# Computational Causal Discovery and its Applications

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# Computational Causal Analytics at U of Minnesota

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Gyorgy Simon, Associate Professor

# Computational Causal Analytics at U of Minnesota



Erich Kummerfeld, Assisstant Professor

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# Where to find material related to this talk?



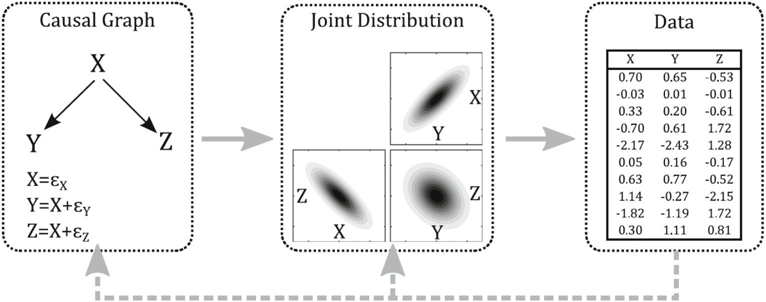
`https://github.com/SisiMa1729/Causal_Feature_Selection`

# Overview

# What is Computational Causal Discovery?

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

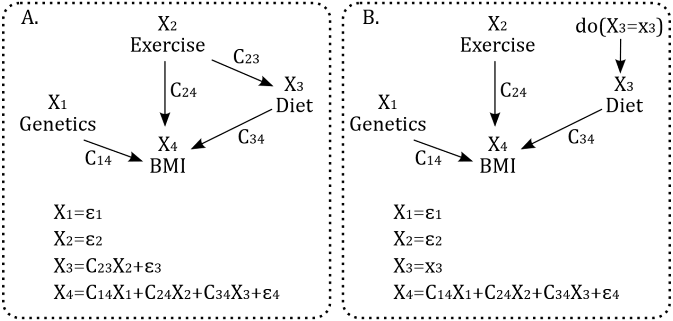
# Discovery of Causal Structure




| X | Y | Z |
|---|---|---|
| 0.70 | 0.65 | -0.53 |
| -0.03 | 0.01 | -0.01 |
| 0.33 | 0.20 | -0.61 |
| -0.70 | 0.61 | 1.72 |
| -2.17 | -2.43 | 1.28 |
| 0.05 | 0.16 | -0.17 |
| 0.63 | 0.77 | -0.52 |
| 1.14 | -0.27 | -2.15 |
| -1.82 | -1.19 | 1.72 |
| 0.30 | 1.11 | 0.81 |

# Estimation of Causal Effect

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

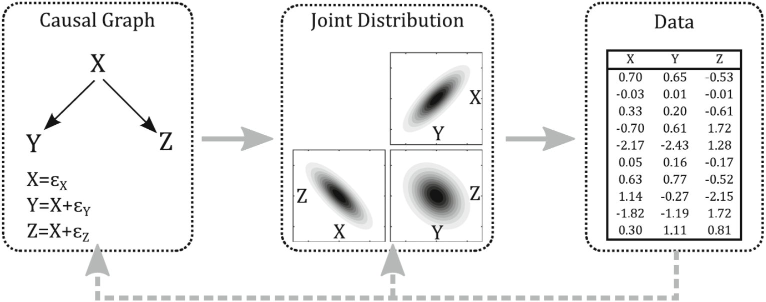



* comment: SEM?

# Discovery of Causal Structure

Correct effect estimation depends on identifying the correct causal structure.

# Discovery of Causal Structure

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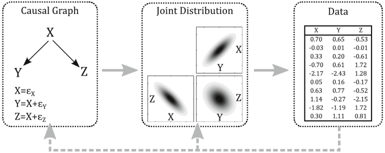
# Discovery of Causal Structure

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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

Computational Causal Discovery

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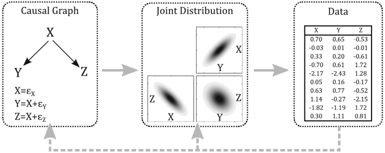
Computational Causal Discovery

Discoverying Causal Structure From Observational Data

Applications of Causal Discovery Methods

# Discovery of Causal Structure

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# Discovery of Causal Structures: Assumptions



Causal Markovian Condition: Every Markovian causal model $M$ induces a distribution $P(X_1, ...X_i, ..., X_n)$ that satisfies the parental Markov condition relative to 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. $X_i \perp V - DE_i | PA_i$

# Discovery of Causal Structures: Assumptions



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 $G$.

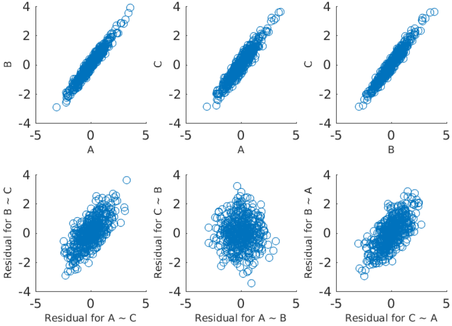
# Discovery of Causal Structures: Assumptions



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

# Causal Graph and Conditional Independency

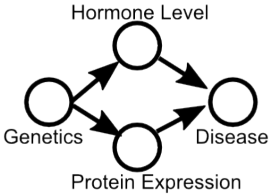
Conditional independence, What does it look like:
$A- > B- > C$; $A < -B < -C$; or $A < -B- > C$




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

# Causal Graph and Conditional Independency

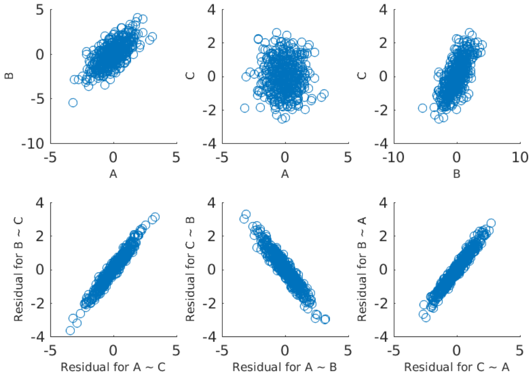
The concept of conditional independence:



# Causal Graph and Conditional Independency

Conditional independence, What does it look like:

$A- > B < -C$




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

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

# Causal Graph and Conditional Independency



Conditional Independence Tests:

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

# Causal Mechanism from Observational Data



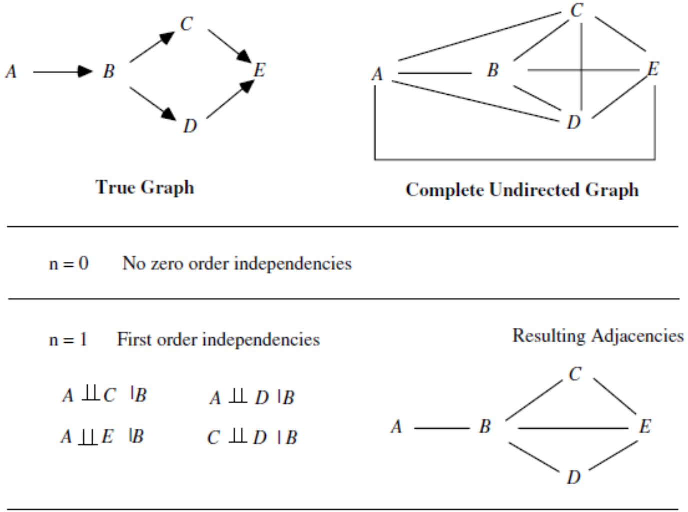
The demonstrated relationships among three variables can be extended to discover causal graphs among any number of variables. Some popular algorithms:

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

# Causal Mechanism from Observational Data



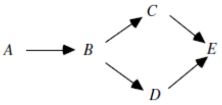
Example: PC algorithm: Skeleton Phase:



# Causal Mechanism from Observational Data



Example: PC algorithm:



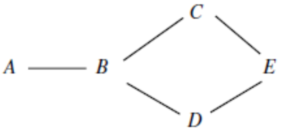

**True Graph**

Skeleton Phase (continued):

n = 2: Second order independencies

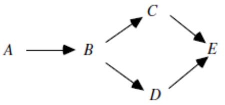
$B \perp\!\!\!\perp E \mid \{C,D\}$

Resulting Adjacencies



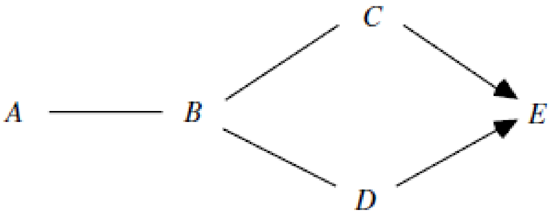
# Causal Mechanism from Observational Data

Example: PC algorithm:




True Graph

Orientation Phase:



# Applications of Causal Discovery Methods

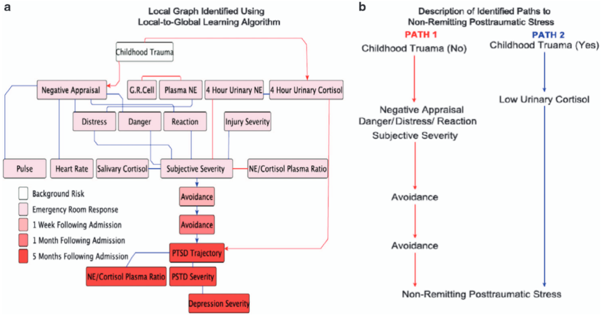


- Causal Mechanism from Observational Data
- Causal Graph Guided Experimentation
- Causal Feature Selection

# Causal Mechanism from Observational Data



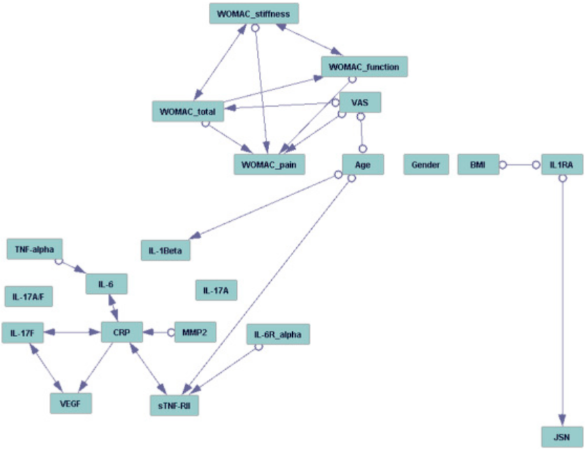
## Biological Mechanisms of PTSD:




[Galatzer-Levy et al., 2017]

# Causal Mechanism from Observational Data

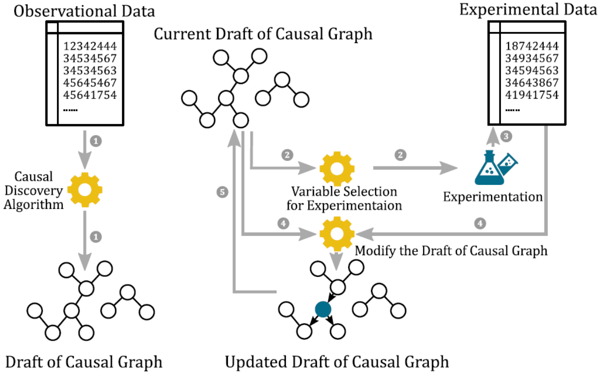
Biological Mechanisms of Osteoarthritis:




[Attur et al., 2015]

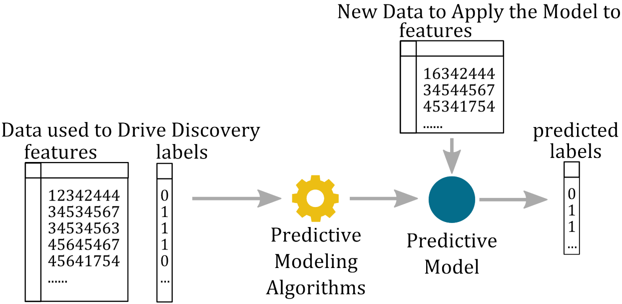
# Causal Graph Guided Experimentation

Reduce number of Experiments needed to fully resolve the causal relations




[Statnikov et al., 2015]

# Causal Feature Selection for Predictive Models



# Causal Feature Selection for Predictive Models



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



**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 redundent features in a optimal feature set according to this definition.

# Information Content of a Feature

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

# Information Content of a Feature



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]

# Information Content of a Feature



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

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

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

**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



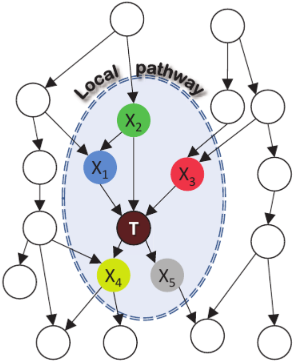
Given the definition of strong, weak and irrelevant variables, what is our stratergy?

- 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






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.

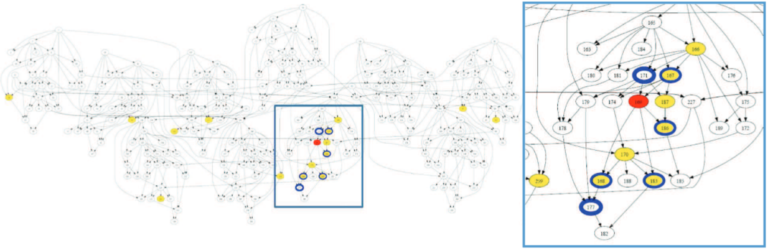
# Benefit of Causal Feature Selection



- 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

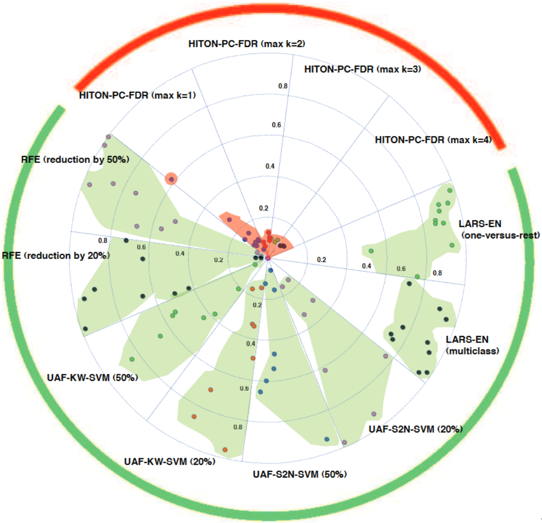
Example: selected features have causal interpretations.



[Aliferis et al., 2010a]

# Benefit of Causal Feature Selection

Example: selected features have causal interpretations.



# Benefit of Causal Feature Selection

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

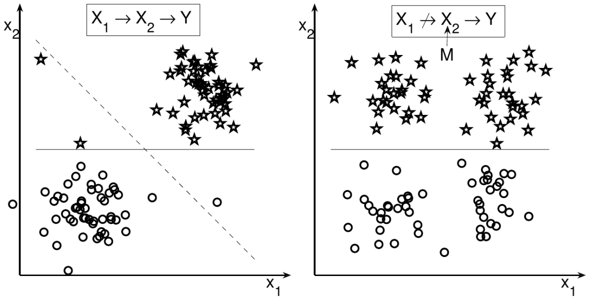
| | ***Predicitivity*** | | ***Reduction*** | |
|---|---|---|---|---|
| Feature selection method | P-value | Nominal winner | P-value | Nominal winner |
| **No feature selection** | 0.1890 | Other | **<0.0001** | HITON-PC |
| **RFE:** 4 variants | 0.9754 | Other | **0.0046** | HITON-PC |
| | 0.8030 |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

[Aliferis et al., 2010a]

# Benefit of Causal Feature Selection



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




(a) No manipulation. (b) Manipulation of $X_2$.

[Guyon et al., 2007]

# Markov Boundary



There are a number of algorithms that discovery the local causal neibourhood 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

- 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.

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Local causal and markov blanket induction for causal discovery and feature selection for classification part i: Algorithms and empirical evaluation.
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