Learning Causal Structure with Kernel-based Dependence Measures

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November 3-4, 2007

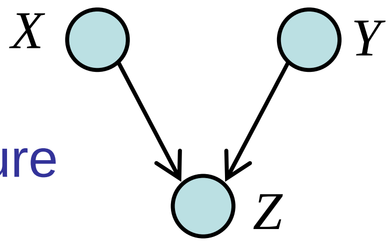
Outline

1. Introduction
2. Kernel measures for dependence
3. Kernel measures for conditional dependence
4. Causal inference with kernels
   – Kernel-based Causal Learning algorithm –
5. Conclusion

Introduction

- Conditional independence in causal learning
  - Determining independence and conditional independence is essential in causal learning.

v-structure



$$\Longleftrightarrow$$

$$X \perp\!\!\!\perp Y$$

and

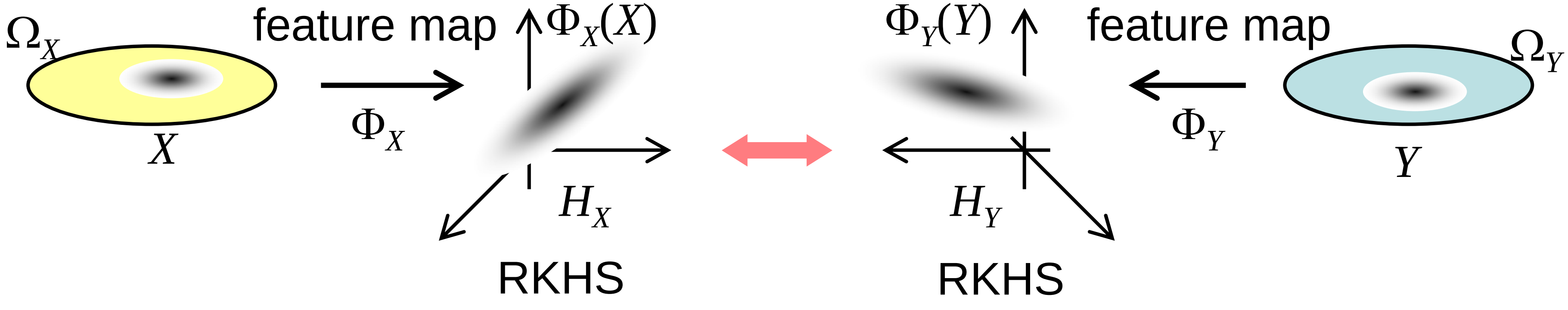
$$X \not\perp\!\!\!\perp Y \mid Z$$

  - But, in practice
    - Dependence for continuous domain is not straightforward.

      How can we estimate mutual information?
    - Many algorithms use linear statistical methods (partial correlation) or discretization.

“Kernel methods” for dependence of variables

- Positive definite kernels have been used for capturing nonlinearity of original data. *e.g*. Support vector machine.
- Kernelization: mapping data into a functional space (RKHS) and apply linear methods on RKHS.
- Recently, kernel methods have been applied for dependence analysis. Covariance structure on RKHS gives dependence and conditional dependence of the original variables.



Positive Definite Kernel and RKHS

- **Positive definite kernel (p.d. kernel)**

  Ω: set. $k : \Omega \times \Omega \to \mathbf{R}$

  k is positive definite if $k(x,y) = k(y,x)$ and for any $n \in \mathbf{N}$, $x_1, \ldots x_n \in \Omega$ the matrix $\left(k(x_i, x_j)\right)_{i,j}$ (Gram matrix) is positive semidefinite.

  – Example: Gaussian RBF kernel $k(x, y) = \exp\left(-\|x - y\|^2 / \sigma^2\right)$

- **Reproducing kernel Hilbert space (RKHS)**

  k: p.d. kernel on Ω.

  $\Rightarrow$ $\exists 1\ H$: reproducing kernel Hilbert space (RKHS)

  1) $k(\cdot, x) \in H$ for all $x \in \Omega$.

  2) $\mathrm{Span}\{k(\cdot, x) \mid x \in \Omega\}$ is dense in H.

  3) $\langle k(\cdot, x), f \rangle_H = f(x)$ (reproducing property)

Feature map / feature vector

$$\Phi : \Omega \to H, \quad x \mapsto k(\cdot, x) \qquad i.e. \quad \Phi(x) = k(\cdot, x)$$

Data: $X_1, \ldots, X_N$ → $\Phi_X(X_1), \ldots, \Phi_X(X_N)$: functional data

Why RKHS?

- By the reproducing property, computation of the inner product on RKHS does not need expansion by basis functions.

$$\langle \Phi(x), \Phi(y) \rangle = k(x, y)$$

$$f = \sum_{i=1}^{N} a_i \Phi(x_i) = \sum_i a_i k(\cdot, x_i), \qquad g = \sum_{j=1}^{N} b_j \Phi(x_j) = \sum_j b_j k(\cdot, x_j)$$

$$\Rightarrow \quad \langle f, g \rangle = \sum_{i,j} a_i b_j k(x_i, x_j)$$

The computational cost essentially depends on the sample size.
Advantageous for high-dimensional data of small sample size.

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Covariance on RKHS

– Linear case (Gaussian):

$$\mathrm{Cov}[X, Y] = E[YX^T] - E[Y]E[X]^T$$: covariance matrix

– On RKHS:

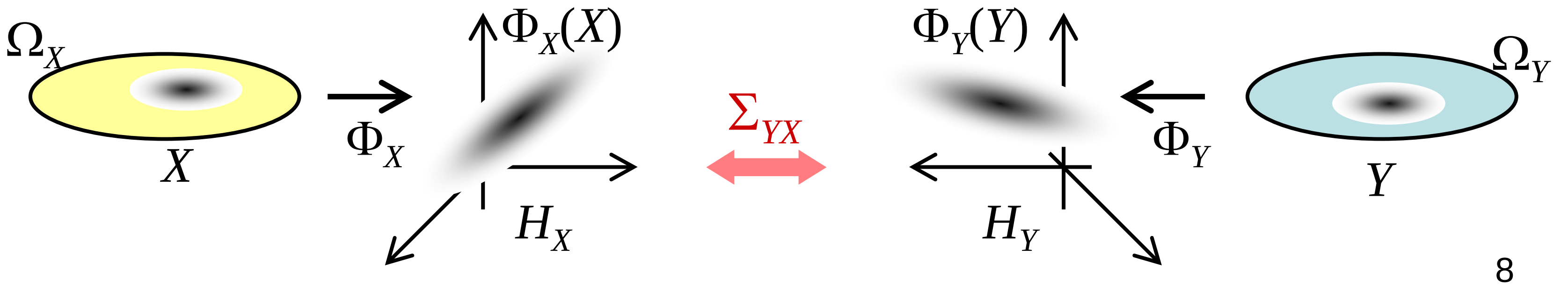
X , Y : random variables on Ω_X and Ω_Y , resp.

Prepare RKHS (H_X, k_X) and (H_Y , k_Y) defined on Ω_X and Ω_Y, resp.

Define random variables on the RKHS H_X and H_Y by

$$\Phi_X(X) = k_X(\cdot, X) \qquad \Phi_Y(Y) = k_Y(\cdot, Y)$$

Define the big (possibly infinite dimensional) covariance matrix Σ_{YX} on the RKHS.



Cross-covariance operator

– Definition

$$\Sigma_{YX} = E[\Phi_Y(Y)\langle\Phi_X(X),\cdot\rangle] - E[\Phi_Y(Y)]E[\langle\Phi_X(X),\cdot\rangle]$$

Σ_{YX} is an operator from H_X to H_Y such that

$$\langle g, \Sigma_{YX} f\rangle = E[g(Y)f(X)] - E[g(Y)]E[f(X)] \quad (= \mathrm{Cov}[f(X), g(Y)])$$

for all $f \in H_X, g \in H_Y$

– *c.f.* Euclidean case

$V_{YX} = \mathrm{E}[YX^T] - \mathrm{E}[Y]\mathrm{E}[X]^T$: covariance matrix

$$(b, V_{YX}a) = Cov[(b,Y),(a,X)]$$

Higher-order moments

Suppose X and Y are **R**-valued, and $k(x,u)$ admits the expansion

$$k(x,u) = 1 + c_1 xu + c_2 x^2 u^2 + c_3 x^3 u^3 + \cdots \qquad \text{e.g.) } k(x,u) = \exp(xu)$$

With respect to the basis $1, u, u^2, u^3, \ldots$, the random variables on RKHS are expressed by

$$\Phi(X) = k(X,u) \sim (1, c_1 X, c_2 X^2, c_3 X^3, \ldots)^T$$

$$\Phi(Y) = k(Y,u) \sim (1, c_1 Y, c_2 Y^2, c_3 Y^3, \ldots)^T$$

$$\Sigma_{YX} \sim \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & c_1^2 Cov[Y,X] & c_1 c_2 Cov[Y,X^2] & c_1 c_3 Cov[Y^3,X] & \cdots \\ 0 & c_2 c_1 Cov[Y^2,X] & c_2^2 Cov[Y^2,X^2] & c_2 c_3 Cov[Y^2,X^3] & \cdots \\ 0 & c_3 c_1 Cov[Y^3,X] & c_3 c_2 Cov[Y^3,X^2] & c_3^2 Cov[Y^3,X^3] & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

The operator Σ_{YX} contains the information on all the higher-order correlation.

Characterization of Independence

- Independence and Cross-covariance operator

If the RKHS's are "rich enough" to express all the moments,

X and Y are independent $\Leftrightarrow$ $\Sigma_{XY} = O$

$\Updownarrow$

$\mathrm{Cov}[f(X), g(Y)] = 0$

or

$E[g(Y) f(X)] = E[g(Y)] E[f(X)]$

for all $f \in H_X, g \in H_Y$

($\Rightarrow$ is always true.

$\Leftarrow$ requires some assumption

Gaussian RBF kernels gives the above equivalence.

$$k(x, y) = \exp\left(-\|x - y\|^2 / \sigma^2 \right)$$

– *c.f.* for Gaussian variables

X and Y are independent $\Leftrightarrow$ $V_{XY} = O$ i.e. uncorrelated

Kernel Dependence Measure

– Hilbert-Schmidt Independence Criteria (HSIC)

$$HSIC(X,Y) = \left\| \Sigma_{YX} \right\|_{HS}^2$$

$$HSIC = 0 \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y$$

– Empirical estimator

$$HSIC_{emp}(X,Y) = \left\| \hat{\Sigma}_{YX}^{(N)} \right\|_{HS}^2 = \mathrm{Tr}\left[G_X G_Y \right]$$

$$G_X = \left(I_N - \tfrac{1}{N}\mathbf{1}_N\mathbf{1}_N^T \right) K_X \left(I_N - \tfrac{1}{N}\mathbf{1}_N\mathbf{1}_N^T \right)$$: centered Gram matrix

$$K_X = \left(k(X_i, X_j) \right)_{i,j=1}^N$$

– Hilbert-Schmidt norm of an operator

$A: H_1 \to H_2$ operator on a Hilbert space

$\{\varphi_i\}, \{\psi_j\}$: complete orthonormal system of H_1 and H_2 (resp.).

$$\|A\|_{HS}^2 = \sum_j \sum_i \left\langle \psi_j, A\varphi_i \right\rangle^2$$

c.f. Frobenius norm of a matrix

Independence Test

- Permutation test for independence
  - Null hypothesis

    $$H_0: \quad X \perp\!\!\!\perp Y$$

  - Permutation test: simulation of the distribution of test statistics under H_0.
    - Make many samples consistent with the null hypothesis by random permutations of the original sample.

      $$\begin{matrix} X_1 & X_2 & X_3 & X_4 & X_5 & X_6 & X_7 \\ Y_1 & Y_2 & Y_3 & Y_4 & Y_5 & Y_6 & Y_7 \end{matrix} \Rightarrow \begin{matrix} X_1 & X_2 & X_3 & X_4 & X_5 & X_6 & X_7 \\ Y_5 & Y_1 & Y_7 & Y_4 & Y_2 & Y_6 & Y_3 \end{matrix} \quad \text{independent}$$

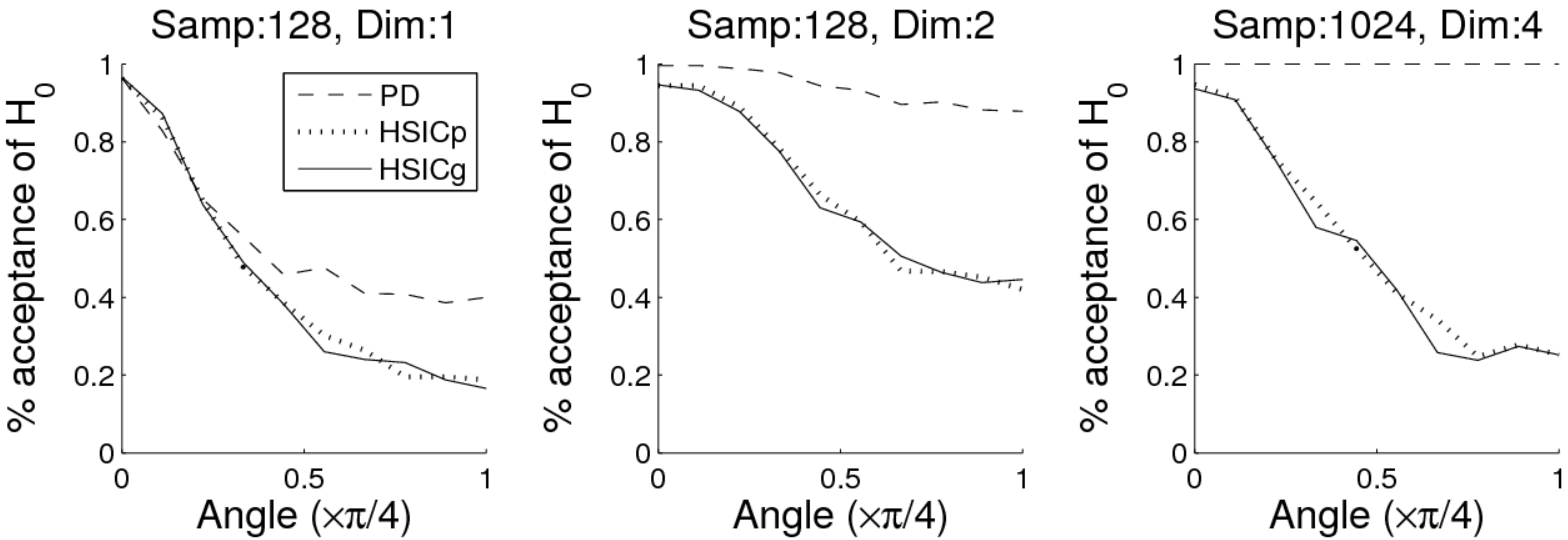
    - Compute the values of test statistics (dependence measure) for the samples.
    - Compute the critical region for a prescribed significance level.

Experiments of independence test

- Synthesized data: two d-dimensional samples

$$(X_1^{(1)},\dots,X_d^{(1)}),\dots,(X_1^{(N)},\dots,X_d^{(N)}) \qquad (Y_1^{(1)},\dots,Y_d^{(1)}),\dots,(Y_1^{(N)},\dots,Y_d^{(N)})$$

  - H_0: X and Y are independent
  - Significance level = 5%



strength of dependence

Power Divergence (Ku&Fine05, Read&Cressie)

- Make partition $\{A_j\}_{j \in J}$: Each dimension is divided into q parts so that each bin contains almost the same number of data.

- Power-divergence

$$T_N = 2I^{\lambda}(X,m) = N \frac{2}{\lambda(\lambda+2)} \sum_{j \in J} \hat{p}_j \left\{ \left(\hat{p}_j \Big/ \prod_{k=1}^{N} \hat{p}_{j_k}^{(k)} \right)^{\lambda} - 1 \right\}$$

I^0 = MI

I^2 = Mean Square Conting.

$\hat{p}_j$: frequency in A_j

$\hat{p}_r^{(k)}$: marginal freq. in r-th interval

- Null distribution under independence

$$T_N \quad \Rightarrow \quad \chi^2_{q^N - qN + N - 1} \qquad (N \to \infty)$$

- Estimation for high-dimensional data is difficult.

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Conditional Covariance on RKHS

- Conditional Cross-covariance operator

  X, Y, Z : random variables on Ω_X, Ω_Y, Ω_Z (resp.).

  (H_X, k_X), (H_Y, k_Y), (H_Z, k_Z) : RKHS defined on Ω_X, Ω_Y, Ω_Z (resp.).

  – Conditional cross-covariance operator $H_X \rightarrow H_Y$

$$\Sigma_{YX|Z} \equiv \Sigma_{YX} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZX}$$

  – c.f. For Gaussian variables

    Conditional covariance of Y given X is equal to

$$V_{YX|Z} \equiv V_{YX} - V_{YZ}V_{ZZ}^{-1}V_{ZX}$$

(conditional covariance matrix)

Conditional independence with kernels

<u>Theorem</u>

Define the augmented variable $\tilde{X} = (X, Z)$ and define a kernel on $\Omega_X \times \Omega_Z$ by

$$k_{\tilde{X}} = k_X k_Z$$

Under some richness assumption, which is satisfied by Gaussian RBF kernels,

$$\Sigma_{Y\tilde{X}|Z} = O \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y \mid Z$$

$$\Sigma_{Y\tilde{X}|Z} = O \quad \Leftrightarrow \quad \Sigma_{\tilde{Y}X|Z} = O \quad \Leftrightarrow \quad \Sigma_{\tilde{Y}\tilde{X}|Z} = O \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y \mid Z$$

Kernel conditional dependence measure

– Hilbert-Schmidt conditional independent criterion

$$HSCIC(X,Y \mid Z) = \left\| \Sigma_{\tilde{Y}\tilde{X}|Z} \right\|_{HS}^{2}$$

– Empirical measure

$$HSCIC_{emp}(X,Y \mid Z) = \left\| \hat{\Sigma}^{(N)}_{\tilde{Y}\tilde{X}} - \hat{\Sigma}^{(N)}_{\tilde{Y}Z} \left(\hat{\Sigma}^{(N)}_{ZZ} + \varepsilon_N I \right)^{-1} \hat{\Sigma}^{(N)}_{Z\tilde{X}} \right\|_{HS}^{2}$$

$$= \mathrm{Tr}\Big[G_X G_Y - 2 G_X (G_Z + N\varepsilon_N I_N)^{-1} G_Z G_Y + G_Z (G_Z + N\varepsilon_N I_N)^{-1} G_X (G_Z + N\varepsilon_N I_N)^{-1} G_Z G_Y \Big]$$

Consistency

If the regularization coefficient satisfies

$$\varepsilon_N \to 0 \qquad N^{1/3}\varepsilon_N \to \infty,$$

then

$$HSCIC_{emp} \to HSCIC \qquad (N \to \infty)$$

Conditional Independence Test

- Permutation test with the kernel measure

$$T_N = \left\| \hat{\Sigma}_{YX|Z}^{(N)} \right\|_{HS}^2$$

– If Z takes values in a finite set $\{1, \ldots, L\}$,

set $A_\ell = \{i \mid Z_i = \ell\}$ $(\ell = 1, \ldots, L)$,

otherwise, partition the values of Z into L subsets $C_1, \ldots, C_L$, and set

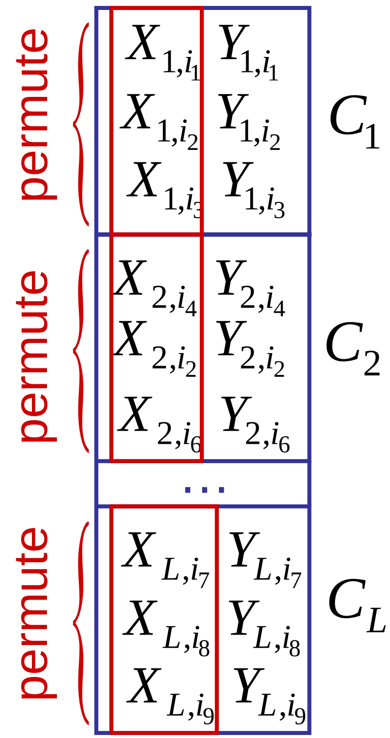
$$A_\ell = \{i \mid Z_i \in C_\ell\} \quad (\ell = 1, \ldots, L).$$

– Repeat the following process B times: ($b = 1, \ldots, B$)

1. Generate pseudo cond. independent data $D^{(b)}$ by permuting X data within each A_ℓ.
2. Compute $T_N^{(b)}$ for the data $D^{(b)}$.

⟶ Approximate null distribution under cond. indep. assumption

– Set the threshold by the $(1\text{-}\alpha)$-percentile of the empirical distributions of $T_N^{(b)}$.



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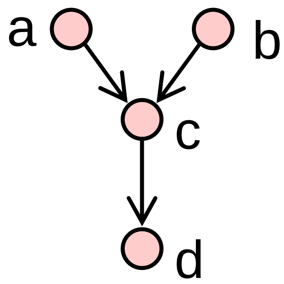
Causal Inference from Non-Experimental Data

- Constraint-based method
  - Determine the (cond.) independence of the underlying probability.
  - Relatively efficient for hidden variables.
- Score-based method
  - Structure learning of Bayesian network
  - Able to use informative prior.
  - Optimization in huge search space.
  - Many methods assume discrete variables (discretization) or parametric model.
- Kernel-based Causal Learning
  - Constraint-based method. A variant of Inductive Causation (IC)

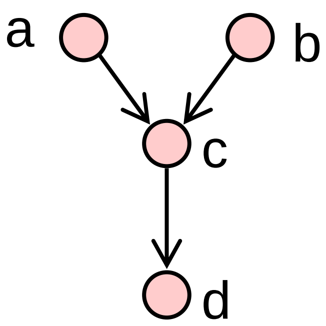
Fundamental Assumptions

- Causal Markov Condition
  - Causal relation is expressed by a DAG, and the probability generating data is consistent with the graph.

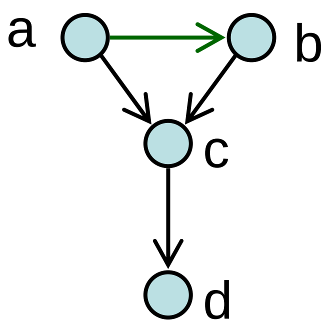


$$p(X) = p(X_a)p(X_b)p(X_c \mid X_a, X_b)p(X_d \mid X_c)$$

- Causal Faithfulness Condition
  - The inferred DAG (causal structure) must express all the independence relations.



true



unfaithful

This includes the true probability as a special case, but the structure does not express $a \perp\!\!\!\perp b$

Inductive Causation

- IC algorithm (Verma&Pearl 90)

  Input – V: set of variables, D: dataset of the variables.

  Output – DAG (specifies an equivalence class, directed partially)

1. For each $(a,b) \in V \times V \ (a \neq b)$, search for $S_{ab} \subset V \setminus \{a,b\}$ such that
   $$X_a \perp\!\!\!\perp X_b \mid S_{ab}$$
   Construct an undirected graph (skeleton) by making an edge between a and b if and only if no set S_{ab} can be found.
2. For each nonadjacent pair (a,b) with $a - c - b$, direct the edges by $a \rightarrow c \leftarrow b$ if $c \notin S_{ab}$
3. Orient as many of undirected edges as possible on condition that neither new v-structures nor directed cycles are created.

Kernel-based Causal Leaning

- Limitations of the previous implementations of IC
  - Linear / discrete assumptions in Step 1.

    e.g. PC-algorithm (Spirtes & Glymour 91) uses partial correlation and χ^2 test.

    Difficulty in testing conditional independence for continuous variables.

    → kernel method!

  - Errors of the skeleton in Step 1 cannot be recovered in the later steps.

    → voting method for direction

Note: The error in Step 1 is inevitable by statistical tests.

■ KCL algorithm (Sun et al. ICML07, Sun et al. 2007)

– Dependence measure: $\hat{\mathbb{H}}_{YX}^{(N)} = HSIC = \left\| \hat{\Sigma}_{YX}^{(N)} \right\|_{HS}^{2}$

– Conditional dependence measure: $\hat{\mathbb{H}}_{YX|Z}^{(N)} \equiv \dfrac{\left\| \hat{\Sigma}_{\tilde{Y}\tilde{X}|Z}^{(N)} \right\|_{HS}^{2}}{\left\| C_{ZZ} \right\|_{HS}^{2}}$

where the operator $C_{ZZ} : H_Z \to H_Z$ is defined by

$$\langle f, C_{ZZ} g \rangle = E\left[f(Z) g(Z) \right]$$

Motivation: make $\left\| \hat{\Sigma}_{YX}^{(N)} \right\|_{HS}^{2}$ and $\left\| \hat{\Sigma}_{\tilde{Y}\tilde{X}|Z}^{(N)} \right\|_{HS}^{2}$ comparable

<u>Theorem</u>

If $(X, Y) \perp\!\!\!\perp Z$, $\left\| \hat{\Sigma}_{\tilde{Y}\tilde{X}|Z}^{(N)} \right\|_{HS}^{2} = \left\| C_{ZZ} \right\|_{HS}^{2} \left\| \hat{\Sigma}_{YX}^{(N)} \right\|_{HS}^{2}$

Outline of KCL algorithm: IC algorithm is modified as follows.

KCL-1: Skeleton by statistical tests with the kernel measure $\hat{\mathbb{H}}^{(N)}_{YX|Z}$

(1) Permutation tests of conditional independence $X \perp\!\!\!\perp Y \mid S_{XY}$

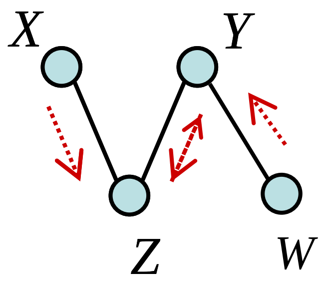
(2) Connect X and Y if no such S_{XY} exists.

The candidates of S_{XY} should be restricted → explained later.

KCL-2: Voting for unshielded triplets

For each triplet $X - Z - Y$ (X and Y not adjacent), compute

$$M_{XY|Z} \equiv \frac{\hat{\mathbb{H}}^{(N)}_{YX|Z}}{\hat{\mathbb{H}}^{(N)}_{YX}}, \quad M_{YZ|X}, \quad M_{ZX|Y}$$



Give a vote to the direction $X \rightarrow Z$ and $Y \rightarrow Z$ if

$$M_{XY|Z} > \max\{M_{YZ|X}, M_{ZX|Y}\}$$

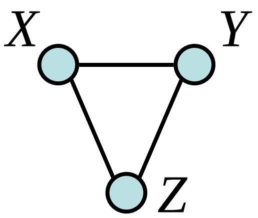
Make an arrow to each edge if a vote is given ("↔" is allowed).

KCL-3: Same as IC-3

KCL-4: Voting for shielded triplets

For each triplet $X - Z - Y$ (X and Y adjacent), compute

$$M_{XY|Z},\ M_{YZ|X},\ M_{ZX|Y}$$



Give a vote to the direction $X \rightarrow Z$ and $Y \rightarrow Z$ if

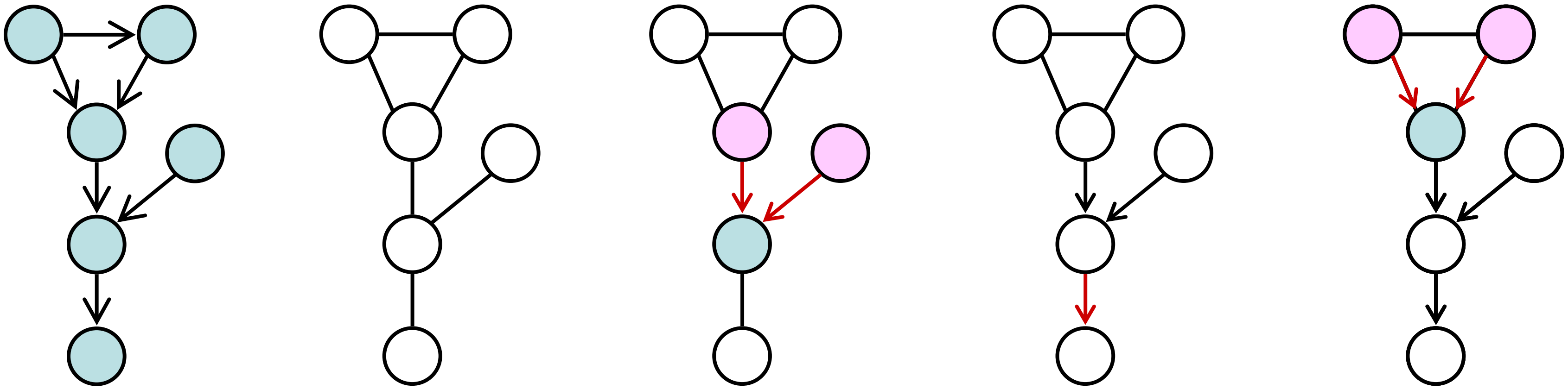
$$M_{XY|Z} > \max\{M_{YZ|X}, M_{ZX|Y}\}$$

Make an arrow to each edge if a vote is given ("$\leftrightarrow$" is allowed).

– The resulting graph is mixed: undirected $—$, directed $\longrightarrow$, or bi-directed $\longleftrightarrow$.

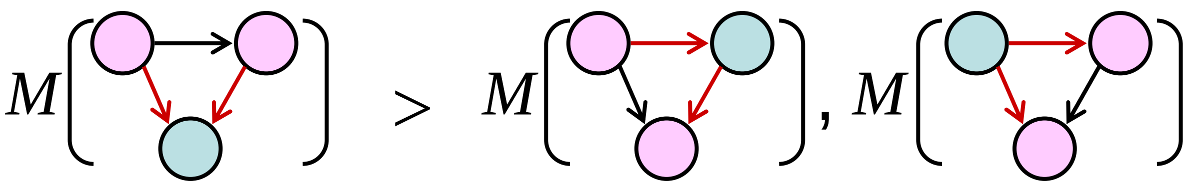
– Motivation of KCL-2 and 4:
  - By inevitable errors in statistical tests, it is preferred that the orientation process be separated from Step 1.
  - Step 4 looks for more directed edges.
    It relies on the heuristic assumption that conditioning common effect strengthens the dependence between the causes.

■ Illustration of KCL



true KCL-1 KCL-2 KCL-3 KCL-4

Heuristic assumption:



Conditioning common effect strengthens the dependence between the causes.

Details of Step 1

Auxiliary partially directed graphs are used for restricting conditioning variables S_{XY} .

- Initialize G by a complete undirected graph.
- 1(a): Unconditional independence tests

  For all pairs (X,Y), apply permutation tests for $X \perp\!\!\!\perp Y$ with $\hat{\mathbb{H}}_{YX}^{(N)}$

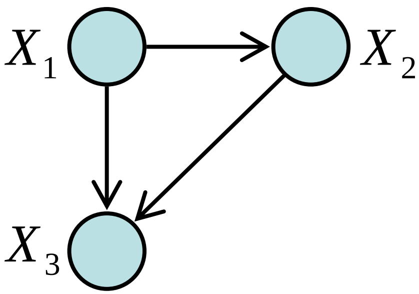
  Remove $X - Y$ if the independence is accepted.
- 1(b): Auxiliary graph

  Orient G by majority votes on all triplets $X - Y - Z$.
- 1(c): Cond. indep. tests $X \perp\!\!\!\perp Y \mid S_{XY}$ with $\hat{\mathbb{H}}_{YX|Z}^{(N)}$ in the auxiliary graph.

  S_{XY}: only variables in the directed (incl. undirected) path between X and Y.
- 1(d): Change the directed edges into undirected ones to make a skeleton G.
- 1(e): Repeat (a)-(d) until nothing changes.

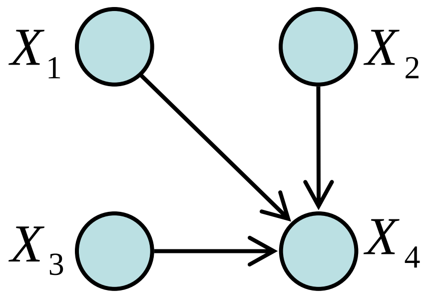
Experiments with Simple Networks

(A)



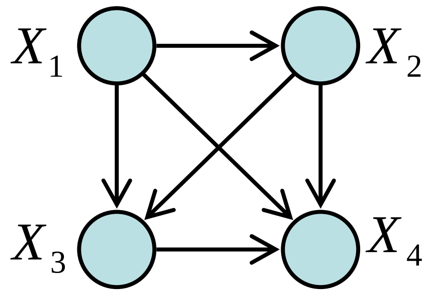
$$P(X_1 = 1) = 0.6$$
$$P(X_2 = X_1 \mid X_1) = 0.8$$
$$X_3 = \text{NoisyOR}(X_1, X_2)$$

(B)



$$P(X_1 = 1) = 0.6$$
$$P(X_2 = 1) = 0.5$$
$$P(X_3 = 1) = 0.4$$
$$X_4 = \text{NoisyOR}(X_1, X_2, X_3)$$

(C)



$$P(X_1 = 1) = 0.6$$
$$P(X_2 = X_1 \mid X_1) = 0.8$$
$$X_3 = \text{NoisyOR}(X_1, X_2)$$
$$X_4 = \text{NoisyOR}(X_1, X_2, X_3)$$

$$X_{n+1} = \text{NoisyOR}(X_1, \ldots, X_n)$$
$$\Leftrightarrow \quad P(X_{n+1} = 1 \mid X_1, \ldots, X_n) = 0.8 \times \left(1 - 0.2^{X_1 + \cdots + X_n}\right) + 0.2$$

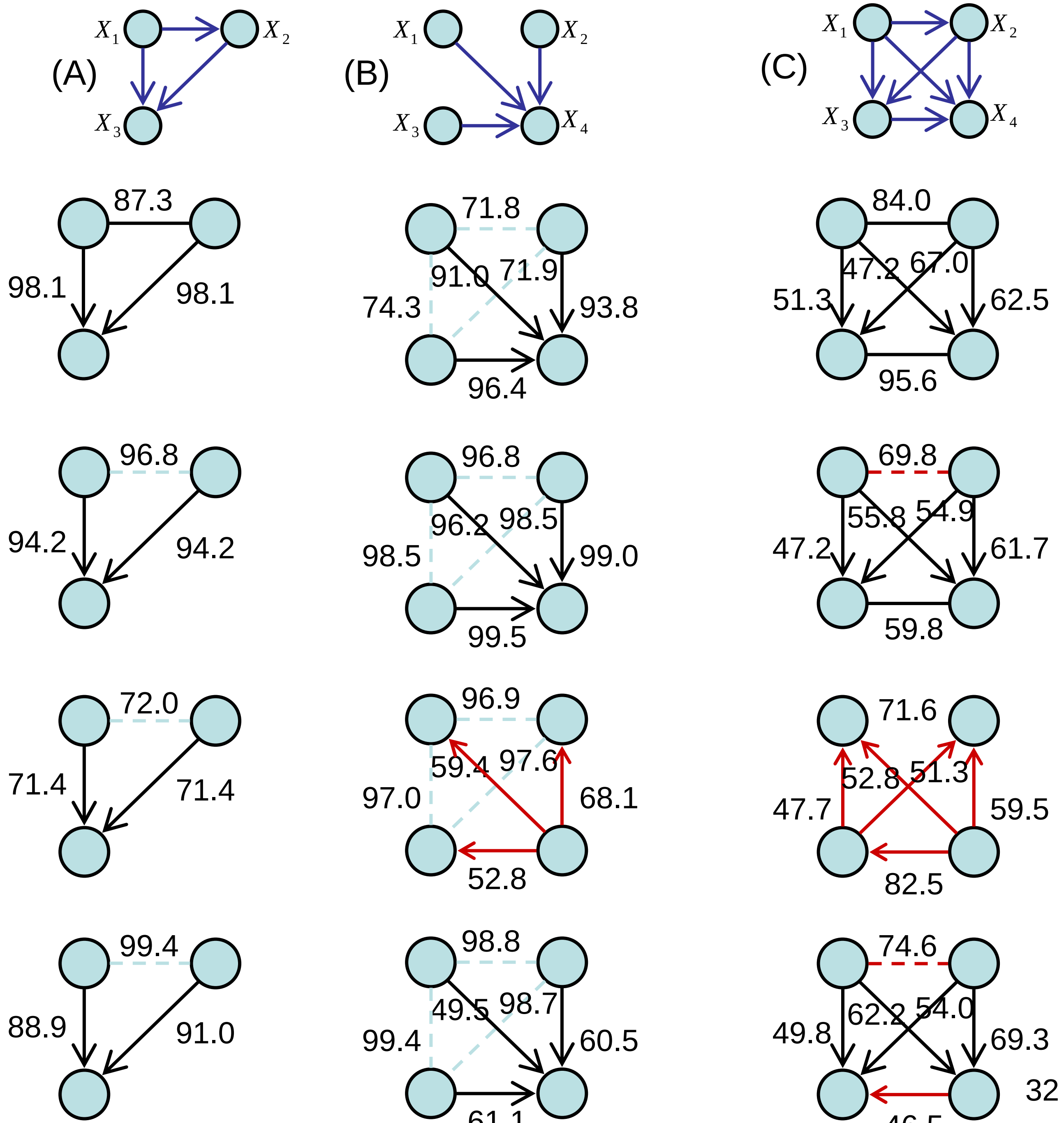
- Results (200 data, 1000 runs)

KCL

PC

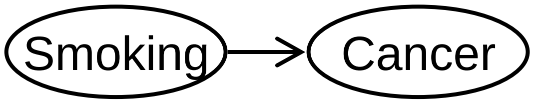
BN-PC (MI is used) [Cheng et al. '02]

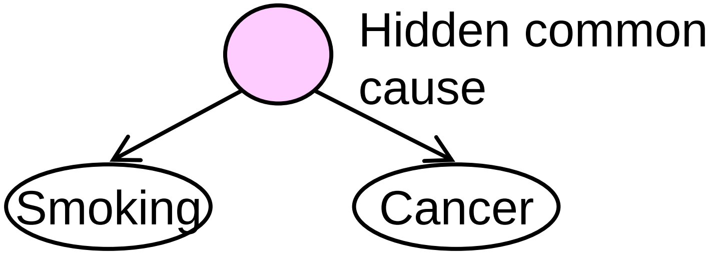
BDe (Score-based) [Heckerman et al. '97]



Hidden Common Cause

– One of the difficulties in causal leaning is possible existence of common hidden causes.





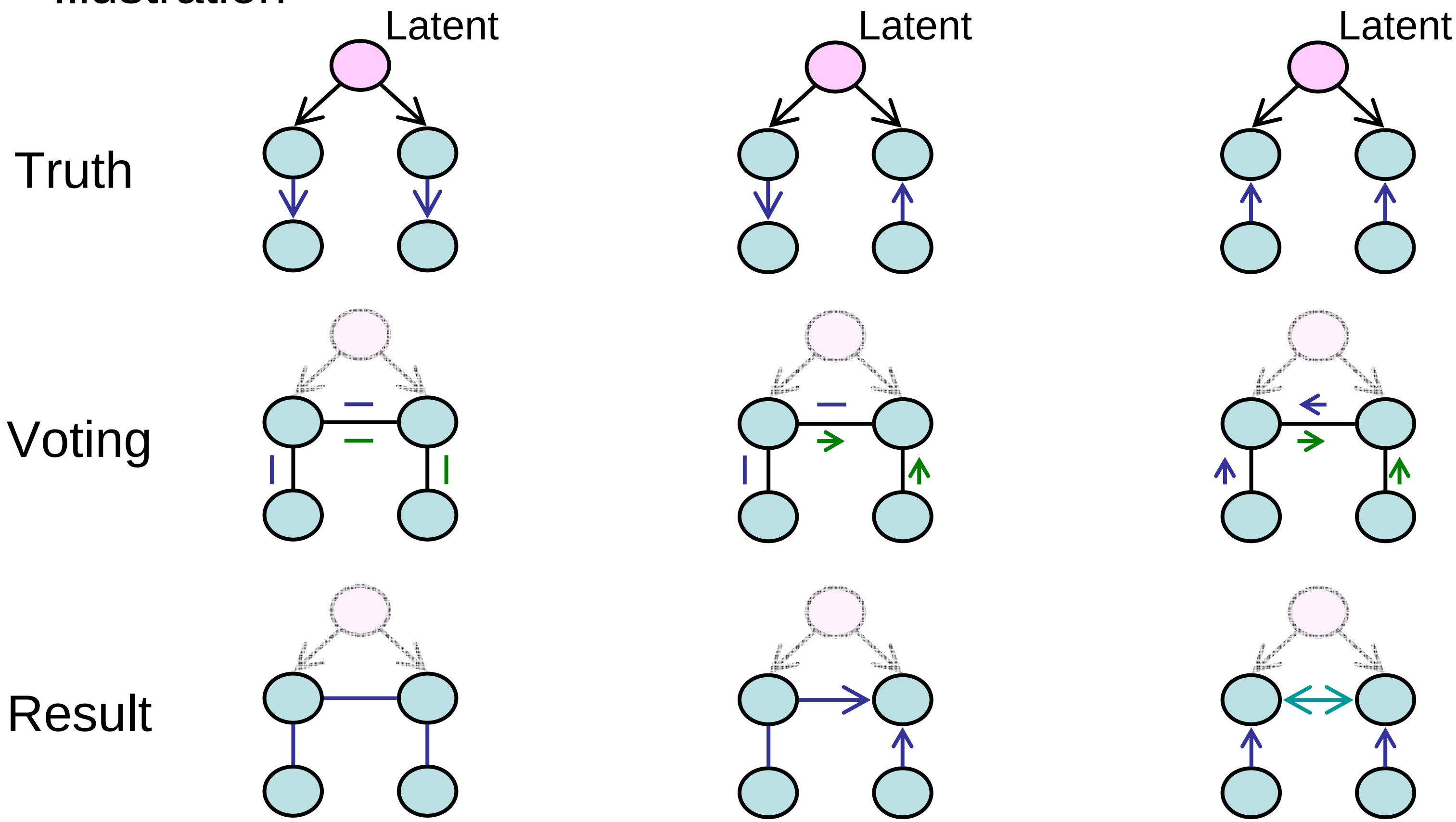
– Some methods can handle hidden variables.

FCI (Fast Causal Inference, Spirtes et al. 93) extends PC to allow hidden variables.

KCL for hidden common causes

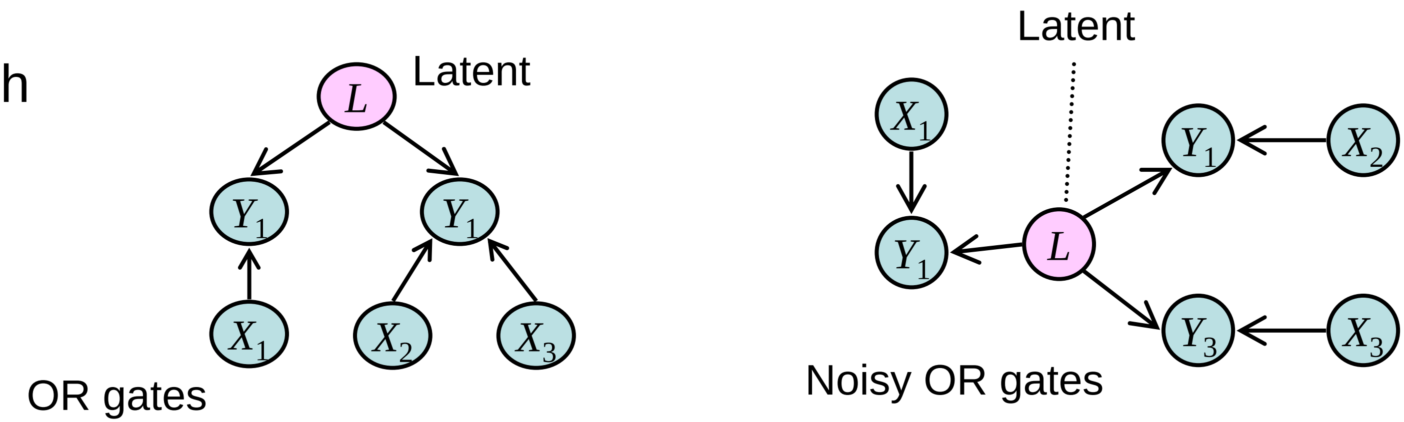
– A bi-directional arrow (↔) given by KCL may suggest existence of a hidden common cause.
Empirically verified in some situations, but no theoretical justification.

– Illustration

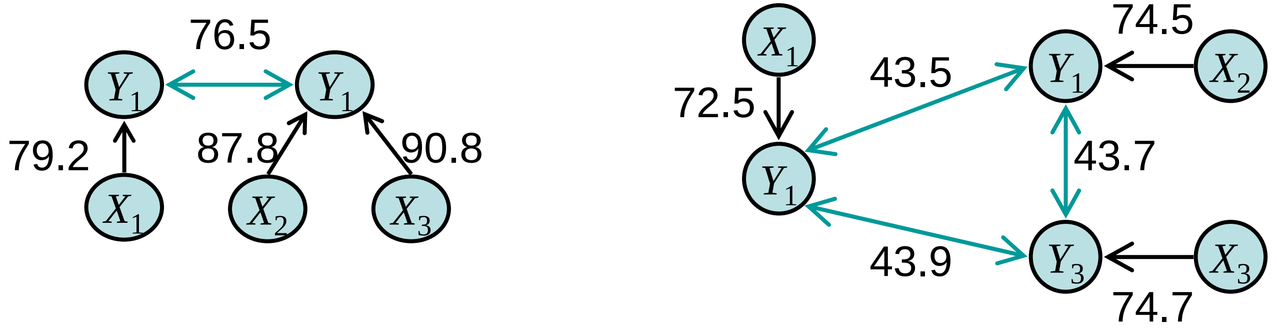


– Experiments (200 data, 1000 runs)

Truth



Result of KCL

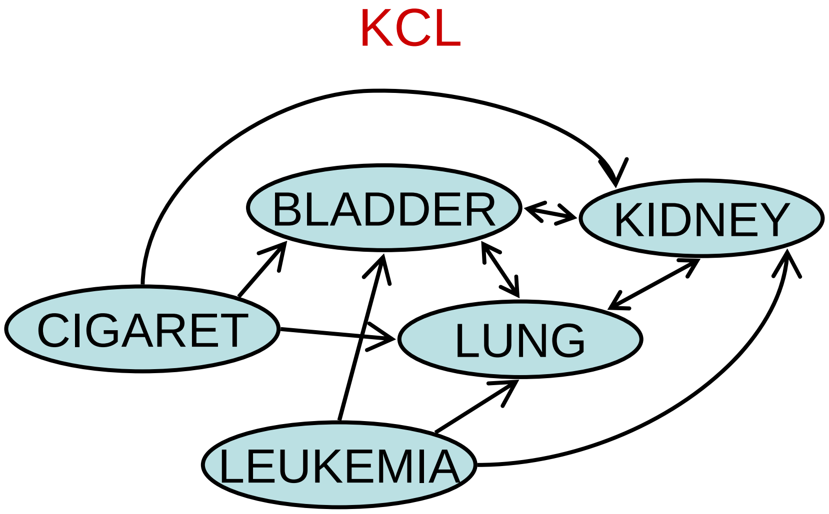


Experiments with Real Data

- Smoking and Cancer
  - Data: 5 continuous variables, $N = 44$

    CIGARET: Cigarettes sales in 43 states in US and District of Columbia

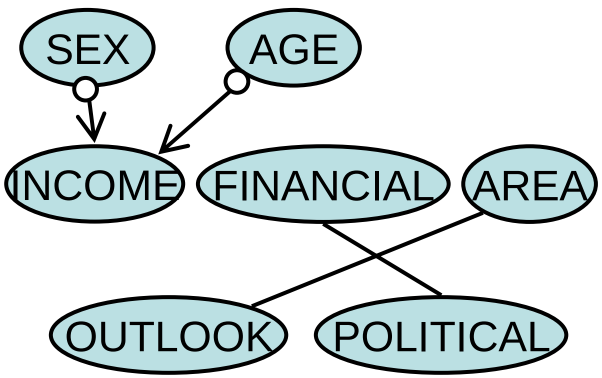
    BLADDER, LUNG, KIDNEY, LEUKEMIA: death rates from various cancers
  - Results



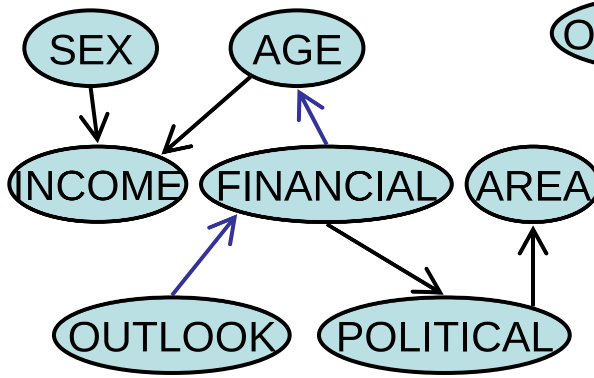
■ Montana Economic Outlook Poll (1992)

– Data: 7 discrete variables, $N = 209$

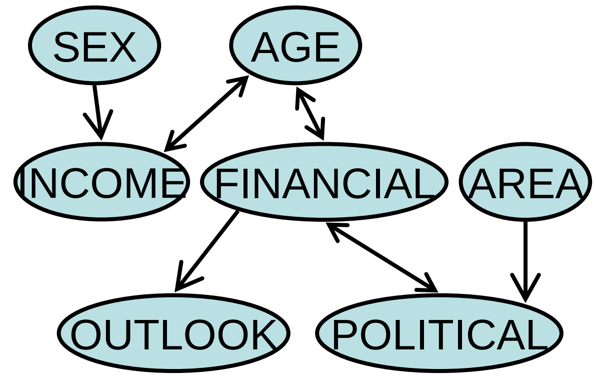
AGE (3), SEX (2), INCOME (3), POLITICAL (3), AREA (3), FINANCIAL status (3, better/same/worse than a year ago), OUTLOOK (2)



FCI



BN-PC



KCL

Conclusion

- Kernel measures of (conditional) dependence
  - Covariance and conditional covariance considered on RKHS provide criterion of independence and conditional independence, resp.
  - Kernel measures are proposed for (conditional) dependence.
- Causal inference from non-experimental data
  - Kernel-based Causal Learning (KCL) algorithm
    - Constraint-based method: A variant of Inductive Causation
      - Conditional independence tests with kernel measures
      - Voting method for orienting edges
    - KCL can handle discrete and continuous domains in a unified way.
    - More theoretical justification is required.

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