation

Causation



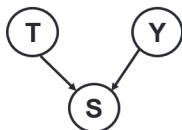
Stable
Actionable
Explainable

Confounding



Spurious Correlation:
T is correlated with Y
ignoring X

Sample Selection



Spurious Correlation:
T is correlated with Y
given S

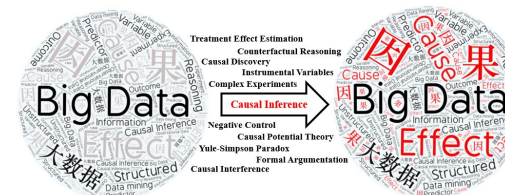
Causal Inference



Causality Regularized

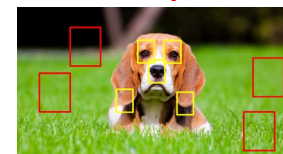
Machine Learning

■ Draw Causation from Big Data



■ Causal Representation/Learning

Stable & Explainable



Fair & Actionable



Thank You!

Kun Kuang

kunkuang@zju.edu.cn

Homepage: <https://kunkuang.github.io/>