Structural Causal Bandits with non-manipulable variables

Sanghack Lee Elias Bareinboim

*We only recently realized about preparing draft presentation so there might be some missing pieces (e.g., animation).

Executive Summary

- **SCM-MAB** = MAB + Causality
  where actions = interventions
- Q: Which interventions *can* be optimal?
  A: Possibly-Optimal Minimal Intervention Set (**POMIS**)
- Q: How to learn *an arm*'s reward from *other arms*?
  A: a generalized identifiability algorithm (**z^2ID**)
- Q: How to utilize **POMIS** and **z^2ID** in bandit algorithm?
  A: modified MAB algorithms for SCM-MAB (**z^2-TS**, **z^2-kl-UCB**)
- Faster convergence: smaller # of arms; more accurate estimation.

Overview

- **Motivation**: why we need to be causally-sensible
- **SCM-MAB** and its **structural properties**
- **SCM-MAB algorithms**
- **Empirical results**
- **Conclusions**

Motivation

Multi-armed bandit (MAB)

A classic, sequential decision-making problem

- Given: a set of **arms** (actions), $\mathbf{A}$
- How: at round t, pull an arm A_t, and get a **reward** Y_{A_t}
- Goal: to minimize cumulative **regret** (or maximize cumulative reward)

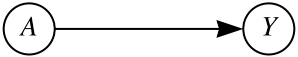
a trade-off between **exploitation** vs. **exploration**

Examples: ad. placement, online news recommendation, packet routing ...

Key **assumption**: arms are *independent* (in a traditional MAB setting)

Multi-armed bandit (MAB)

The reward mechanism can be understood as (at its simplest form possible),



Can we be agnostic to the mechanism between A and Y?
What if there exists a complex (causal) mechanism?

MAB through Causal Lens

Structural Causal Model (SCM) $\mathcal{M} = \langle \mathbf{U}, \mathbf{V}, \mathbf{F}, P(\mathbf{U}) \rangle$:

- $\mathbf{U}$: unobserved variables
- $\mathbf{V}$: observed variables
- $\mathbf{F}$: a set of functions for $\mathbf{V}$
- $P(\mathbf{U})$: a joint distribution over $\mathbf{U}$ ($\sim$randomness)

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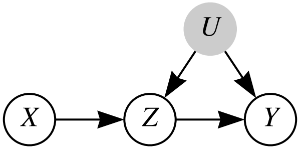
A causal graph $\mathcal{G}$ conforming to $\mathcal{M}$ looks like **DAG** + **bidirected edges** for unobserved confounders (UCs).[1]



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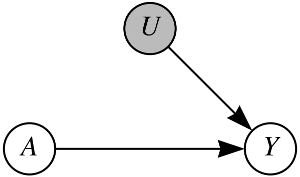
$$
\begin{tikzcd}
X \arrow[r] & Z \arrow[r] \arrow[r, dashed, bend left, leftrightarrow] & Y
\end{tikzcd}
$$

[1] among $\mathbf{U}$, only UCs will be visualized.

MAB through Causal Lens

An example with a traditional MAB problem



- a bandit algorithm plays an arm a by *doing* $do(a)$,
- get a reward, e.g.,

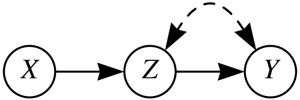
$$Y = f(a, u) = \mu_a + u,$$

where, e.g., $U \sim \mathcal{N}(0, 1)$.

(with time step t implicit)

MAB through Causal Lens — a worst case scenario?

Given an underlying causal mechanism,



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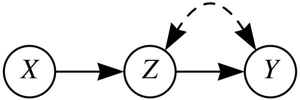

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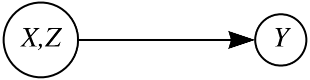

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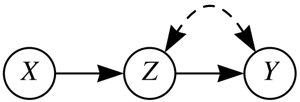

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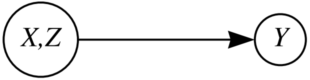

Insensitive to the structure: $\mathbf{A} = \mathfrak{X}_X \times \mathfrak{X}_Z$ (simultaneously)
Sensitive to the structure: $\mathbf{A} = \bigcup_{\mathbf{W} \subseteq \{X,Z\}} \mathfrak{X}_{\mathbf{W}}$ (all combinations)

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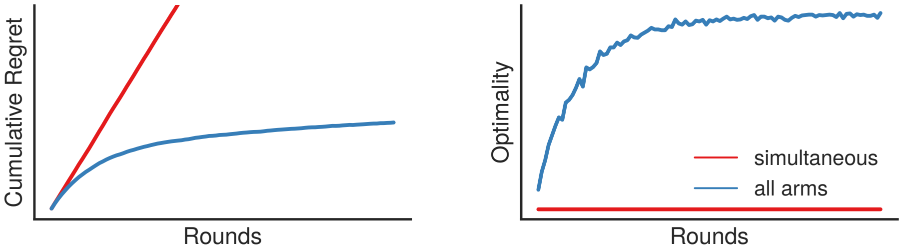

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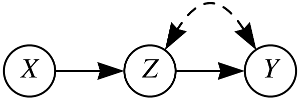

$\mathcal{M} = \langle \{U_X, U_Y, U_Z, U_{YZ}\}, \{X, Y, Z\}, \mathbf{F}, P(\mathbf{U}) \rangle$ where $\mathbf{F}$ is

$$
\begin{aligned}
X &\leftarrow U_X \\
Z &\leftarrow U_Z \oplus X \oplus U_{YZ} \\
Y &\leftarrow U_Y \oplus Z \oplus U_{YZ}
\end{aligned}
$$

and $P(U_X = 1) = 0.6$, $P(U_Y = 1) = 0.15$, $P(U_Z = 1) = 0.11$, $P(U_{YZ} = 1) = 0.51$.

MAB through Causal Lens — a worst case scenario?

Can we do better than ‘all subsets’ approach if we are aware of the underlying causal graph?

SCM-MAB

SCM-MAB, definition

A **SCM-MAB** is $\langle M, Y, \mathbf{N} \rangle$:

- a SCM $\mathcal{M} = \langle \mathbf{U}, \mathbf{V}, \mathbf{F}, P(\mathbf{U}) \rangle$,
- a reward variable $Y \in \mathbf{V}$,
- non-manipulable variables $\mathbf{N} \subseteq \mathbf{V} \setminus \{Y\}$

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Therefore,

- Actions: $\mathbf{A} = \{\mathbf{x} \in \mathfrak{X}_{\mathbf{X}} | \mathbf{X} \subseteq \mathbf{V} \setminus \mathbf{N} \setminus \{Y\}\}$ (including observation)
- Reward distribution: $P(Y|do(\mathbf{X} = \mathbf{x}))$ (or $P_{\mathbf{x}}(Y)$) $(\forall_{\mathbf{x} \in \mathbf{A}})$
- Expected reward: $\mu_{\mathbf{x}} = \mathbb{E}[Y|do(\mathbf{x})]$

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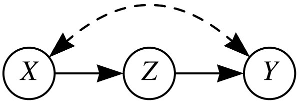
<u>Assumption: we access to the causal graph $\mathcal{G}$ without knowing $\mathbf{F}$ nor $P(\mathbf{U})$.</u>

SCM-MAB examples



- No non-manipulable variable
- Intervention sets: $\emptyset$, $\{X\}$, $\{Z\}$, $\{X, Z\}$
- Arms: $do(\emptyset)$, $do(X = 0)$, $do(X = 1)$, $\ldots$, $do(X = 1, Z = 1)$

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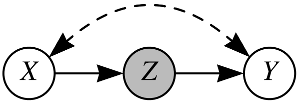
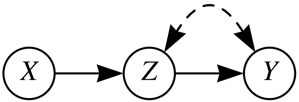


- Z is non-manipulable
- Intervention sets: $\emptyset$, $\{X\}$
- Arms: $do(\emptyset)$, $do(X = 0)$, $do(X = 1)$
- e.g., diet $\rightarrow$ cholesterol $\rightarrow$ health

SCM-MAB examples



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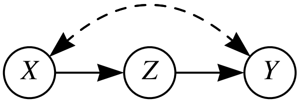
Structural Properties in SCM-MAB

Arms are **dependent** through underlying causal mechanism in SCM-MAB.

1. **Equivalence**: two arms share the **same** reward distribution



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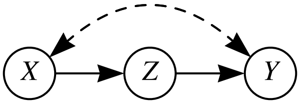

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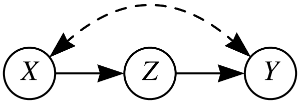

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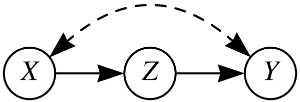

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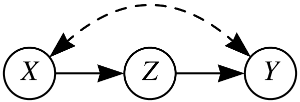

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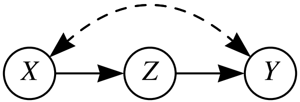
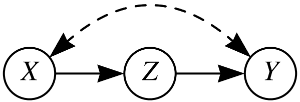
$$P_x(y) = \sum_z P(z|x) \sum_{x'} P(y|z, x')P(x')$$



Structural Property 1: Equivalence

Consider a graph:



$\mu_{x,z} = \mu_z$ based on Rule 3 of *do*-calculus (Pearl, 2000), $(Y \perp\!\!\!\perp X | Z)_{\mathcal{G}_{\overline{X,Z}}}$

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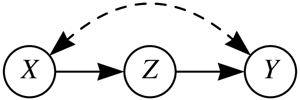

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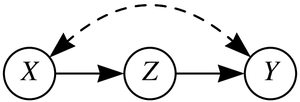

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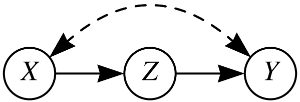

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Find out **minimal** sets of variables with **unique** rewards.

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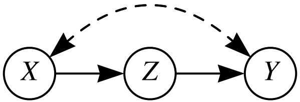

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Definition (Minimal Intervention Set (MIS))

Given $\langle \mathcal{G}, Y, \mathbf{N} \rangle$, a set of variables $\mathbf{X} \subseteq \mathbf{V} \setminus \{Y\} \setminus \mathbf{N}$ is said to be a *minimal intervention set* if there is no $\mathbf{X}' \subset \mathbf{X}$ such that $\mu_{\mathbf{x}'} = \mu_{\mathbf{x}}$ for every SCM conforming to $\mathcal{G}$ where $\mathbf{x}' \in \mathfrak{X}_{\mathbf{X}'}$ that is consistent with $\mathbf{x}$.

Structural Property 2: Partial-orderedness

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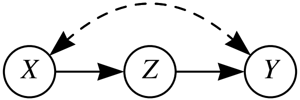

$\mu_x = \sum_z \mu_z P(z|x) \leq \sum_z \mu_{z^*} P(z|x) = \mu_{z^*}$.
Note that, there is no partial-order between $\emptyset$ and μ_z.

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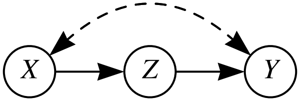

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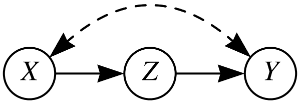

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Find out sets of variables that is not **dominated** by other sets.

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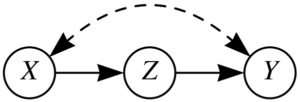

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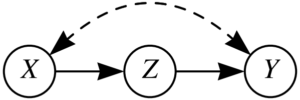

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Definition (Possibly-Optimal Minimal Intervention Set (POMIS))

Given $\langle \mathcal{G}, Y, \mathbf{N} \rangle$, let $\mathbf{X}$ $\in$MISs. If there exists a SCM conforming to $\mathcal{G}$ st

$$\mu_{\mathbf{x}^*} > \forall_{\mathbf{W} \in \text{MISs} \setminus \{\mathbf{X}\}} \mu_{\mathbf{w}^*},$$

then $\mathbf{X}$ is a *possibly-optimal minimal intervention set* wrt $\langle \mathcal{G}, Y, \mathbf{N} \rangle$.

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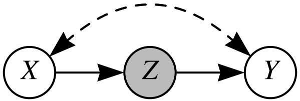

Since $do(z)$ becomes impossible, $do(x)$ is **not** dominated by other arms.
Note that, there is no partial-order between $\emptyset$ and μ_x.

Implication: play $do(\emptyset)$ and $do(x)$.

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Structural Property 3: Relating (POMISs) Arms

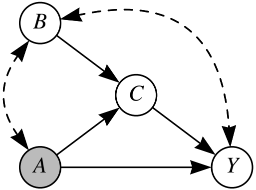
- Q: how are samples from $\{do(\mathbf{z})\}_{\mathbf{Z} \in \text{POMIS}}$ related to $do(\mathbf{x})$?

Structural Property 3: Relating (POMISs) Arms

- Q: how can we express $P_{\mathbf{x}}(\mathbf{v}')$ with $\{P_{\mathbf{z}}\}_{\mathbf{Z}\in\text{POMIS}}$?

- ID: $P_{\mathbf{x}}(\mathbf{v}')$ from $P(\mathbf{v})$ (SP, 2006)
- zID: $P_{\mathbf{x}}(\mathbf{v}')$ from $P_{\mathbf{z}'}(\mathbf{v})$ for $\mathbf{Z}' \subseteq \mathbf{Z}$ (BP, 2012)
- **z²ID**: $P_{\mathbf{x}}(\mathbf{v}')$ from a set of experiments (this paper)

Structural Property 3: Relating POMISs — an example



POMISs are $\emptyset$, $\{B\}$, and $\{C\}$.

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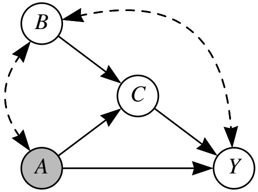
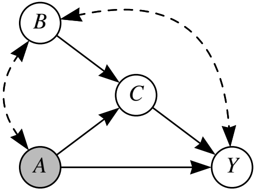


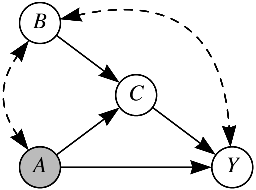
POMISs are $\emptyset$, $\{B\}$, and $\{C\}$.
Can we express $P(y)$ with $P_b(\mathbf{v})$ only?

Structural Property 3: Relating POMISs — an example



POMISs are $\emptyset$, $\{B\}$, and $\{C\}$.
Can we express $P_c(y)$ with $P_b(\mathbf{v})$ and/or $P(\mathbf{v})$?

Structural Property 3: Relating POMISs — an example



POMISs are $\emptyset$, $\{B\}$, and $\{C\}$.

$$P(y) = \sum\nolimits_{a,b,c} P_b(c|a) P_c(a,b,y)$$

$$P_b(y) = \sum\nolimits_{a,c} P(c|a,b) \sum\nolimits_{b'} P(y|a,b',c) P(a,b')$$

$$P_c(y) = \sum\nolimits_{a,b} P(y|a,b,c) P(a,b)$$

$$P_c(y) = \sum\nolimits_{a} P_b(y|a,c) P_b(a)$$

SCM-MAB algorithms

Incorporating Structural Properties into MAB algos.

What we know,

- **POMIS**: all arms vs. possibly-optimal arms
- **expressions**: utilize samples from other arms

Incorporating Structural Properties into MAB algos.

What we know,

- **POMIS**: all arms vs. possibly-optimal arms
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Two algorithms we considered:

- **Thompson sampling**: posterior sample for expected reward
  $\rightarrow$ approximate ‘posterior distribution’ w/ all available data.
- **kl-UCB**: upper bounds computed for expected reward
  $\rightarrow$ adjust ‘upper bound’ by taking account samples from other arms.

SCM-MAB algorithm: modified TS

taking advantage of **POMIS** and **z²ID**.

function z^2-TS$(\mathcal{G}, Y, \mathbf{N}, T)$

$\mathbb{Z} \leftarrow \mathbb{P}^{\mathbf{N}}_{\mathcal{G},Y}$

$\mathbf{A} \leftarrow \{\mathbf{x} \in \mathfrak{X}_{\mathbf{X}} \mid \mathbf{X} \in \mathbb{Z}\}$

$\hat{\boldsymbol{\theta}}_{\mathbf{x}} \leftarrow \{P_{\mathbf{x}}(y)\} \cup \{\text{z}^2\text{ID}(\mathcal{G}, y, \mathbf{x}, \mathbb{Z}')\}_{\mathbb{Z}' \subseteq \mathbb{Z} \setminus \{\mathbf{X}\}}$ **for** $\mathbf{x} \in \mathbf{A}$

$\mathbf{D} \leftarrow \{D_{\mathbf{x}} = \emptyset\}_{\mathbf{x} \in \mathbf{A}}$

for t in $1, \ldots, T$ **do**

  for $\mathbf{x} \in \mathbf{A}$ **do**

    $\hat{\theta}_{\mathbf{x}}, \hat{s}^2_{\mathbf{x}} \leftarrow \text{bMVWA}(\mathbf{D}, \hat{\boldsymbol{\theta}}_{\mathbf{x}})$

    Find $\hat{\alpha}_{\mathbf{x}}, \hat{\beta}_{\mathbf{x}}$ such that Beta$(\hat{\alpha}_{\mathbf{x}}, \hat{\beta}_{\mathbf{x}})$ matching $\hat{\theta}_{\mathbf{x}}, \hat{s}^2_{\mathbf{x}}$

    $\theta_{\mathbf{x}} \sim \text{Beta}(\hat{\alpha}_{\mathbf{x}}, \hat{\beta}_{\mathbf{x}})$

  $\mathbf{x}' \leftarrow \arg\max_{\mathbf{x} \in \mathbf{A}} \theta_{\mathbf{x}}$

  Sample $\mathbf{v}$ by $do(\mathbf{x}')$ and append $\mathbf{v}$ to $D_{\mathbf{x}'}$

SCM-MAB algorithm: modified kl-UCB

taking advantage of **POMIS** and **z²ID**.

function z^2-KL-UCB$(\mathcal{G}, Y, \mathbf{N}, T, f \leftarrow \ln(t) + 3\ln(\ln(t)))$

Initialize $\mathbb{Z}, \mathbf{A}$, $\{\hat{\boldsymbol{\theta}}_{\mathbf{x}}\}_{\mathbf{x}\in\mathbf{A}}$, $\mathbf{D}$

$(\forall_{\mathbf{x}\in\mathbf{A}})$ Sample $\mathbf{v}$ by $do(\mathbf{x})$, and append $\mathbf{v}$ to $D_{\mathbf{x}}$

for t in $|\mathbf{A}|, \ldots, T$ **do**

$\hat{\theta}_{\mathbf{x}}, \hat{s}^2_{\mathbf{x}} \leftarrow$ bMVWA$(\mathbf{D}, \hat{\boldsymbol{\theta}}_{\mathbf{x}})$ **for** $\mathbf{x} \in \mathbf{A}$

$\hat{N}_{\mathbf{x}} \leftarrow \hat{\theta}_{\mathbf{x}}(1 - \hat{\theta}_{\mathbf{x}})/\hat{s}^2_{\mathbf{x}}$; $\hat{t} \leftarrow \sum_{\mathbf{x}} \hat{N}_{\mathbf{x}}$

$$\boldsymbol{\mu} = \left\{ \sup \left\{ \mu \in [0,1] : \mathrm{KL}(\hat{\theta}_{\mathbf{x}}, \mu) \leq \frac{f(\hat{t})}{\hat{N}_{\mathbf{x}}} \right\} \right\}_{\mathbf{x}\in\mathbf{A}}$$

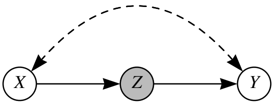
$\mathbf{x}' \leftarrow \arg\max_{\mathbf{x}\in\mathbf{A}} \mu_{\mathbf{x}}$

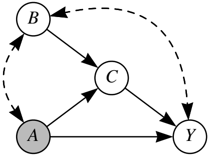
Sample $\mathbf{v}$ by $do(\mathbf{x}')$, and append $\mathbf{v}$ to $D_{\mathbf{x}'}$

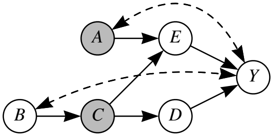
Empirical Evaluation

Experimental settings

- **4** strategies: Brute-force, MIS, POMIS, POMIS+
- **2** base MAB algorithms: Thompson sampling (TS), kl-UCB
- **3** SCM-MAB problems, binary $\mathbf{V}$



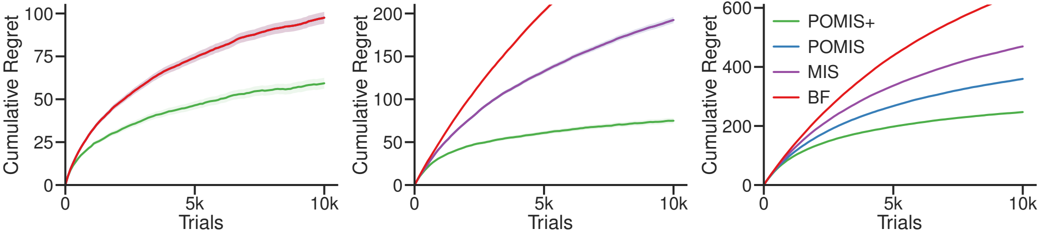




- **1000** simulations

Experimental results (average cumulative regret)

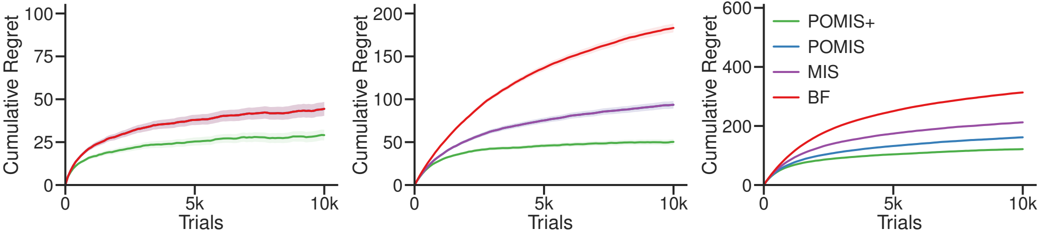
base algorithm: kl-UCB



Performance: POMIS+ $>$ POMIS $\geq$ MIS $\geq$ Brute-force

Experimental results (average cumulative regret)

base algorithm: TS

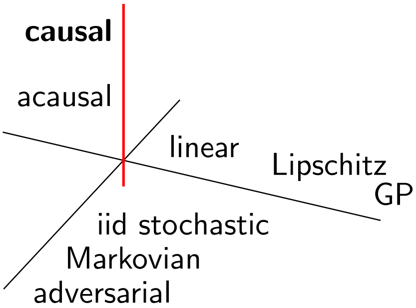


Performance: POMIS+ $>$ POMIS $\geq$ MIS $\geq$ Brute-force

Conclusions

Bandit Landscape

Dimensions: functional assumptions, bandit type, reward type, etc.
We generalized MABs into a *causal* dimension.



SCM-MAB: stochastic iid reward, nonparametric, bandit feedback

Conclusions

We studied how to take advantage of a known causal graph in bandit setting:

- introduced: **SCM-MAB** w/ non-manipulability constraints
- characterized: Possibly-Optimal Minimal Intervention Set (**POMIS**)
- devised: $\mathbf{z^2}$**ID** to connect arms
- designed: SCM-MAB algorithms: $\mathbf{z^2}$**-TS**, $\mathbf{z^2}$**-kl-UCB**

Conclusions

We studied how to take advantage of a known causal graph in bandit setting:

- introduced: **SCM-MAB** w/ non-manipulability constraints
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Mahalo!

(= thank you)