

# Computational Causal Discovery and its Applications

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# Computational Causal Analytics at U of Minnesota

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Causal  
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Causal  
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Discovering  
Causal  
Structure  
From  
Observational  
Data

Applications  
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Methods

Constantin Aliferis, Professor, Director of IHI at UMN



Gyorgy Simon, Associate Professor



# Computational Causal Analytics at U of Minnesota

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Erich Kummerfeld, Assistant Professor



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# Where to find material related to this talk?

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[github.com/SisiMa1729/CausalAnalytics\\_Intro](https://github.com/SisiMa1729/CausalAnalytics_Intro)  
[github.com/SisiMa1729/Causal\\_Feature\\_Selection](https://github.com/SisiMa1729/Causal_Feature_Selection)

# Overview

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- 1 Computational Causal Discovery
- 2 Discovering Causal Structure From Observational Data
- 3 Applications of Causal Discovery Methods

# What is Computational Causal Discovery?

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- Discovery of Causal Structure
- Estimation of Causal Effect
- Using a combination of observational data, experimental data, and prior knowledge.

# Discovery of Causal Structure

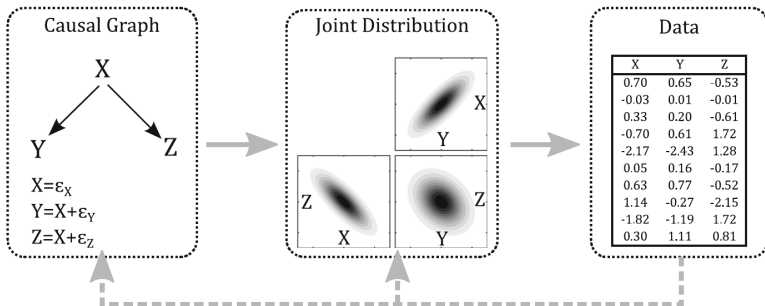
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# Estimation of Causal Effect

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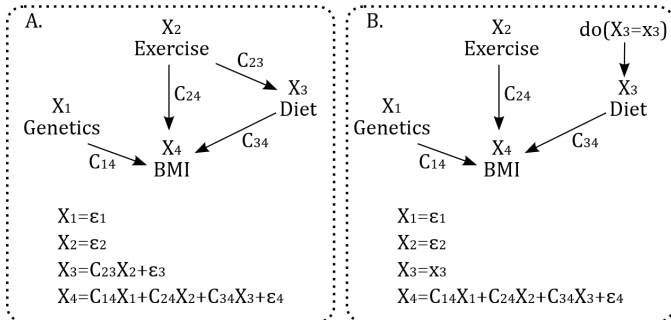
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$E(Y|do(X = x)) - E(Y|do(X = x'))$  is the average effect on  $Y$  when changing  $X$  from  $x$  to  $x'$



\* comment: SEM?



# Discovery of Causal Structure

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Correct effect estimation depends on identifying the correct causal structure.

# Discovery of Causal Structure

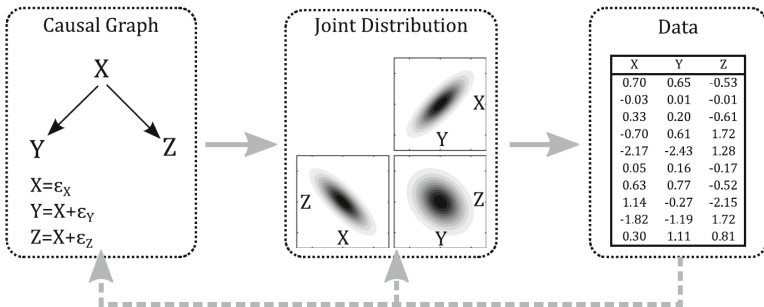
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# Discovery of Causal Structure

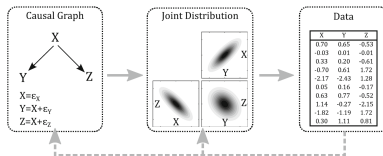
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- score based method (maximize likelihood of data given causal structure)
- constraint-based (joint distribution of data is constrained by causal structure)
- hybrid of the above two

# Discovery of Causal Structure

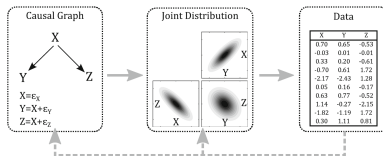
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- score based method (maximize likelihood of data given causal structure)
- constraint-based (joint distribution of data is constrained by causal structure)
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# Discovery of Causal Structures: Assumptions

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Causal Markovian Condition: Every Markovian causal model  $M$  induces a distribution  $P(X_1, \dots, X_i, \dots, X_n)$  that satisfies the parental Markov condition relative to causal diagram  $G$  associated with  $M$ ; that is, each variable  $X_i$  is independent of all its nondescendants, given its parents in  $G$ . i.e.

$$X_i \perp V - DE_i | PA_i$$

This results in the important decomposition of the joint distribution  $P(X_1, \dots, X_i, \dots, X_n) = \prod_i^n P(X_i | PA_i)$

# Discovery of Causal Structures: Assumptions

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**Faithfulness Condition:** Let  $G$  be a causal graph and  $P$  a probability distribution generated by  $G$ .  $G$  and  $P$  satisfies the faithfulness condition if and only if every conditional independence true in  $P$  is entailed by the Causal Markovian condition applied to  $G$ .

# Discovery of Causal Structures: Assumptions

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Intuitively, causal Markov condition and faithfulness condition establish a one to one relationship between the causal graph (more precisely, Markov equivalent class) and the joint probability distribution. This correspondence makes causal discovery possible.

# Causal Graph and Conditional Independency

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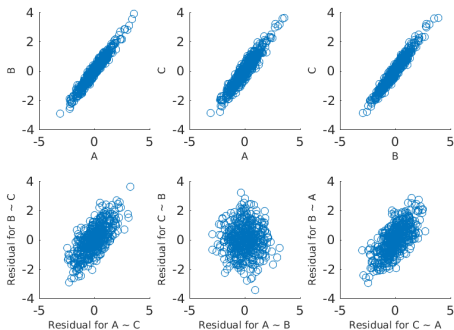
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Conditional independence, What does it look like:

$A \rightarrow B \rightarrow C$ ;  $A \leftarrow B \leftarrow C$ ; or  $A \leftarrow B \rightarrow C$



$A \not\perp B, A \not\perp C, B \not\perp C$

$A \not\perp B|C, A \perp C|B, B \not\perp C|A$



# Causal Graph and Conditional Independency

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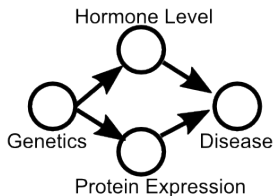
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The concept of conditional independency:



# Causal Graph and Conditional Independency

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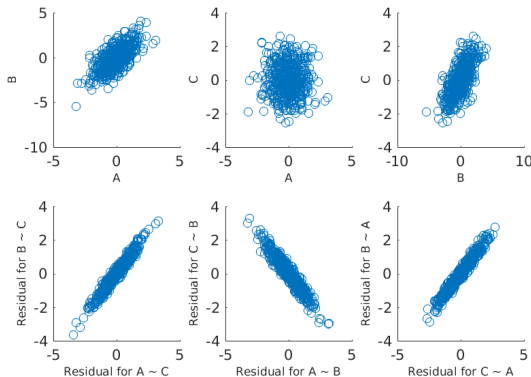
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Conditional independency, What does it look like:

$$A \perp\!\!\!\perp B \mid C$$



$$A \not\perp\!\!\!\perp B, A \perp\!\!\!\perp C, B \not\perp\!\!\!\perp C$$

$$A \not\perp\!\!\!\perp B \mid C, A \not\perp\!\!\!\perp C \mid B, B \not\perp\!\!\!\perp C \mid A$$

# Causal Graph and Conditional Independency

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## Conditional Independence Tests:

- fisher's test
- $\chi^2$ ,  $g^2$
- conditional mutual information, distance correlation
- comparison of nested models

# Causal Mechanism from Observational Data

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The demonstrated relationships among three variables can be extended to discover causal graphs among any number of variables.

Some popular algorithms:

- constraint based: SGS, PC, HITON-PC, FCI
- score based: GES, FGES
- hybrid: MMHC, GFCI

# Causal Mechanism from Observational Data

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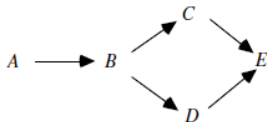
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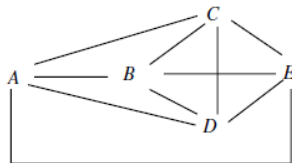
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Example: PC algorithm: Skeleton Phase:



True Graph



Complete Undirected Graph

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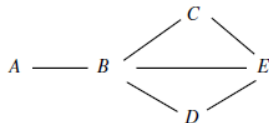
$n = 0$  No zero order independencies

---

$n = 1$  First order independencies

$A \perp\!\!\!\perp C \mid B$        $A \perp\!\!\!\perp D \mid B$   
 $A \perp\!\!\!\perp E \mid B$        $C \perp\!\!\!\perp D \mid B$

Resulting Adjacencies



# Causal Mechanism from Observational Data

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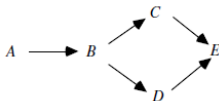
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Example: PC algorithm:



True Graph

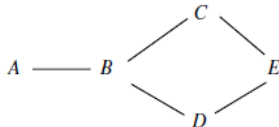
Skeleton Phase (continued):

---

$n = 2$ : Second order independencies

$$B \perp\!\!\!\perp E \mid \{C, D\}$$

Resulting Adjacencies



# Causal Mechanism from Observational Data

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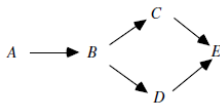
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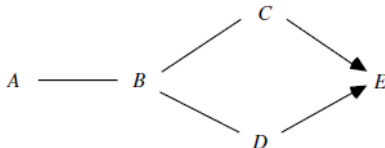
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Example: PC algorithm:



True Graph

Orientation Phase:



Note: Markov equivalent class

# Applications of Causal Discovery Methods

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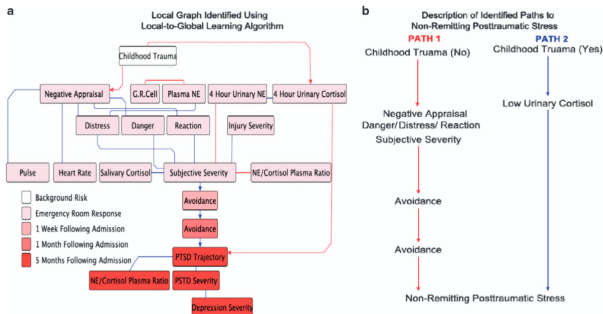
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- Causal Mechanism from Observational Data
- Causal Graph Guided Experimentation
- Causal Feature Selection



# Causal Mechanism from Observational Data

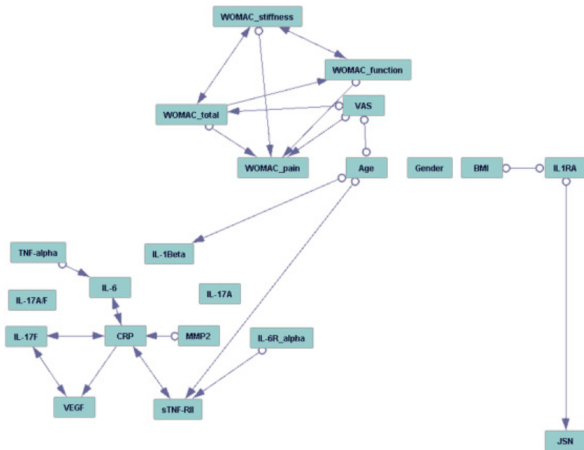
## Biological Mechanisms of PTSD:



[Galatzer-Levy et al., 2017]

# Causal Mechanism from Observational Data

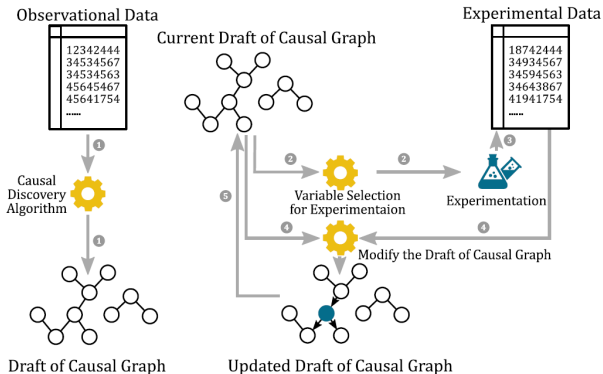
## Biological Mechanisms of Osteoarthritis:



[Attur et al., 2015]

# Causal Graph Guided Experimentation

Reduce number of Experiments needed to fully resolve the causal relations



[Statnikov et al., 2015]

# Causal Feature Selection for Predictive Models

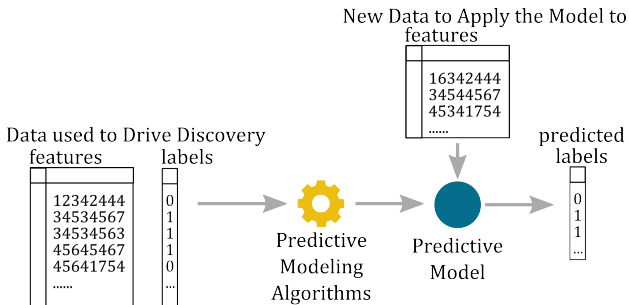
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# Causal Feature Selection for Predictive Models

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## Goals of Feature Selection:

- Improve model predictivity
- Enhance model interpretability
- Increase cost-efficiency for model deployment

Causal feature selection is well-suited for these goals.

# Optimal Feature Set

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**Optimal feature set:** Given a data set  $\mathbb{D}$  (a sample from distribution  $\mathbb{P}$ ) for variables  $\mathbf{V}$ , a learning algorithm  $\mathbb{L}$ , and a performance metric  $\mathbb{M}$ , a feature set  $\mathbf{X} \subseteq \mathbf{V}$  is an optimal feature set of  $T$  if  $\mathbf{X}$  maximizes the performance metric  $\mathbb{M}$  for predicting  $T$  using learner  $\mathbb{L}$  in the dataset  $\mathbb{D}$ .

[Statnikov et al., 2013, Kohavi and John, 1997]

Note: Optimal here is defined with respect to predictivity.

There could be redundant features in a optimal feature set according to this definition.

# Information Content of a Feature

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The contribution of a given feature to the predictive performance of a model depends on what other features are present in the model.

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Let  $\mathbf{S}_i = \mathbf{V} - V_i$ , the set of all features except  $V_i$

**Strong relevance:** A feature  $V_i$  is strongly relevant to  $T$  iff there exists some  $v_i$ ,  $t$ , and  $s_i$  for which  $p(V_i = v_i, \mathbf{S}_i = s_i) > 0$ , such that  $p(T = t | V_i = v_i, \mathbf{S}_i = s_i) \neq p(T = t | \mathbf{S}_i = s_i)$ .

[Kohavi and John, 1997]



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Strongly relevant features are conditionally dependent of  $T$  given all other measured variables. In other words, knowing the value of features  $V_i$  gives additional information regarding the target of interest, even when we know the value of all other features.

[Kohavi and John, 1997]

# Information Content of a Feature

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Let  $\mathbf{S}_i = \mathbf{V} - V_i$ , the set of all features except  $V_i$

**Weak relevance:** A feature  $V_i$  is weakly relevant to  $T$  iff it is not strongly relevant, and  $\exists S'_i \subset S_i$  and some  $v_i, t$ , and  $s'_i$  for which  $p(V_i = v_i, \mathbf{S}'_i = s'_i) > 0$ , such that  $p(T = t | X_i = v_i, S'_i = s'_i) \neq p(T = t | S'_i = s'_i)$ .

[Kohavi and John, 1997]

# Selection based on combination of features

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Knowing the value of weakly relevant variable  $V_i$  do not give additional information regarding the target of interest, when we know the value of all other features; however if we only know the value of a subset of all other measured variables, knowing the value of  $V_i$  may provide additional information.

[Kohavi and John, 1997]

# Selection based on combination of features

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**Irrelevance:** A feature  $V_i$  is relevant if it is either weakly relevant or strongly relevant; otherwise, it is irrelevant.

Irrelevant features neither provide information regarding the target by itself nor in combination with any other features.

[Kohavi and John, 1997]

# Selection based on combination of features

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Given the definition of strong, weak and irrelevant variables, what is our strategy?

- Strongly relevant features should always be selected.  
Omitting Strongly relevant features will compromise predictive performance.
- Weakly relevant features do not improve predictive performance if all strongly relevant features are selected.
- Irrelevant features do not improve predictive performance.

[Kohavi and John, 1997]

# Relationship between Causality and Feature Selection

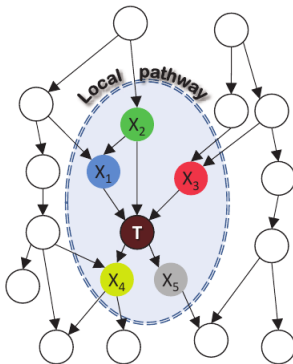
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The Markov Boundary (direct causes + direct effects + direct causes of direct effects) is the minimal feature set that contain all information regarding the target of interest (i.e. strongly relevant) under faithfulness.

# Benefit of Causal Feature Selection

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- selected features have causal interpretations
- selected feature set is generally smaller compared to non-causal methods
- model generalize better under certain type of distribution shift

## Benefit of Causal Feature Selection

# Computational Causal Discovery

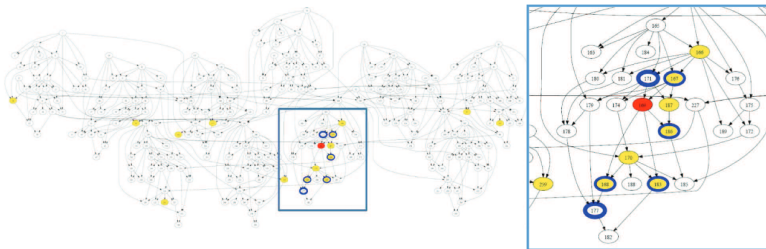
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Example: selected features have causal interpretations.

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# Discovering Causal Structure From Observational Data

## Applications of Causal Discovery Methods

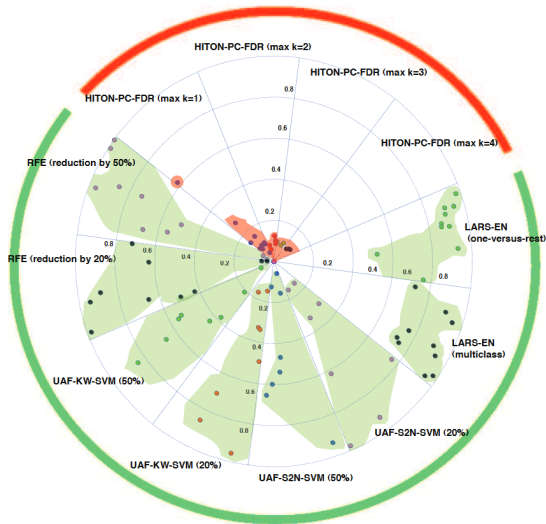


[Aliferis et al., 2010a]



# Benefit of Causal Feature Selection

Example: selected features have causal interpretations.



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# Benefit of Causal Feature Selection

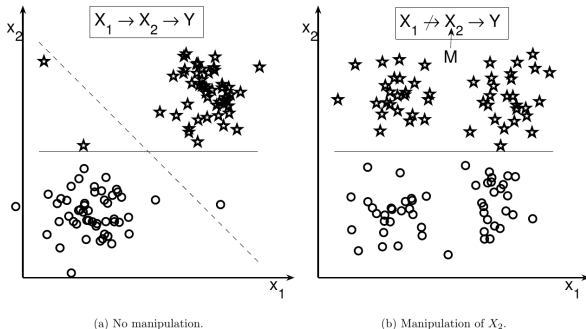
Example: selected feature set is generally smaller compared to non-causal methods, without compromising predictive performance.

Feature selection method	<i>Predictivity</i>		<i>Reduction</i>	
	P-value	Nominal winner	P-value	Nominal winner
<b>No feature selection</b>	0.1890	Other	<0.0001	HITON-PC
<b>RFE: 4 variants</b>	0.9754	Other	<b>0.0046</b>	HITON-PC
	0.8030	Other	<b>0.0042</b>	HITON-PC
	0.1312	HITON-PC	0.3634	HITON-PC
	0.1008	HITON-PC	0.6816	Other
	0.2248	Other	<b>0.0028</b>	HITON-PC
<b>UAF-KruskalWallis-SVM: 4 variants</b>	<b>0.0098</b>	Other	<b>0.0004</b>	HITON-PC
	1.0000	HITON-PC	0.1414	HITON-PC
	0.3232	HITON-PC	0.3998	HITON-PC
	0.0710	Other	<b>0.0018</b>	HITON-PC
	0.0752	Other	<b>0.0030</b>	HITON-PC
<b>UAF-Signal2Noise-SVM: 4 variants</b>	0.4420	HITON-PC	0.7850	HITON-PC
	0.2820	HITON-PC	0.6604	HITON-PC
	0.5046	Other	<0.0001	HITON-PC
	0.9782	HITON-PC	<0.0001	HITON-PC
	0.6980	HITON-PC	<b>0.0044</b>	HITON-PC
<b>UAF-Neal-SVM: 4 variants</b>	0.3806	HITON-PC	<b>0.0186</b>	HITON-PC
	0.6064	HITON-PC	0.3252	HITON-PC
	0.5050	HITON-PC	0.1338	Other
<b>Random Forest Variable Selection: 2 variants</b>	1.0000	Other	0.1112	HITON-PC
	0.0832	HITON-PC	0.5216	Other
	0.3033	Other	<0.0001	HITON-PC
<b>LARS-Elastic Net: 2 variants</b>	0.3033	Other	<0.0001	HITON-PC
	0.3033	Other	<0.0001	HITON-PC
	0.3033	Other	<0.0001	HITON-PC

[Aliferis et al., 2010a]

# Benefit of Causal Feature Selection

Example: Model built with causal feature selection methods generalize better under certain distribution shifts.



[Guyon et al., 2007]

# Markov Boundary

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There are a number of algorithms that discovery the local causal neighbourhood of the data.

- PC-simple[Bühlmann et al., 2010]
- HITON-PC[Aliferis et al., 2003, Aliferis et al., 2010a, Aliferis et al., 2010b]
- HITON-MB[Aliferis et al., 2010a, Aliferis et al., 2010b]
- MMPC [Tsamardinos et al., 2006]
- IAMB[Tsamardinos et al., 2003]
- MBFS[Ramsey, 2006]

# Take Home Message

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- Causal structural discovery methods can identify causal relationships from observational and experimental data with and without domain knowledge.
- Computational causal discovery methods have wide applications in knowledge discovery and predictive modeling.
- [github.com/SisiMa1729/CausalAnalytics\\_Intro](https://github.com/SisiMa1729/CausalAnalytics_Intro)
- [github.com/SisiMa1729/Causal\\_Feature\\_Selection](https://github.com/SisiMa1729/Causal_Feature_Selection)

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