Dynamical Causality

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Aristotle (BC384 \sim 322) developed "four causes" to explain change: material cause, formal cause, efficient cause (or moving cause), and final cause (or purpose cause)

Causal Model

• Statistical model (non-time-series data)

(Statistical learning, neural network, machine learning)

Criterion: correlation

• Causal model (non-time-series data)

(Neyman-Rubin structural causal model, Judea Pearl's causal calculus)

Criterion: independence, do-calculus, OOD

• Dynamical model-1 (time-series data, statistical model)

(Granger causality, transfer entropy)

Criterion: prediction $x(t) \rightarrow y(t+1)$

预测

• Dynamical model-2 (time-series data, dynamical model)

(embedding causality, embedding entropy)

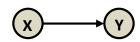
Criterion: inverse mapping $Y(t) \rightarrow X(t-1)$

逆重构/逆映射

$$x_{t+1} = \hat{f}(x_t)$$

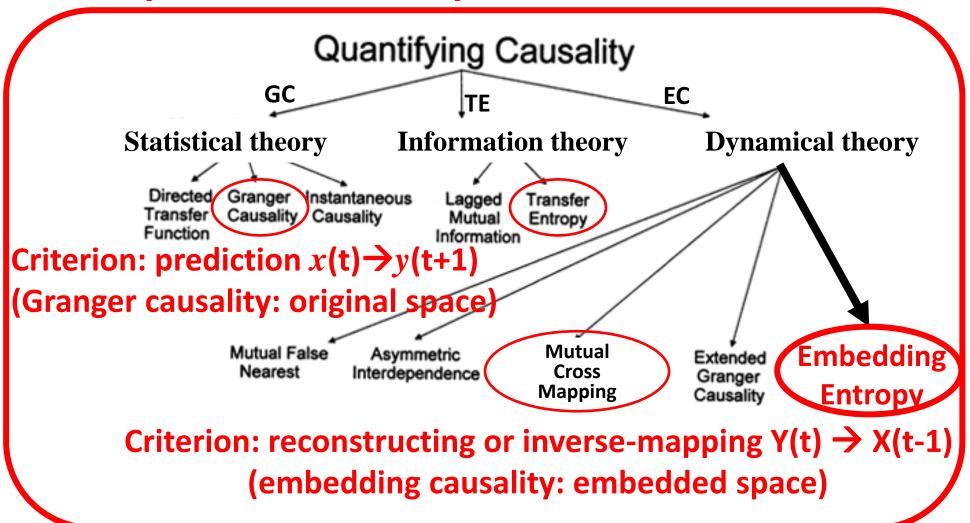
$$y_{t+1} = g(x_t, y_t)$$





Existing models for time-course data

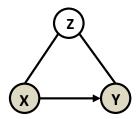
Dynamical Causality: uniform framework



Causality Definition

 Cause: X causes Y if and only if changing X leads to a change in Y while keeping everything else constant.

Effect: causal effect is the magnitude by which Y is changed by one unit change in X.



Dynamical Causality (DC)

$$x_t = f(x_{t-1}, ..., x_{t-p}, ...)$$

 $x_t = (x_{1,t}, x_{2,t}, ..., x_{n,t}); f = (f_1, f_2, ..., f_n)$

• H_1 of DC: $x_i \rightarrow x_j$, dynamics of x_j depends on x_i , i.e.

 $\exists k \in \{1, 2, ..., p\}$, such that

$$\frac{\partial f_j}{\partial x_{i,t-k}} \neq 0 \qquad \text{for almost any sampled } t$$

causal $x_{i} \xrightarrow{x_{i}} x_{j}$ $x_{j,t} = f(x_{t-1}, x_{i,t-1})$

• H_0 of DC: dynamics of x_i does not depend on x_j , i.e.

 $\forall k \in \{1, 2, ..., p\}$, such that

$$\frac{\partial f_j}{\partial x_{i,t-k}} = 0 \qquad \text{for almost any sampled } t$$

non-causal

$$x_i \longrightarrow x_j$$

$$x_{j,t} = f(x_{t-1} \setminus x_{i,t-1})$$

Direct DC: explicit dependence; Indirect DC: implicit dependence

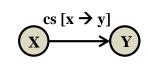
Causal Strength

- Ho: model error with no effect from x to y
- H1: model error with an effect from x to y

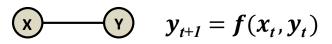
Causal strength: $cs[x\rightarrow y] = D[H_1 | H_0]$

- cs: causality strength
- *D*: distance function

$$x_{t+1} = f(x_t)$$
$$y_{t+1} = g(x_t, y_t)$$



1. Regression Theory (dynamical model-1: prediction)



Granger Causality (GC)

如果使用X的信息,Y的预测误差减少:X → Y

Using X reduced the prediction error of Y: $X \rightarrow Y$

If
$$\sigma(y_{t+1} | \Lambda_t, x_t) < \sigma(y_{t+1} | \Lambda_t)$$

 $\Lambda_t = \{ \text{past terms of } y_t \text{, excluding } x_t \} ; x_t = \{ \text{past terms of } x_t \}$

Then $X \rightarrow Y$

x(t) predicts y(t+1)



Nobel Prize

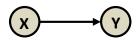
Granger Causal Effect

(original state space: x, y)

• H0:
$$y_{t+1} = \sum_{k=0}^{p} a_k y_{t-k} + \varepsilon_{2t}$$
• H1:
$$y_{t+1} = \sum_{k=0}^{p} a_k y_{t-k} + \sum_{k=0}^{p} b_k x_{t-k} + \varepsilon_{1t}$$

• Causal strength:
$$CS_{x\to y} = In\epsilon_2^2 - In\epsilon_1^2$$

 $cs[x\to y] = D[H1 | H0]$



Granger Causality (GC)

If **X** past values provide statistically significant information about **Y** future, **X** is said to Granger-cause **Y**.

Questions?

It is applicable for a strong associated network

- Linear causality
- Non-separability of X and Y (false negative or H_0 underestimation)
- cutoff error for p
- Weak/moderate coupling
- indirect causality

Criterion: prediction

2. Information Theory (dynamical model-1: prediction)

Transfer Entropy (TE)

 $(\mathbf{x}) \longrightarrow (\mathbf{y})$ $\mathbf{y}_{t+1} = f(\mathbf{x}_t, \mathbf{y}_t)$

(original state space: *x*,*y*)

如果使用X的信息,Y的不确定性减少: X→Y Using X reduced the uncertainty of Y: X→Y

Granger causality: linear

$$cs[x\rightarrow y] = D[H1 \mid H0]$$

Transfer entropy: nonlinear

$$T_{X \to Y} = H(Y^t | Y^{t-1}) - H(Y^t | Y^{t-1}, X^{t-1}),$$

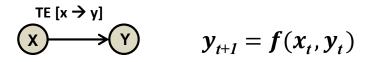
= MI(Y^t, X^{t-1}|Y^{t-1}) > 0 (causal)

Granger causality is the linear version of transfer entropy.

- Question? 1. Separability (false negative or H0 underestimation),
 - 2. Strong association problem,
 - 3. Cutoff error of p

$$x(t)$$
 predicts $y(t+1)$

TE Causal Effect



• H0:
$$H(\varepsilon_{2t}) = H(y_t | y_{t-1}, ..., y_{t-p})$$

• H1:
$$H(\varepsilon_{1t}) = H(y_t | y_{t-1}, ..., y_{t-p}; x_{t-1}, ..., x_{t-p})$$

• Causal strength: $TE_{x \to y} = |H(\epsilon_1)-H(\epsilon_2)|$

separability of *X* and *Y* (false negative or H0 underestimation), strong association problems! cutoff error problem of *p*!

Transfer entropy measures the decrease of uncertainty by considering y



Embedding Causality

(Delay embedding space: *X,Y*)

Y的邻居也是对应X空間的邻居: $X \rightarrow Y$

Original state space → Delay embedding space

Advantages: no requirement on separability, nonlinear, no cut-off

Criterion: Inverse-mapping (逆映射) Y(t) inverse-maps to X(t-1)

Delay Embedding

From original space x to embedded space X

Causal inference at embedded space, not at original space!

Original space in
$$R: x_1, x_2, ..., x_t, ...$$

Embedded space in $R^L: X_1, X_2, ..., X_t$, ...

 X_t represents the state of whole system, including information of other variable y_t

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_L \end{bmatrix}, \begin{bmatrix} x_2 \\ x_3 \\ \vdots \\ x_{L+1} \end{bmatrix}, \dots, \begin{bmatrix} x_t \\ x_{t+1} \\ \vdots \\ x_{t+L-1} \end{bmatrix}, \dots$$



Randomly distributed embedding making short-term high-dimensional data predictable

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One variable can possibly describe another variable!

(Y may include the information of X)

Cross Mapping

Application to many areas, i.e. economics, ecological systems, bio-systems, AI

Ho is not appropriate in GC and TE

 One variable y can topologically construct whole dynamics, and thus also includes the information of x, from the embedding theorem.

H0 : assume no effect from x to y

$$y_{t+1} = \sum_{k=0}^{p} a_k y_{t-k} + \varepsilon_{2t}$$

incorrect due to its past time points!



Non-separability problem for GC and TE

- The information of one variable could be generically entangled with the whole system.
- H_1 data should not be used to construct H_0 model.

GC and TE

 H_1 hypothesis with H_1 data

$$x_{t+1} = \sum_{k=0}^{p} c_k x_{t-k} + \varepsilon_{2t}$$

$$y_{t+1} = \sum_{k=0}^{p} a_k y_{t-k} + \sum_{k=0}^{p} b_k x_{t-k} + \varepsilon_{1t}$$



H₀ hypothesis but with H₁ data

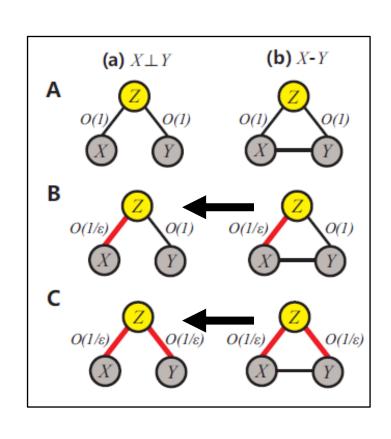
$$x_{t+1} = \sum_{k=0}^{p} c_k x_{t-k} + \varepsilon_{2t}$$
$$y_{t+1} = \sum_{k=0}^{p} a_k y_{t-k} + \varepsilon_{1t}$$

Summary of non-separability problem:

- Causal variables could be both explicit and implicit in the dynamics of the effect variable, and thus only removing the explicit causal variable to construct a H_0 model is improper and actually influence the dynamical behaviors of the whole system.
- The data sampled from H_1 should not be used to approximate the H_0 model because their dynamics could be different.

False negative problem!

Strong association problem for TE



Strong associated network



$$p(x, \mathbf{y}) = \frac{1}{Z_{\epsilon}} \exp\left(-\frac{1}{\epsilon}\phi(x, \mathbf{y}) - \psi(x, \mathbf{y})\right)$$

$$CMI(X, Y|Z) = CMI_0 + \epsilon CMI_1 + \epsilon^2 CMI_2 + O(\epsilon^3)$$

A: $CMI(X, Y|Z) \sim O(1)$

TE

B: $CMI(X, Y|Z) \sim O(\varepsilon)$

Scale error

C: CMI(X,Y|Z)~ $O(\varepsilon^2)$

False negative problem!

Zhao et al. **PNAS** 2016 Shi et al. **IEEE/ACM TCBB** 2018 Shi et al. **Sci China Math** 2018



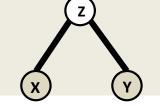
Part mutual information for quantifying direct associations in networks

Zhao et al. PNAS 2016

Juan Zhao^{a,1}, Yiwei Zhou^{a,b,1}, Xiujun Zhang^a, and Luonan Chen^{a,b,c,2}

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Zhao et al. **PNAS** 2016 (one side) Shi et al. **IEEE/ACM TCBB** 2018 (two sides) Shi et al. **Sci China Math** 2018 (two sides)

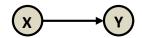


PMI algorithm and kernel PMI algorithm for network inference

Do运算: 后门规则 Back-door criterion

$$p^*(y|z) = \sum_{y} p(y|z,x)p(x)$$

Statistical model cannot mathematically prove that y changes accordingly if x changes, and thus validation experiment is generally required



Cutoff error problem for p for GC and TE

$$x_{t} = f(x_{t-1}, ..., x_{t-p}) + \epsilon_{x,t}$$

$$y_{t} = g(x_{t-1}, ..., x_{t-p}, y_{t-1}, ..., y_{t-p}) + \epsilon_{y,t}$$

Cutoff errors : ϵ_x , ϵ_y

Dynamical Causality (DC)

Dynamical System:

$$x_t = f(x_{t-1}, ..., x_{t-p}, ...)$$

with $x_t = (x_{1,t}, x_{2,t}, ..., x_{n,t}); f = (f_1, f_2, ..., f_n)$

• Dynamical Causality: $x_i \rightarrow x_j$, dynamics of x_j depends on x_i , i.e.

 $\exists k \in \{1, 2, ..., p\}$, such that

$$\frac{\partial f_j}{\partial x_{i,t-k}} \neq 0 \qquad \text{for almost any sampled } t$$

causal



$$x_{i,t} = f(x_{t-1}, x_{i,t-1})$$

• Non-Dynamical Causality: dynamics of x_i does not depend on x_j , i.e.

 $\forall k \in \{1, 2, ..., p\}$, such that

$$\frac{\partial f_j}{\partial x_{i,t-k}} = 0$$

for almost any sampled t

non-causal

$$(x_i) \longrightarrow (x_j)$$

$$x_{j,t} = f(x_{t-1} \setminus x_{i,t-1})$$

Direct DC: explicit dependence; Indirect DC: implicit dependence

DC includes Granger Causality (GC), Transfer Entropy (TE) and Embedding Causality (EC)

Causal representation



$$y_{t} = f(y_{t-1}, ..., y_{t-p}, x_{t-1}, ..., x_{t-p}; \varepsilon_{y})$$

$$x_{t} = g(x_{t-1}, ..., x_{t-p}; \varepsilon_{x})$$

where ε_y is all remaining terms of x_{t-i} , y_{t-j} ; ε_x is all remaining terms of x_{t-i}



$$0 = -y_t + f(y_{t-1}, ..., y_{t-p}, x_{t-1}, ... x_{t-p}; \varepsilon_y) = F(y_t, ..., y_{t-p}, x_{t-1}, ... x_{t-p}; \varepsilon_y)$$

$$\text{hence} \rightarrow 0 = F(Y_t, X_{t-1}; \varepsilon_y)$$

$$\text{where } Y_t = (y_t, ..., y_{t-p}); X_{t-1} = (x_{t-1}, ..., x_{t-p})$$

(x,y)观测空间2p+1,流形自由度d,所以约束2p+1-d; 当 2p+1-d> p (y的个数)时可用隐函数定理

Thus, from implict function theorem for F: $X_{t-1} = H(Y_t, \varepsilon_y)$ with $\varepsilon_y \neq 0$

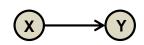
$$X_{t-1} = H(Y_t, \varepsilon_v)$$
 with $\varepsilon_v \neq 0$

y是果,包含x的信息,可重构(x,y)全空间,所以当p>2d时,Y可以表征X的空间 Further, from Takens' embedding theorem for $f: X_{t-1} = H(Y_t)$ with $\varepsilon_v = 0$ (Eliminating ε_{v} if p+1>2d; note generally $Y_{t}\neq G(X_{t-1})$)



Therefore, we have $X_{t-1} = H(Y_t)$ for numerical causal inference (functional continuity of $H \rightarrow$ neighbor cross-mapping) Current effect reconstructs past cause (现在的果重建过去的因)

Key observations



Past cause reconstructs current effect (过去的因重建现在的果)

Prediction function $y_t = H(y_{t-1}, x_{t-1})$ 预测 by time-series data in original space (x_t, y_t)

is equivalent to



Current effect reconstructs past cause (现在的果重建过去的因)

Inverse-mapping function $X_{t-1} = H(Y_t)$ 逆重构 by cross-mapping data in delay embedding space (X_{t-1}, Y_t)

$$X_{t-1} = (x_{t-1}, x_{t-2}, ..., x_{t-p}); Y_t = (y_t, y_{t-1}, ..., y_{t-p})$$

Benefits: solving non-separability, strong association, cut-off problems!

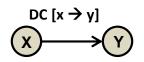
An example of inverse-mapping

Model
$$x(t+1) = c \ x(t) + d$$
 仅用Y能描述 x ,则 $x \rightarrow Y$ 仅用Y能描述 x ,则 $x \rightarrow Y$
$$x(t) = y(t+1)/b - ay(t)/b \rightarrow x(t-1) = x(t)/c - d/c = c \ y(t+1)/b - ac \ y(t)/b - d/c$$
 or $\mathbf{X}(t-1) = [x(t), x(t-1)] = [1/b, -a/b; c/b, -ac/b] [y(t+1), y(t)] + [0, -d/c] = \mathbf{AY}(t) + [0, -d/c]$ We can represent $\mathbf{x}(t+1)$ in terms of \mathbf{y} ! (finite terms of $\mathbf{y} \rightarrow \mathbf{cross-map}$ to \mathbf{x} ; $\mathbf{x}(t+1) = f(y(t+1), y(t), \dots)$)

But we cannot represent y(t+1) in terms of x! (finite terms of $x \neq cross-map$ to y; $y(t+1) \neq f(x(t+1),x(t),...)$)

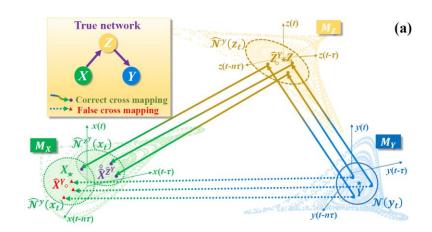
y has all information on x but x has no information on extra dynamics of y (i.e. a y(t))

Dynamical Causal Effect



• H0: $Corr(X(t),X^{Y}(t)|H0)=0$

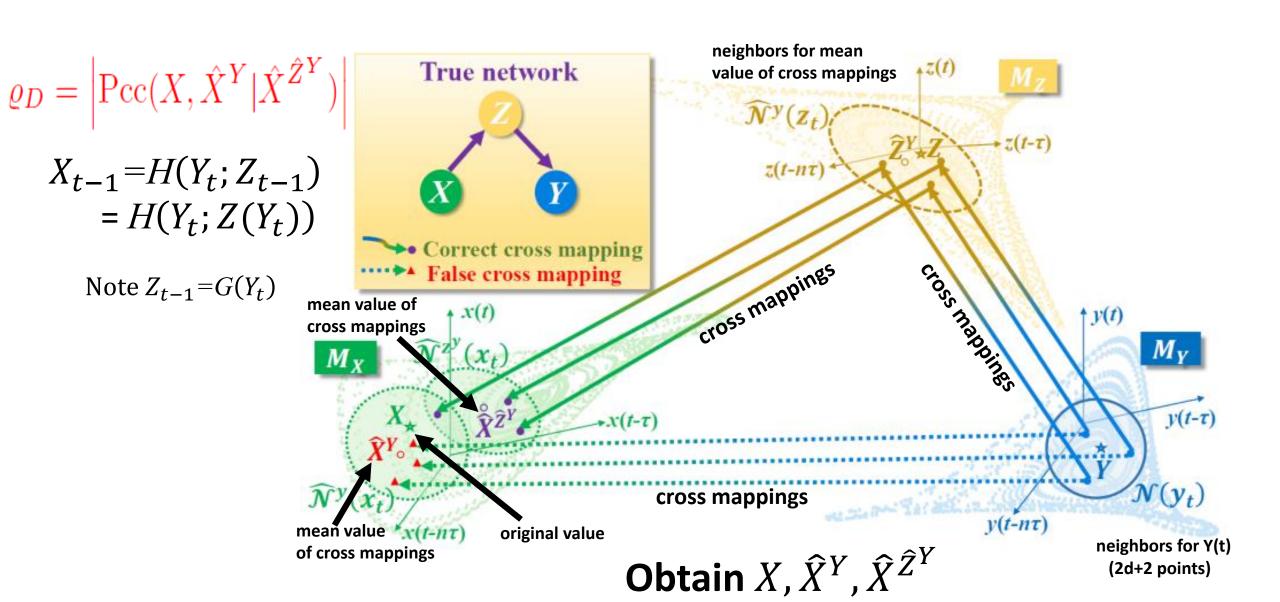
• H1: $Corr(X(t),X^{Y}(t)|H1)=1$



Causal strength: Corr(X(t),X^Y(t)|X^{ZY}(t))

$$\varrho_D = \left| \operatorname{Pcc}(X, \hat{X}^Y | \hat{X}^{\hat{Z}^Y}) \right|$$

Partial Cross Mapping (PCM)



Indirect and direct causality

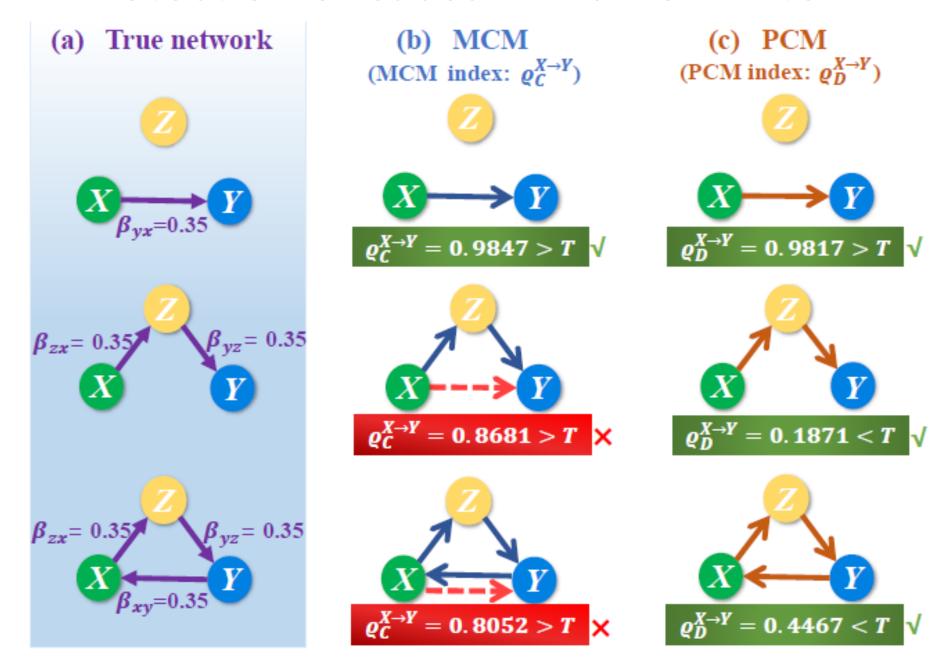
MCM: mutual cross mapping (indirect causality)

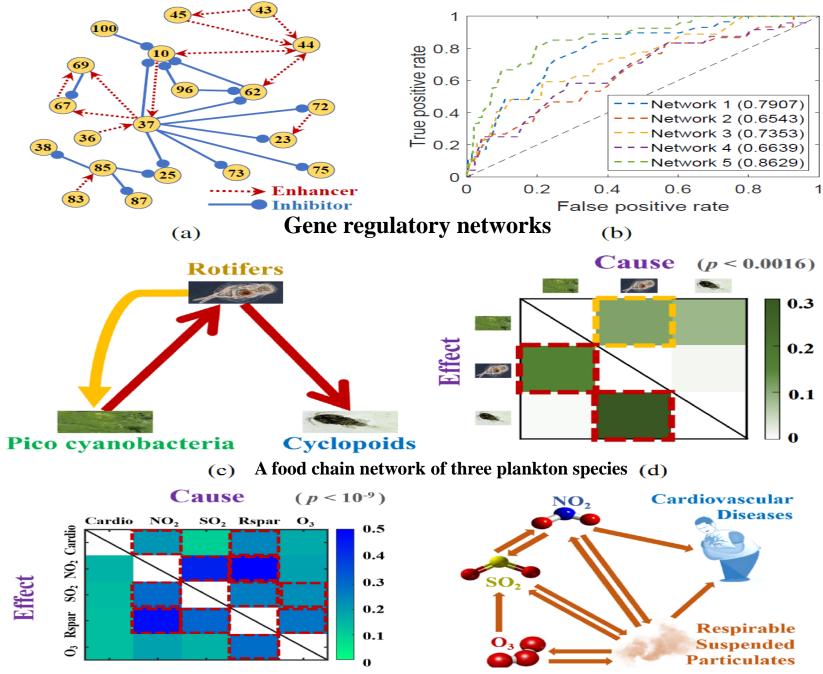
$$\varrho_C = \left| \operatorname{Corr}(X, \hat{X}^Y) \right|$$

PCM: partial cross mapping (direct causality)

$$\varrho_D = \left| \operatorname{Pcc}(X, \hat{X}^Y | \hat{X}^{\hat{Z}^Y}) \right|$$

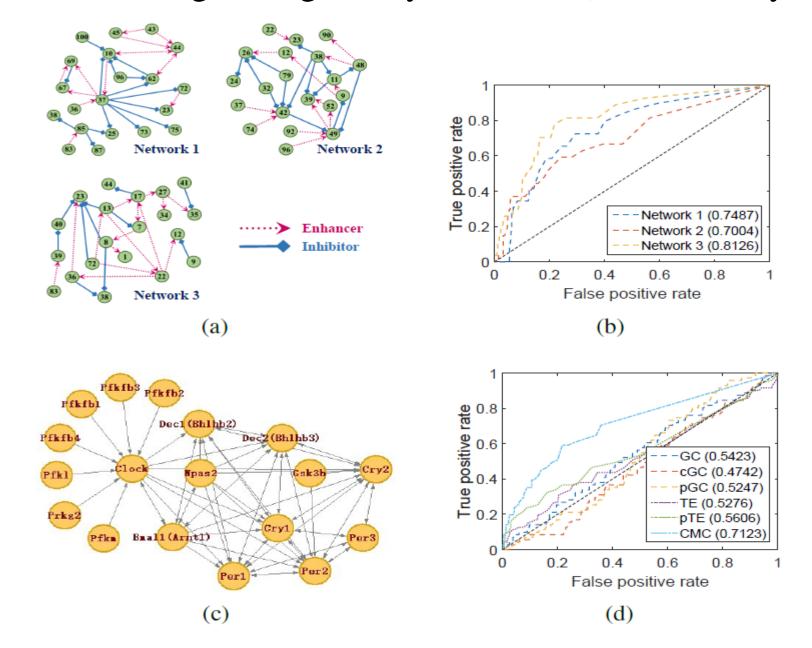
Detection of causal links from X to Y





Interactions between air pollutants and cardiovascular diseases (Hong Kong)

Results in real gene regulatory networks (circadian rhythms)





Dynamical model can mathematically prove that Y changes accordingly if X changes

ARTICLE



https://doi.org/10.1038/s41467-020-16238-0

OPEN

Partial cross mapping eliminates indirect causal influences

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10

 $CM \rightarrow MCM \rightarrow PCM$

Linear combination problem *Wi*?

动力学因果性和嵌入熵

Dynamical Causality by Embedding Entropy

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Embedding Entropy (EE)

$$TE[y \rightarrow x] = H(x_t/x_{t-1}) - H(x_t/y_{t-1}, x_{t-1}) = MI(x_t, y_{t-1}/x_{t-1})$$

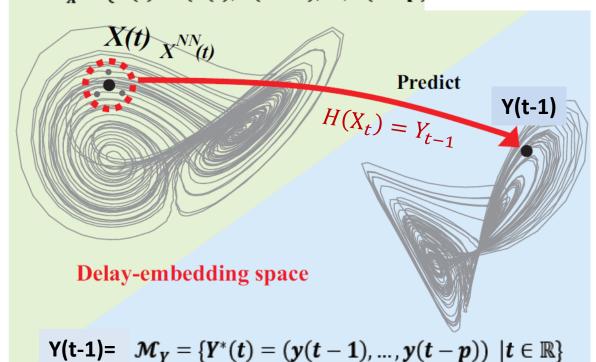
$$EE[y \rightarrow x] = H(Y_{t-1}) - H(Y_{t-1} | X_t^{NN}) = MI(Y_{t-1}, X_t^{NN})$$



TE: state space x,y; EE: embedding space X,Y

TE: past points y_{t-1} ; EE: neighbor points X_t^{NN}

$$\mathcal{M}_X = \{X(t) = (x(t), x(t-1), ..., x(t-p)) \text{ TE: conditional } y \text{ to } x; \text{ EE: conditional } X \text{ to } Y$$



 $H_0: EE[y \rightarrow x] = 0$

 $H_1: EE[y \rightarrow x] = H(Y) - H(Y|X^{NN})$

 $cs[x\rightarrow y] = D[H1 I H0]$

X^{NN}: neighbors of X

由X重构Y:加上X邻居的信息后,Y的不确定性减少(射影函数的连续性)强关联问题!

 x_t : original variable X_t : embedded variable

 $Y_{t-1} = H(X_t)$

Current effect reconstructs past cause (现在的果重建过去的因)

Embedding entropy (EE)



$$x(t) = \widehat{F}[x(t - \Delta t), x(t - 2\Delta t), \dots, x(t - p\Delta t)] + \epsilon_t$$

= $\widehat{F}[x_1(t - \Delta t), \dots, x_1(t - p\Delta t), \dots, x_n(t - \Delta t), \dots, x_n(t - p\Delta t)] + \epsilon_t$

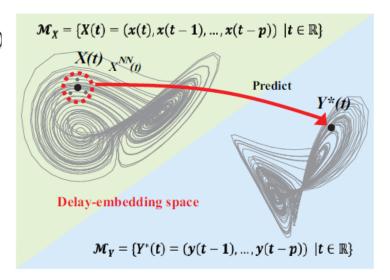
- ➤ Implicit function theorem (necessary condition)
- Takens' embedding theorem (sufficient condition)

$$Y^*(t) = h(X(t), \epsilon_{x,t})$$

$$X(t) = (x(t), x(t - \Delta t), \dots, x(t - p\Delta t))^T \in \mathbb{R}^{p+1}$$

$$Y^*(t) = (y(t - \Delta t), \dots, y(t - p\Delta t))^T \in \mathbb{R}^p$$

$$\text{EE}[y \to x] = \text{MI}(Y^*, X^{NN}) = H(Y^*) - H(Y^*|X^{NN}).$$



 X^{NN} denotes the p+2 NNs of X, i.e., $X^{NN}(t)=(X^{[1]}(t),X^{[2]}(t),\ldots,X^{[p+2]}(t))$

Solving linear problem of MCM, non-separability, false negative, cutoff problem!

$$H(Y_t) = -\sum p(Y_t) \log p(Y_t)$$

Features of Embedding Entropy

$$EE[y \rightarrow x] = H(Y_{t-1}) - H(Y_{t-1} | X_t^{NN}) = MI(Y_{t-1}, X_t^{NN})$$



- 1. Use entropy to solve the <u>nonlinear problem</u>.
- 2. Use embedding mapping and implicit function from *Y* to *X*, to solve the **non-separability problem**.
- 3. Use X^{NN} instead of X in the delay embedding manifold to avoid the <u>strong association problem</u>.
- 4. Use implicit function theorems, solve **cutoff problem** of p.

$$H(Y_t) = -\sum p(Y_t) \log p(Y_t)$$

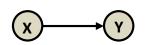
Detecting Dynamical Causality by Cross Mapping

Hirata & Aihara. Phys. Rev. E 81. 016203, 2010 (CM)
Sugihara et al. Science 338, 496, 2012 (MCM)
Leng et al. Nature Communications 11, 2632, 2020 (PCM)
Shi et al. Journal of Royal Society Interface, 2022 (EE)

A neighborhood of M_Y is that of the corresponding M_X



Dynamical Causality from X to Y

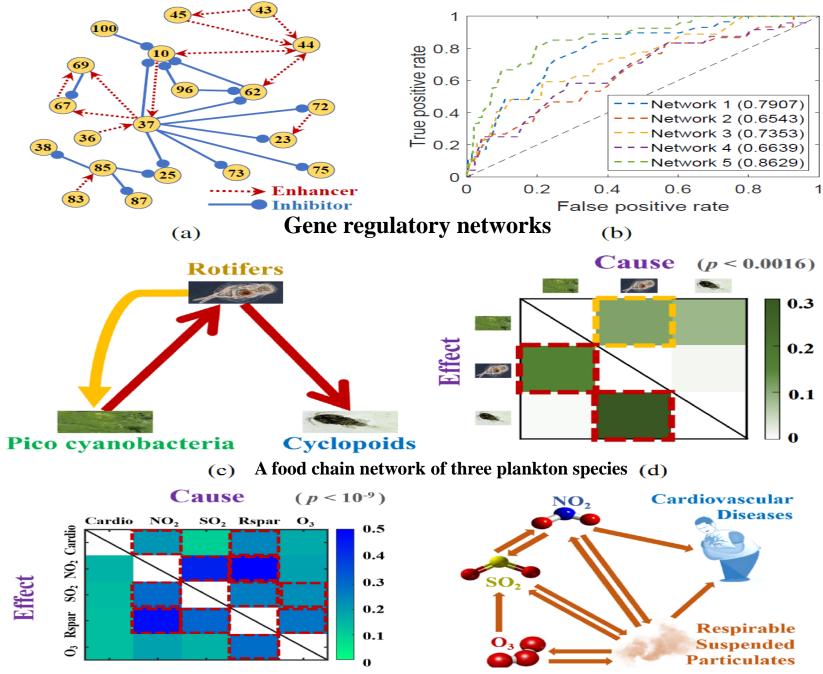


where M_X :delayed-coordinate reconstruction of X, M_Y :delayed-coordinate reconstruction of Y.

2010 2012 2020 2022 .

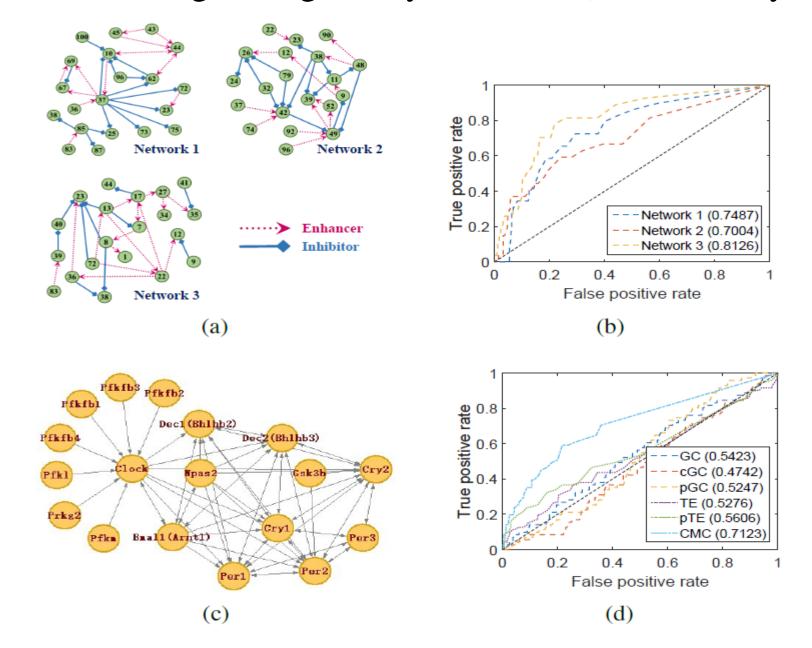
2010 2012

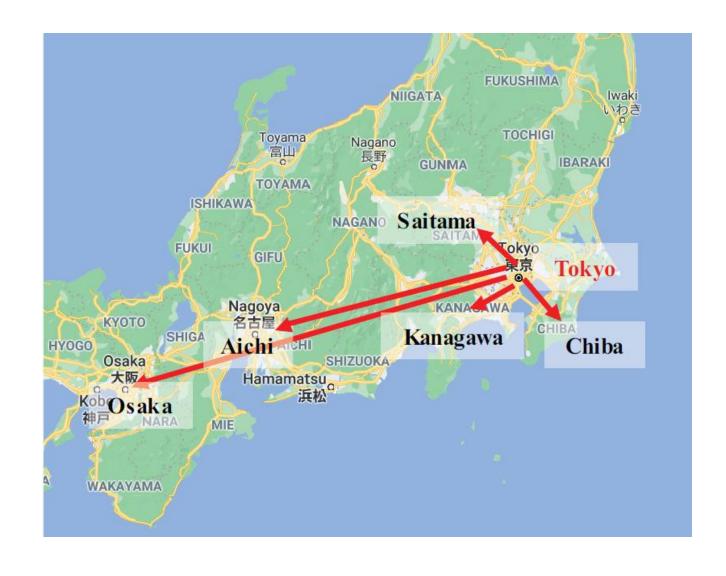
cross-mapping (CM) \rightarrow mutual cross-mapping (MCM) \rightarrow partial cross-mapping (PCM) \rightarrow embedding entropy (EE)



Interactions between air pollutants and cardiovascular diseases (Hong Kong)

Results in real gene regulatory networks (circadian rhythms)



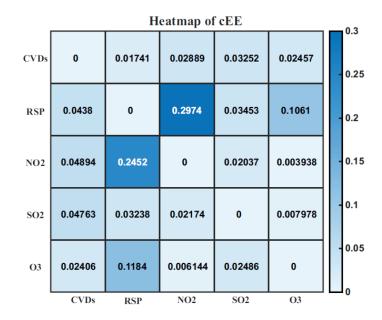


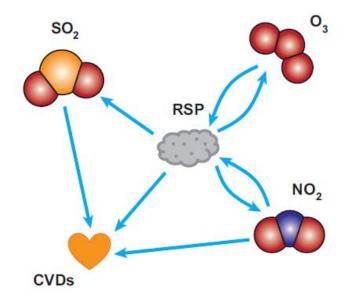
The 5 most affected prefectures by Tokyo

Real dataset 2: Hong Kong air pollution and cardiovascular diseases(CVDs)

Hong Kong from March 1995 to November 1997 (1032 days in total)

- Air pollutants: NO_2 , SO_2 , respirable suspended particulate (RSP), and O_3 (in $\mu g/m^3$)
- CVDs: daily number of CVD admissions to major hospitals in Hong Kong



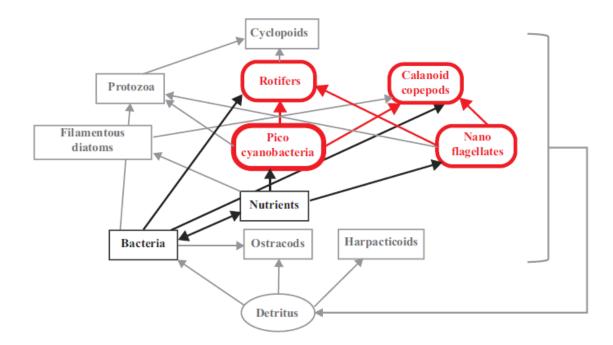


By cEE (65% quantile as the threshold value)

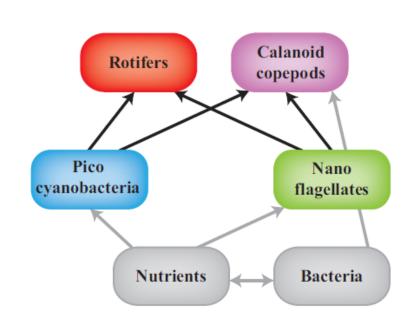
Real dataset 3: Food chain network

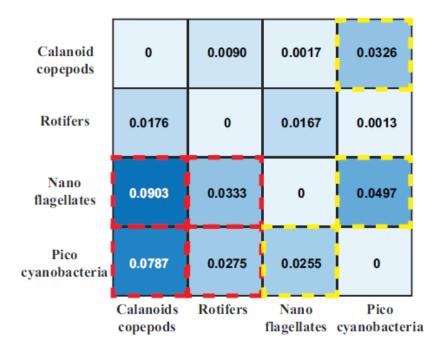
An 8-year mesocosm experiment of a plankton community isolated from the Baltic Sea (1032 days).

• Four species: calanoid copepods, rotifers, nanoagellates, and picocyanobacteria



Result of cEE





Red square: True positive

Yellow square: False positive caused by hidden variables

EE for Inverse-Mapping

Causal Inference

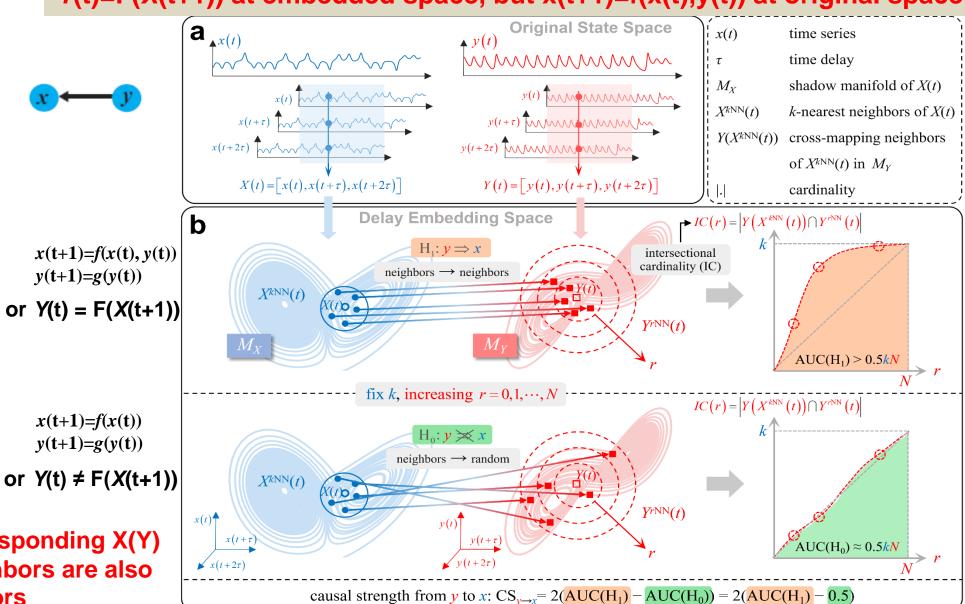
Cross-Mapping Cardinality (CMC)
 (time series data)

Neighboring Cross-Mapping Entropy (NME)
 (non-time series)

 Counterfactual-Invariant Diffusion-based GNN Explainer (CIDER) (non-time series)

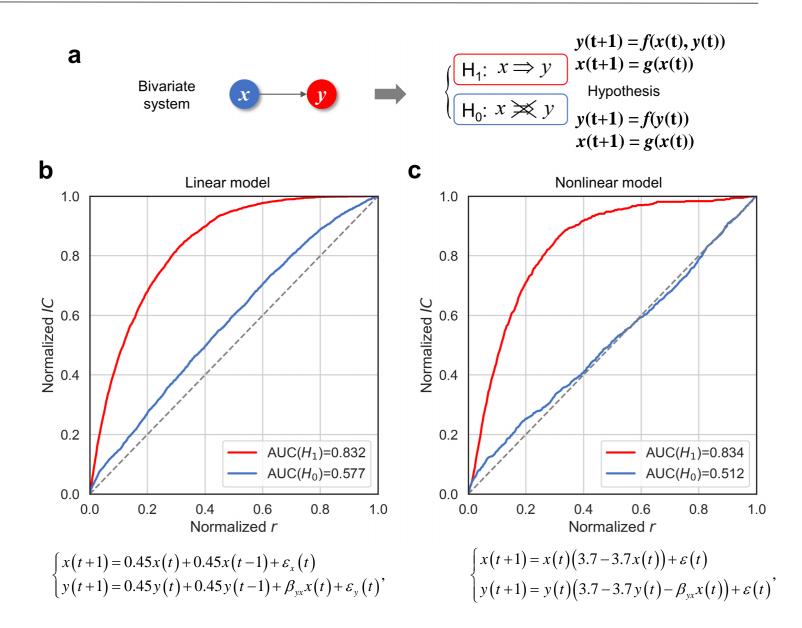
Luonan Chen (Chinese Academy of Sciences)

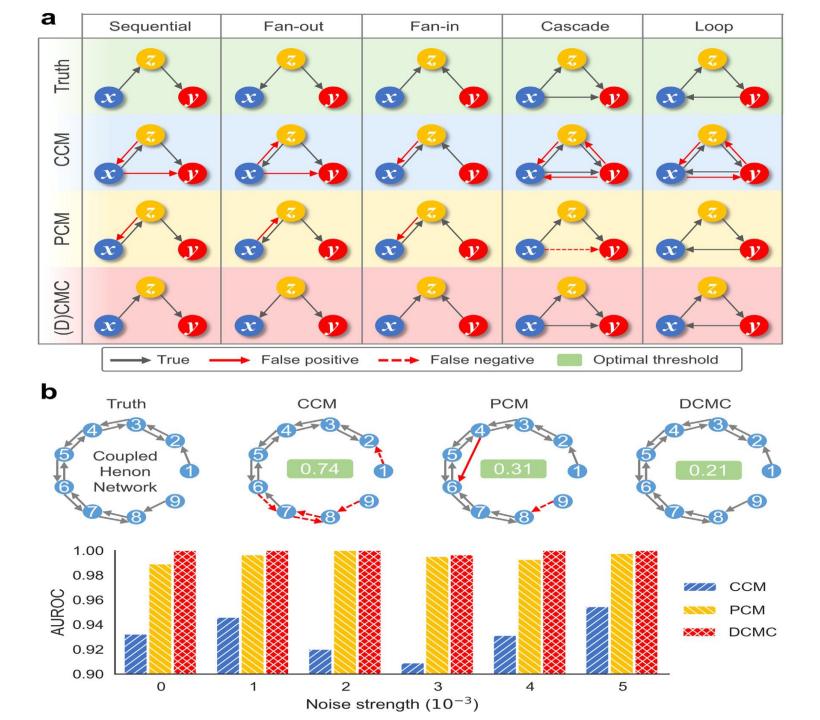
Reverse Mapping or Reverse Reconstruction Y(t)=F(X(t+1)) at embedded space, but x(t+1)=f(x(t),y(t)) at original space



The corresponding X(Y) of Y neighbors are also X neighbors

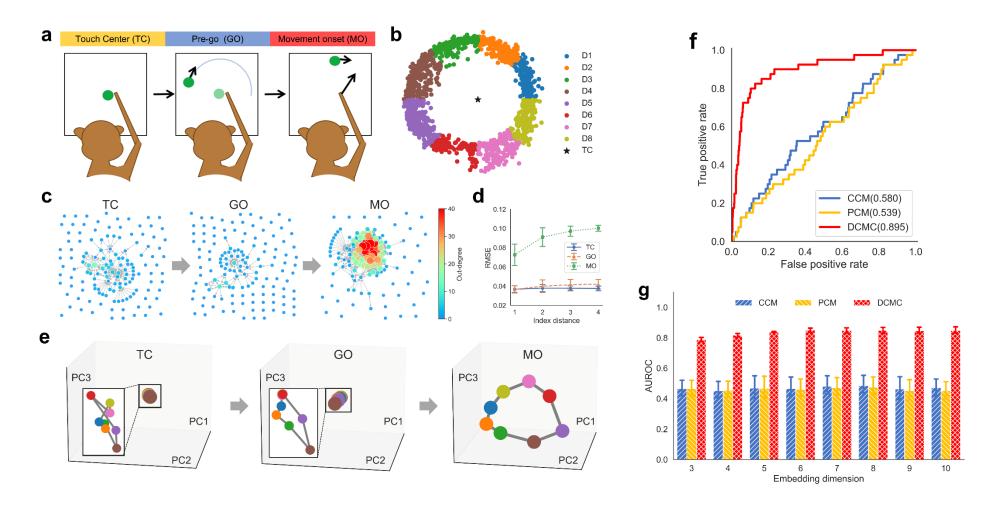
Results





Results

Neural network of the rhesus monkey's motor cortex



Acknowledgments

Jifan Shi, Siyang Leng, Kazuyuki Aihara,
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- Huanfei Ma,
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- Wei Lin,
 Fudan University

Part mutual information: Zhao et al. PNAS 2016 Randomly distributed embedding: Ma et al. PNAS 2018

Partial cross-mapping: Leng et al. Nature Communications 2020

Embedding entropy: Shi et al. J. R. Soc. Interface 2022