Nonlinearity of nature and its challenges

Journal Club
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The scientific method

System

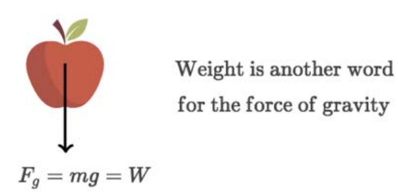
Observe and describe

Discern pattern, find rules (deduction)

Using the language of mathematics

$F = mg$

Prediction



Compare predicted with observed reality

Nonlinearity: Disclaimer

- Nomenclature mostly from classical and quantum mechanics.
- Mathematical and intuitive approach possible.
- In biology, pioneered and mostly used by (however still few) ecologists.
- Usually ignored in molecular biology.

Goals of this JC

- Show you how insights gained in one field of science may, if understood and taken advantage of, fertilize other fields.
- Discuss how scientific questions may impact, and even alter, everyday epistemology.
- Show conceptual relevance without necessarily understanding the full mathematical scope.

Phase space and dimensionality

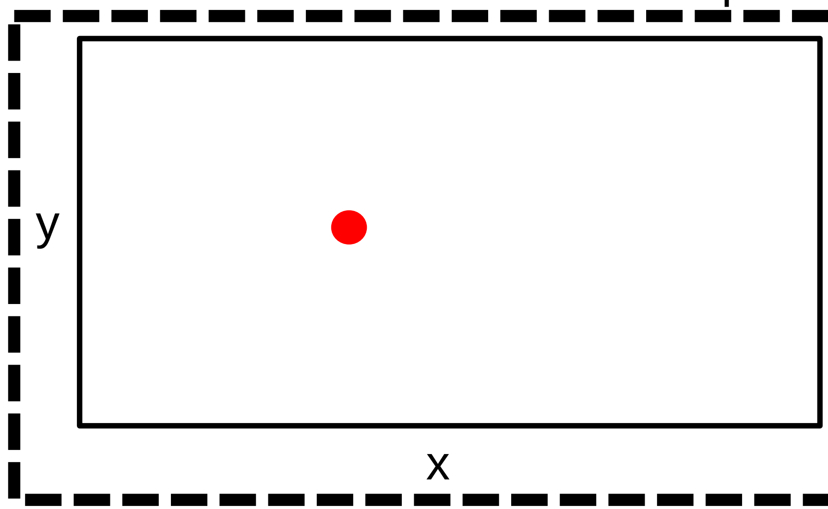
System

Infinite number of variables

Representation

Surrogate to represent system

Phase space



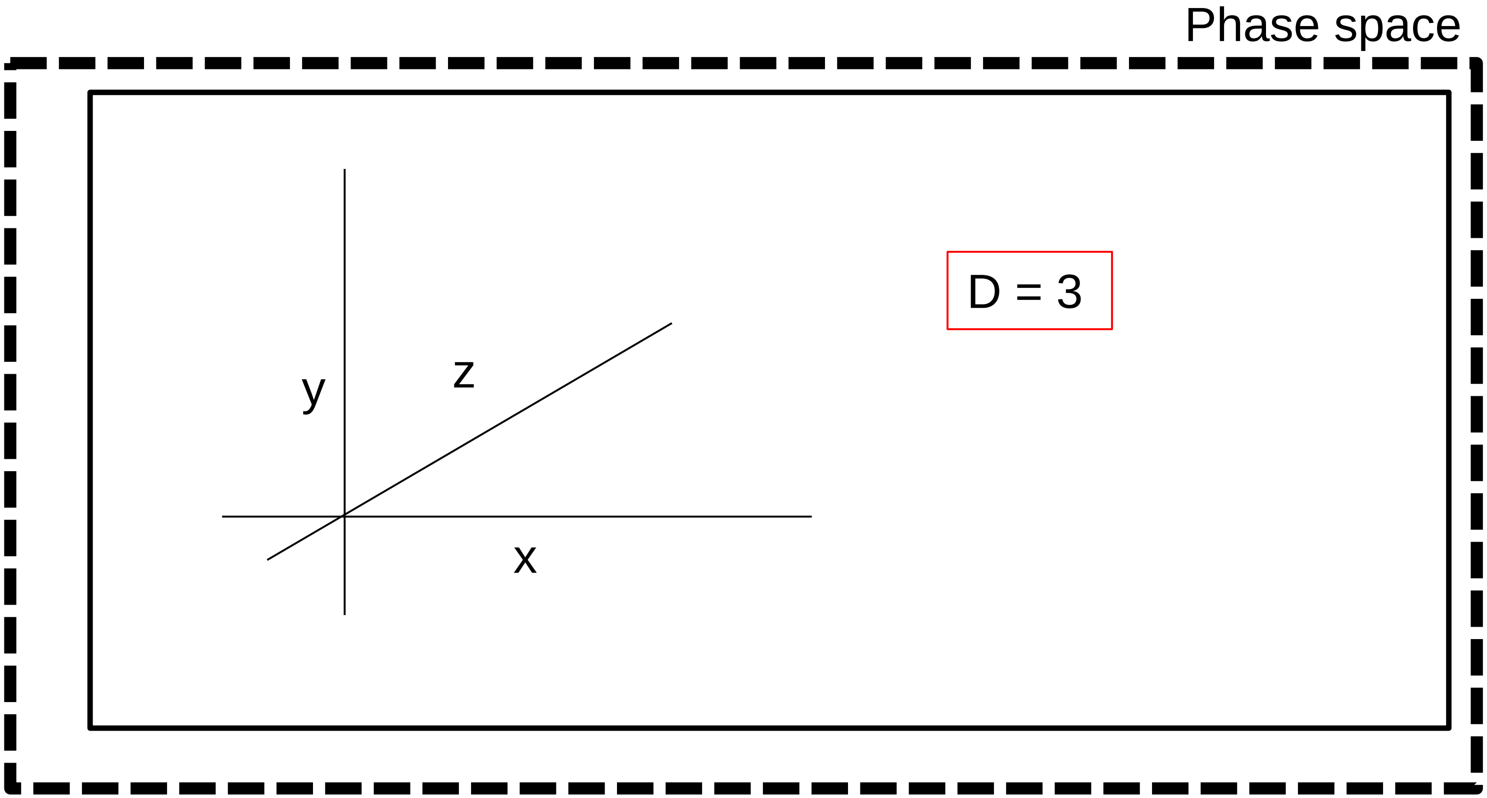
● Possible state of the system

Trajectory/ orbit

x e.g. density of clouds

y e.g. humidity

Phase space and dimensionality



Amount of variables required to represent system: **Dimensionality**
The more dimensions, the higher the **degree of freedom**

Relationship of phenomena

- The world is not static and changes over time: **Dynamics** → usually nonlinear.
- If sensitive to **initial conditions** (e.g. chaos theory) → usually nonlinear.
- Something like $f(x) = mx + k$ → certainly linear.

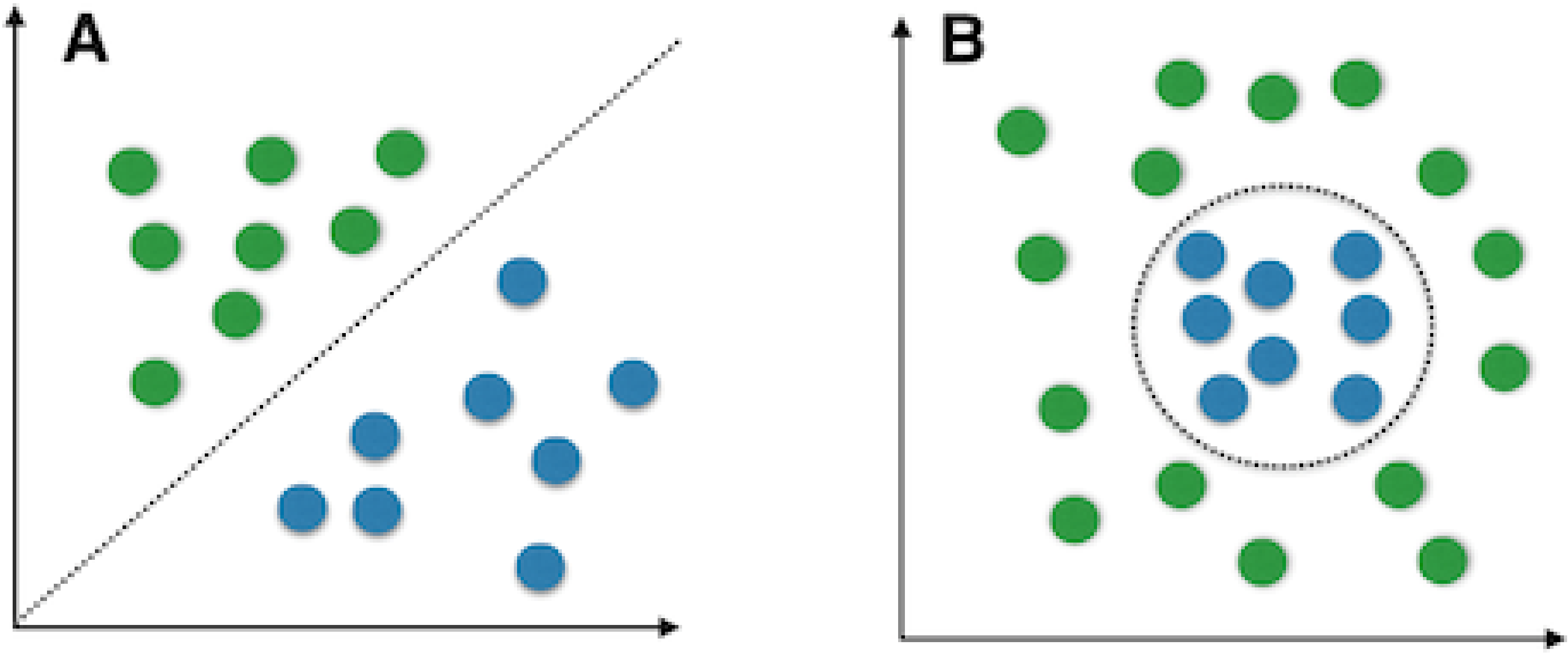
Linear systems

- Change in variable at initial time → change in same or different variable at later time that is **linearly proportional** to change at initial time.
- Linear systems satisfy the property of **superposition**: The combination of two solutions for a linear system is also a solution: $f(x + y) = f(x) + f(y)$.
- System **can be simplified**, sum of simplified solutions (addressing the full complexity of the system) are still valid.
- Rather easily solvable.

Nonlinear systems

- Change in variable at initial time → change in same or different variable at later time is **not proportional** to change at initial time.
- Often, they show exponential sensitivity to initial conditions.
- Individual solutions cannot be superimposed → Cope with **entire complexity** of problem.
- Solutions require high **computational power**.
- These systems are **ubiquitous in nature** and concern all fields of science!

Linear vs. nonlinear problems



Separability!

Linearity is an exception

- Example linear system: Dampened oscillator:

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = 0$$

$$m\ddot{x} + b\dot{x} + kx = 0$$

with $x_1 = x$
and $x_2 = \dot{x}$

$$\dot{x}_1 = x_2$$

$$\dot{x}_2 = \ddot{x} = -\frac{b}{m}\dot{x} - \frac{k}{m}x = -\frac{b}{m}x_2 - \frac{k}{m}x_1$$

- Since x_i on the right side appear first power, the system is called **linear**. Otherwise, system would be **nonlinear**.

Linearity is an exception

- Example nonlinear systems:
  - Gene expression
  - Neuronal network formation
  - Morphogenesis
  - Weather
  - Fish population/overfishing
  - Spread of infectious disease with TIME
  - Pulsating stars (non-chaotic)
  - Other stars (chaotic)
  - Economics (stock market, e.g.)
- Common sense assumptions:
  - System is static
  - We are in equilibrium

Why should we consider nonlinear systems?

- Because we may not be at **equilibrium** when we measure.
- Because **TIME** may heavily influence the outcome of our studied system.
- Because our data might heavily rely on initial states and display **mirage correlations**.
- (Because some of us would like to make a lot of money on the stock market…)

Detecting Causality in Complex Ecosystems

George Sugihara,[1]* Robert May,[2] Hao Ye,[1] Chih-hao Hsieh,[3]* Ethan Deyle,[1]
Michael Fogarty,[4] Stephan Munch[5]

Identifying causal networks is important for effective policy and management recommendations on climate, epidemiology, financial regulation, and much else. We introduce a method, based on nonlinear state space reconstruction, that can distinguish causality from correlation. It extends to nonseparable weakly connected dynamic systems (cases not covered by the current Granger causality paradigm). The approach is illustrated both by simple models (where, in contrast to the real world, we know the underlying equations/relations and so can check the validity of our method) and by application to real ecological systems, including the controversial sardine-anchovy-temperature problem.

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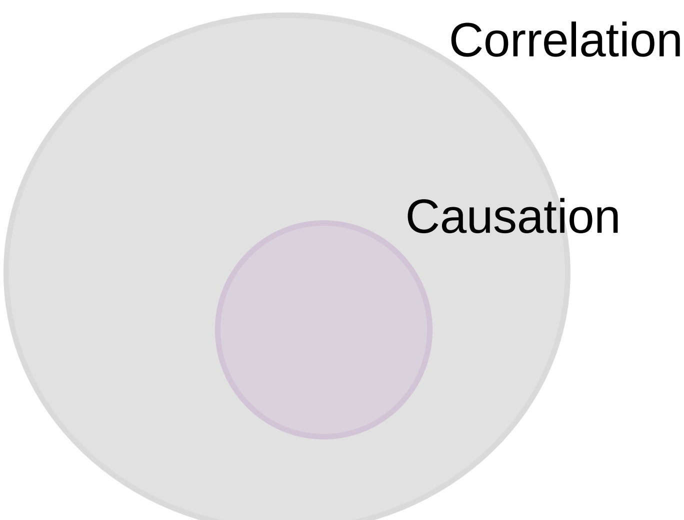
Implications: Correlation and causation

Shark attacks

Ice cream sales

Implications: Correlation and causation

- Bishop Berkeley (1710): «*Correlation does not necessarily imply causation*.»



Detecting causality in complex systems

- Imagine you have reason to believe that the laws «governing» your system have to be mathematically described with a **nonlinear difference equation**.

System

Observe and describe

Discern pattern, find rules (deduction)

$$F(x,y) = x^2 - xy + y^2$$

Multiple solutions, complex behaviour, chaos, bifurcations.

The Coupled Logistic Map: A Simple Model for the Effects of Spatial Heterogeneity on Population Dynamics

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(*Received on* 3 *August* 1993, *Accepted in revised form on* 19 *October* 1994)

$$\boxed{\begin{aligned} X(t+1) &= X(t)[r_x - r_x X(t) - \beta_{x,y} Y(t)] \\ Y(t+1) &= Y(t)[r_y - r_y Y(t) - \beta_{y,x} X(t)] \end{aligned}}$$

- Simple model of two elusively coupled logistic maps → two species logistic model.

Causation without correlation?

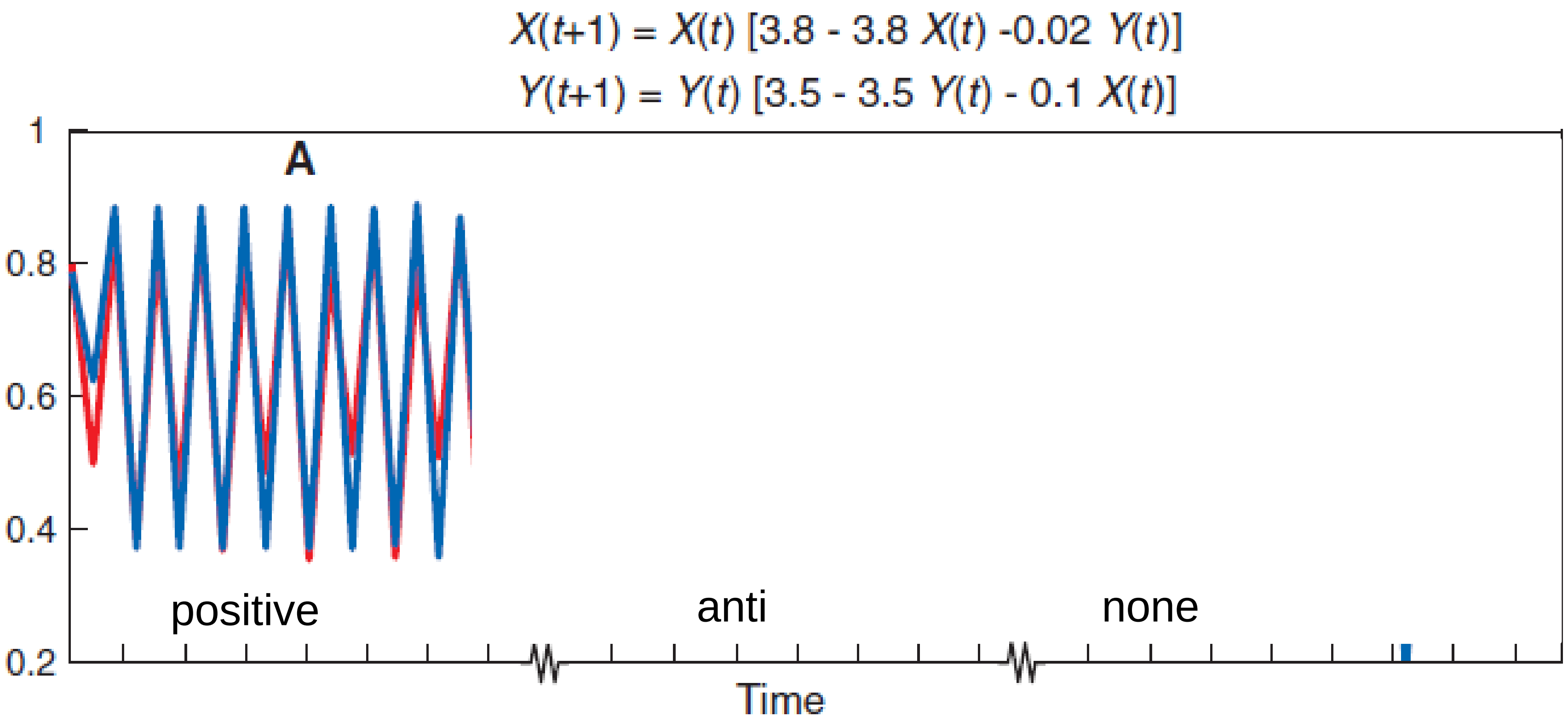
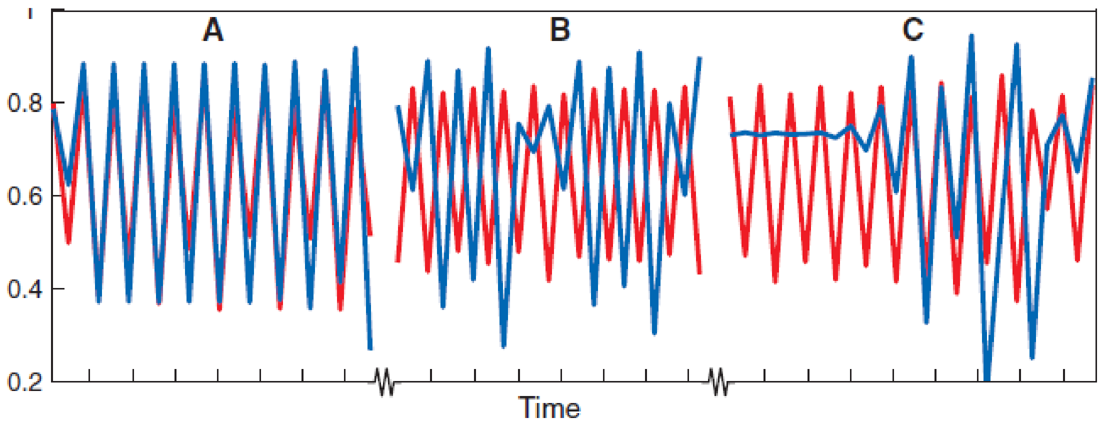


Fig. 1. Mirage correlations. (**A** to **C**) Three samples from a single run of a coupled two-species nonlinear logistic difference system with chaotic dynamics. Variables *X* (blue) and *Y* (red) appear correlated in the first time segment (A), anticorrelated in the second time segment (B), and lose all coherence in the third time segment (C) with alternating interspersed periods of positive, negative, and zero correlation. Although the system is deterministic and dynamically coupled, there is no long-term correlation ($n = 1000$, $\rho = 0.0054$, $P = 0.864$).

Correlation and causation



- Conclusion: Variables are not causally related since they are uncorrelated?
- But they are, mathematically, causally related.

Predictive causality

- Importance to define causal relationships also in nonlinear, i.e. predominating, systems in nature.

- Apply principal of Granger causality?

Granger causality (economics)

If

$$\sigma^2\{(X|\overline{U})\} < \sigma^2\{(X|\overline{U - Y})\}$$

is true, then Y «Granger causes» X.

Problematic if Y contains information on X, i.e. is not fully uncoupled → This is exactly what happens in dynamic (coupled) systems where information about Y is contained in all other variables, whereby it cannot be subtracted from the universe of all possible variables.

Granger theorem only applies if world is fully stochastic.

Convergent cross mapping

- If X causes Y, then Y contains information about X that can be used to predict X.
- States of X can be reconstituted from history of Y.
- Causation can be tested by mesauring extent to which historical record of Y values can reliably estimate states of X → correlation **coefficient ρ**.

Finding correlations

Convergent cross mapping

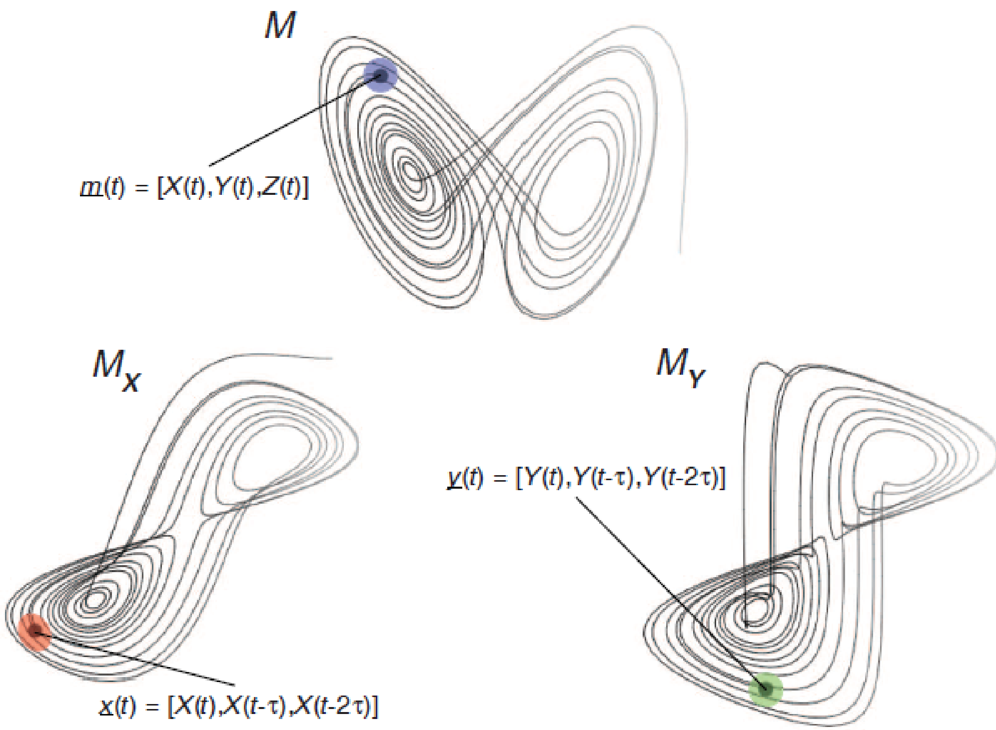


Fig. 2. Convergent cross mapping (CCM) tests for correspondence between shadow manifolds. This example based on the canonical Lorenz system (a coupled system in *X*, *Y*, and *Z*; eq. S7 without *V*) shows the attractor manifold for the original system (*M*) and two shadow manifolds, M_X and M_Y, constructed using lagged-coordinate embeddings of *X* and *Y*, respectively (lag = τ). Because *X* and *Y* are dynamically coupled, points that are nearby on M_X (e.g., within the red ellipse) will correspond temporally to points that are nearby on M_Y (e.g., within the green circle). That is, the points inside the red ellipse and green circle will have corresponding time indices (values for *t*). This enables us to estimate states across manifolds using *Y* to estimate the state of *X* and vice versa using nearest neighbors (*3*). With longer time series, the shadow manifolds become denser and the neighborhoods (ellipses of nearest neighbors) shrink, allowing more precise cross-map estimates (see movies S1 to S3).

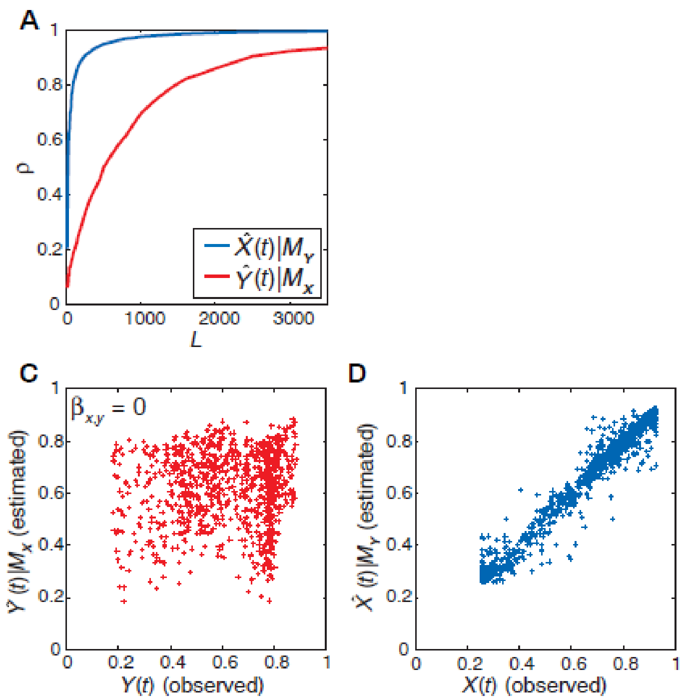
Based on Lorenz attractor for coupled nonlinear system

$$\dot{X} = a(Y - X)$$
$$\dot{Y} = X(b - Z) - Y$$
$$\dot{Z} = XY - cZ$$

Takens' Theorem

Convergent Cross Mapping

Detecting causation with CCM



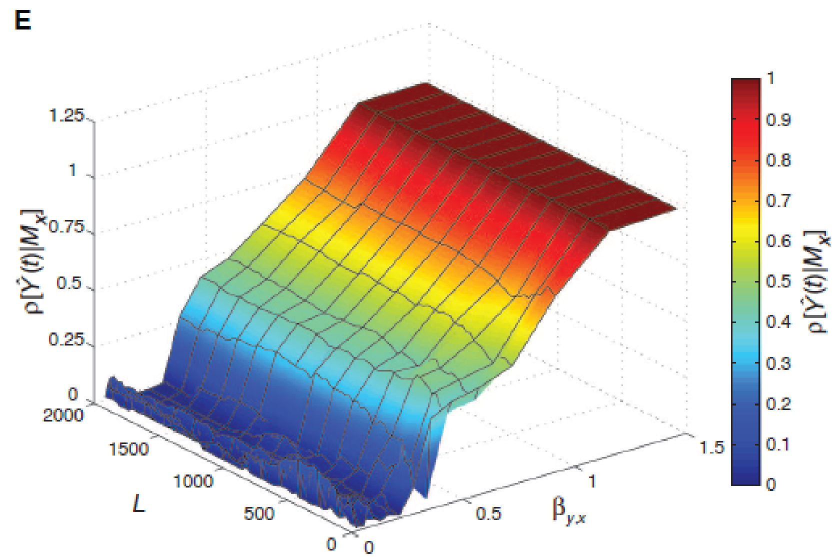


Fig. 3. Detecting causation with CCM. With convergence, the skill of cross-map estimates, indicated by the correlation coefficient (ρ), increases with time-series (library) length L. (**A**) CCM for Eq. 1, Fig. 1, where the effect of X on Y is stronger than in the reverse: $\beta_{y,x} > \beta_{x,y}$. Consequently, cross mapping X using M_Y converges faster than cross mapping Y using M_X. (**B**) Summary of this effect for Eq. 1, $L = 400$. (**C** to **E**) When Y (red) has no effect on X (blue) (i.e., $\beta_{x,y} = 0$), (C) shows that cross mapping of Y using M_X fails; however, the cross map of X succeeds (D) because the time series for Y contains information about the dynamics of X. (E) demonstrates nonconvergence of $\hat{Y}(t)$ as a function of forcing strength when $\beta_{x,y} = 0$. Convergence only occurs as a special case if strong forcing causes the system to collapse dimensionality (dark red plateau at high $\beta_{y,x}$), thus removing the dynamics of Y.

Causal networks

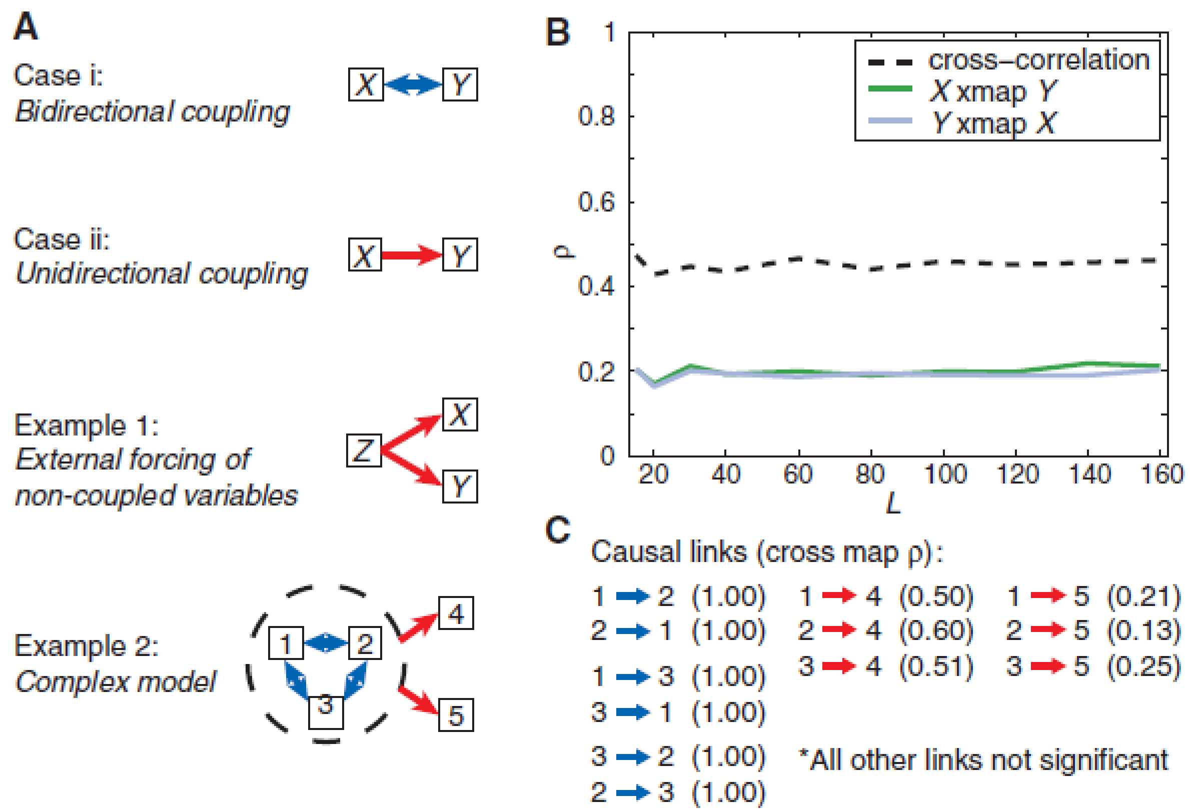


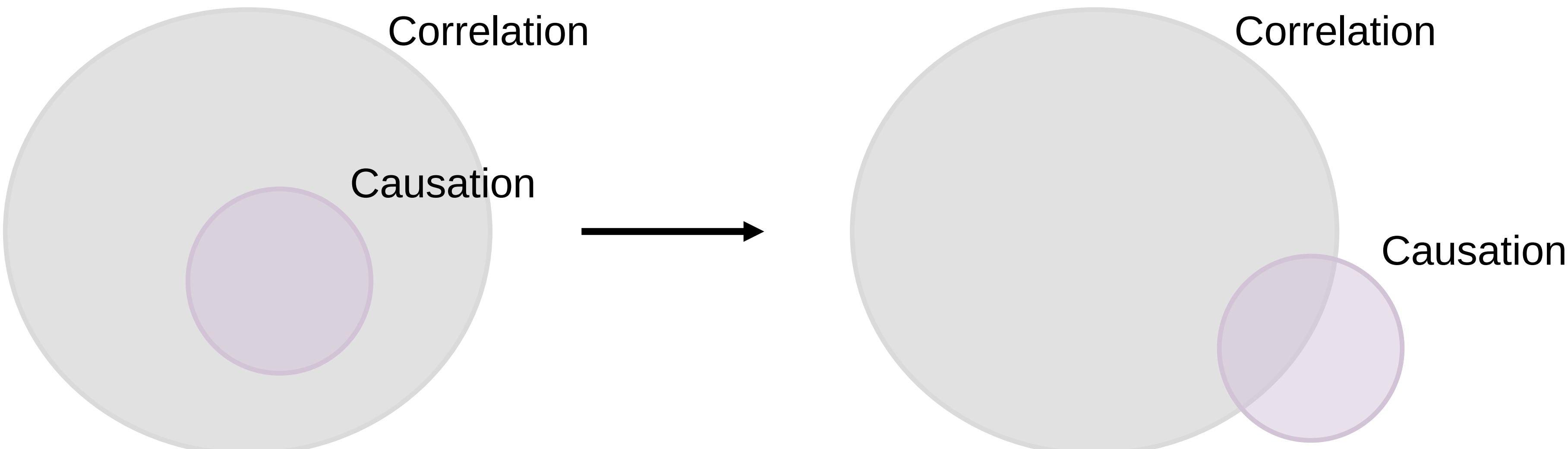
Fig. 4. Model causal networks. (**A**) Schematics of causal networks: two base cases and two model examples showing external forcing of noncoupled variables. (**B**) Cross-map results for example 1: external forcing of noncoupled variables. Cross-correlation erroneously suggests that *X* and *Y* are interacting, whereas cross mapping correctly shows that there is no interaction. (**C**) Cross-map results for the complex five-species model example. All significant ($P < 0.05$) mappings are given and indicate that species 1, 2, and 3 (the subsystem in the circle) all interact mutually (case i), but interact only asymmetrically as external forcing variables with respect to 4 and 5 (case ii), which do not interact directly themselves.

Summary

- CCM allows predictive modelling of nonlinear systems (including variable feedback loops) and detection of correlation.
- Regulatory actions (climate change, overfishing, e.g.), economics, data analysis and experimental design.

Implications: Correlation and causation

- Bishop Berkeley (1710): «*Correlation does not necessarily imply causation*.»
- George Sugihara (nonlinear dynamics): «*Lack of correlation does not imply lack of causation*.»



TIME SERIES ANALYSIS

Information leverage in interconnected ecosystems: Overcoming the curse of dimensionality

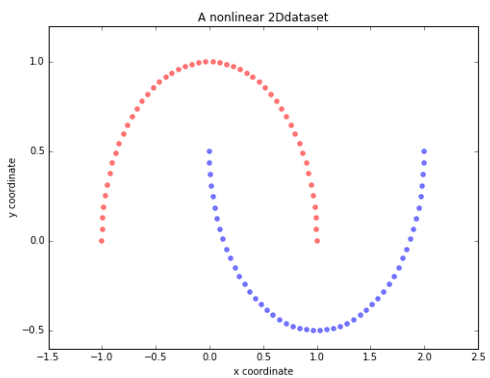
Hao Ye and George Sugihara*

The curse of dimensionality

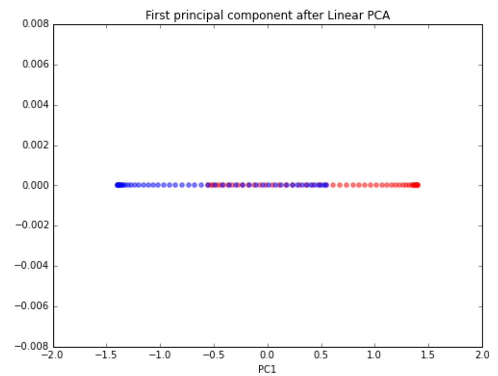
- Complexity → obstacle to overcome!
- In variety of fields including ecology, finance, neuroscience, medicine…
- Approach 1: Reduce systems to linearly independent components.

The curse of dimensionality

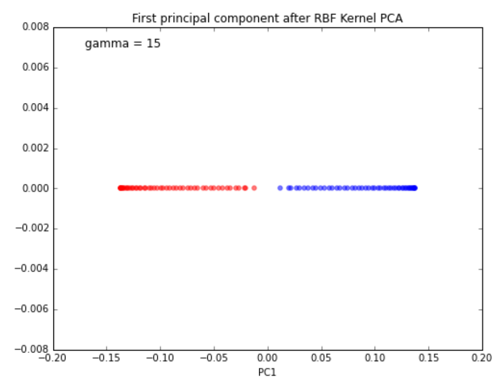
Dimensionality reduction primer



PCA

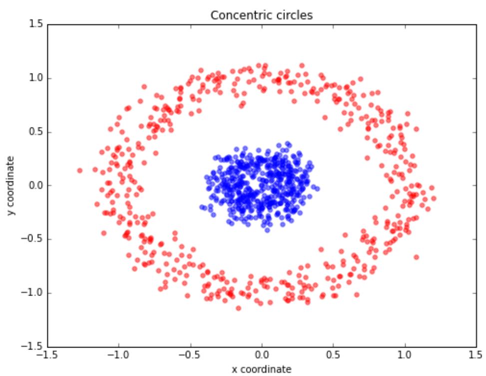


K-PCA

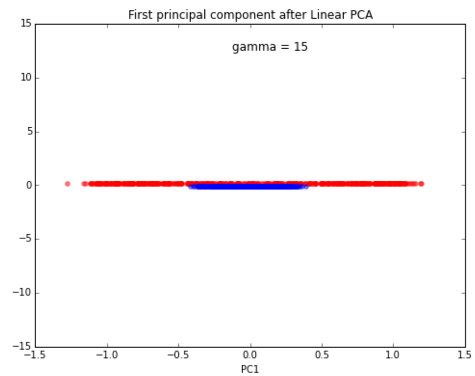


The curse of dimensionality

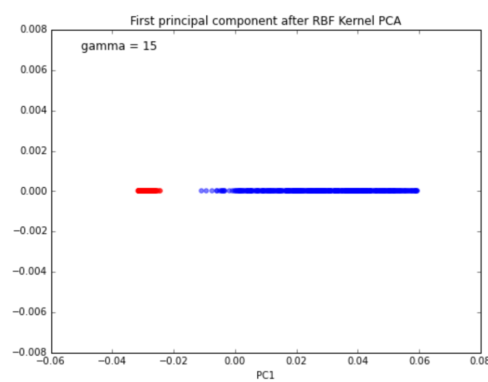
Dimensionality reduction primer



PCA

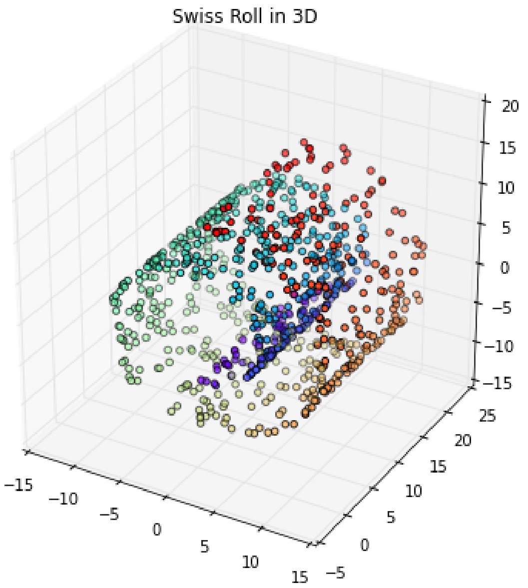


K-PCA



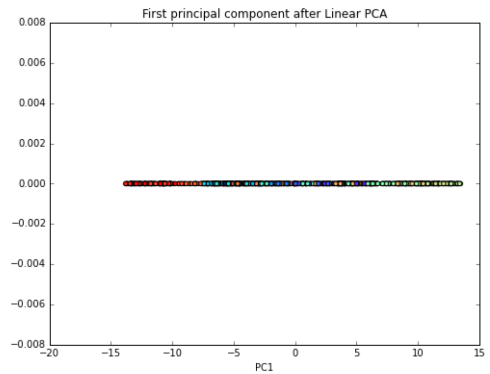
The curse of dimensionality

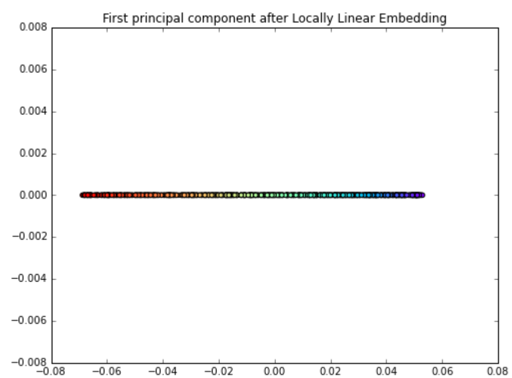
Dimensionality reduction primer



PCA

LLE





The curse of dimensionality

- Dimensionality reduction → assume that causal factors
  - do not interact with each other,
  - have effects that are independent or additive (as is valid for truly linear systems that can be superimposed).

The curse of dimensionality

- Complexity → obstacle to overcome!
- In variety of fields including ecology, finance, neuroscience, medicine…
- Approach 2: Use complex equation-based models → often too many parameters to be precisely determined.

Empirical dynamic modeling

Time series

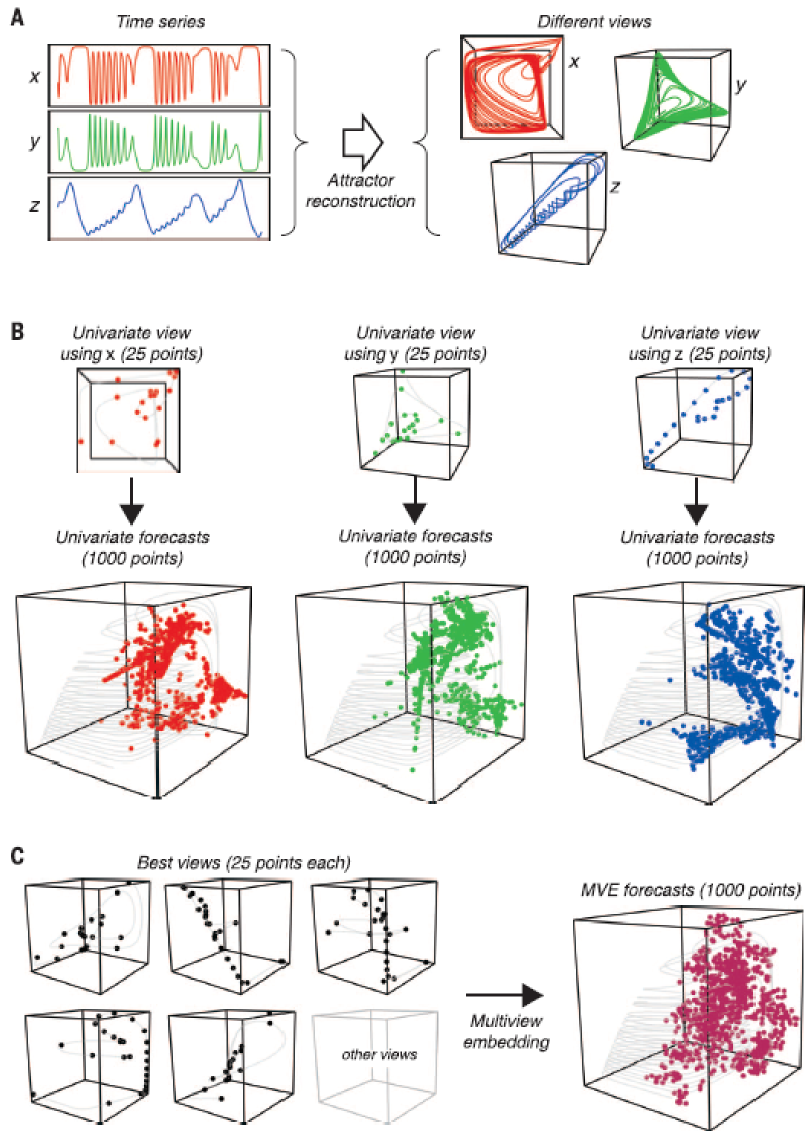
Lag of single or multiple variables

Takens' theorem

Reconstruction of attractor manifold

As seen with CCM

Multiview embedding



Multiview embedding

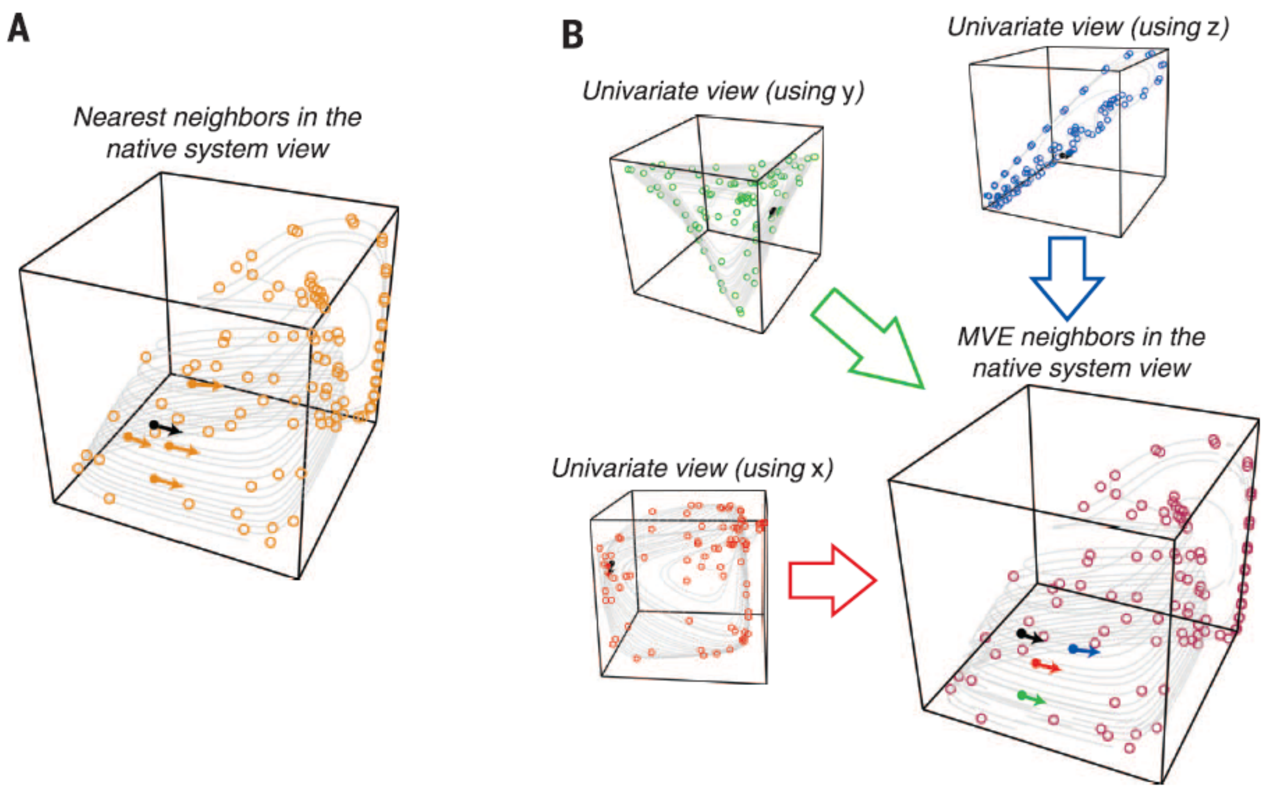


Fig. 2. Nearest-neighbor selection on attractor manifolds. (**A**) In the native system view, the nearest neighbors (solid orange points) to the target point (black) are used to predict the future trajectory. (**B**) MVE selects the single nearest neighbor in each of the different views to produce a more robust model. Here, the nearest neighbors (red, green, and blue) to the target point (black) from the three univariate views (based on lags of *x*, *y*, or *z*, respectively) are used to forecast the future behavior of the target.

Comparison

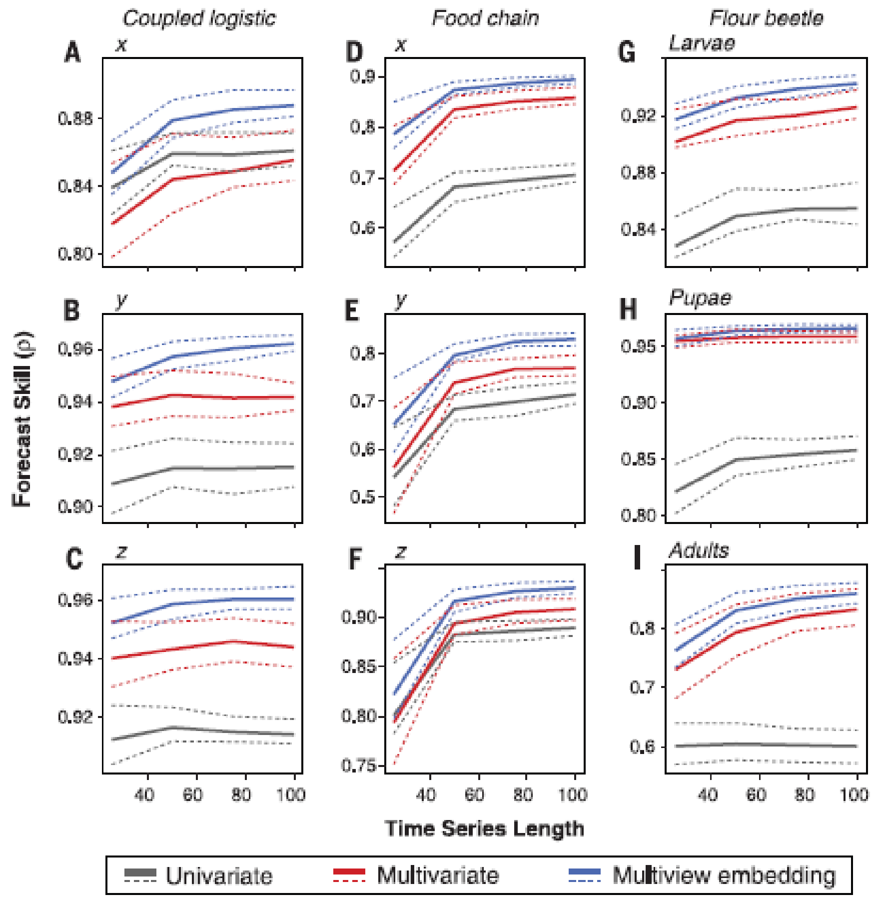


Fig. 3. Comparison of forecast skill for univariate, multivariate, and MVE methods on simulated data with 10% observational error. (**A** to **C**) Forecast skill (ρ, correlation between observations and predictions) versus library size for variables *x*, *y*, and *z* in the three-species coupled logistic. Solid lines indicate average values over 100 randomly sampled libraries; dashed lines denote upper and lower quartiles. (**D** to **F**) Same as (A) to (C) but for the three-species food-chain model (*20*). (**G** to **I**) Same as (A) to (C) but for the flour beetle model (*25*).

Conclusions

- Main innovation of MVE is to leverage interconnectedness of complex systems.
- Noise-mitigating aspects of MVE are potentially useful for applications such as signal processing or nonlinear system control.
- High-dimensionality may be a curse – but complexity can be advantage promoting better clarity and prediction.

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