

ERGODIC THEORY AND DYNAMICAL PROCESS MODELING

FOUNDATIONS FOR CONTINUUM COMPUTATIONAL MECHANICS

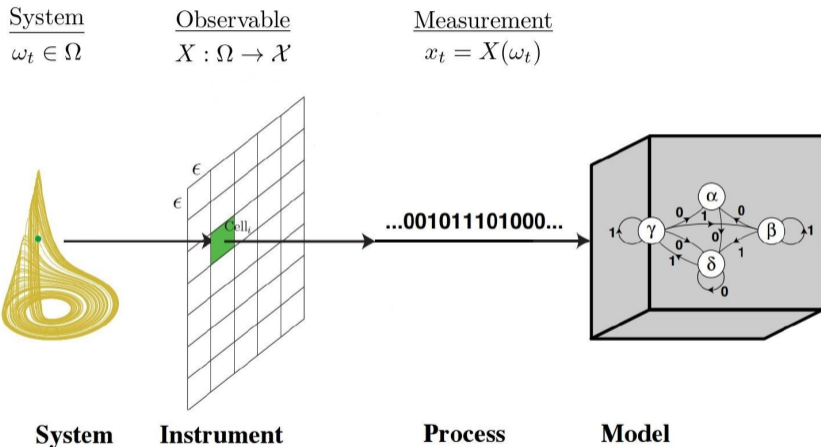
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NONLINEAR MODELING AND SYMBOLIC PROCESSES

How does chaos generate randomness?



Systematic and rigorous method for converting a continuous dynamical system into a fully-discrete, i.e. *symbolic*, stochastic process.

NONLINEAR MODELING AND SYMBOLIC PROCESSES

Symbolic processes are the objects traditionally modeled by computational mechanics,

Studied through *ϵ -machines*

Unique minimal sufficient statistic of past for predicting the future,
generated by *causal equivalence relation*:

$$\text{past}_i \sim_{\epsilon} \text{past}_j \iff \Pr(\text{Future}|\text{past}_i) = \Pr(\text{Future}|\text{past}_j)$$

- ▶ optimal prediction
- ▶ (causal) structure, organization
- ▶ directly calculate entropy rate
- ▶ process memory and complexity

NONLINEAR MODELING AND SYMBOLIC PROCESSES

When does nonlinear modeling work? – *generating partitions*

discrete-time dynamical system $(\Omega, \Phi : \Omega \rightarrow \Omega)$ – e.g. Poincare Map

$$\omega_{n+1} = \Phi(\omega_n)$$

partition phase space with *measurement function* $G_{\mathbb{P}} : \Omega \rightarrow \mathcal{A}$

$\mathbb{P}_i \cap \mathbb{P}_j = \emptyset$ and $\bigcup_{i=0}^N \mathbb{P}_i = \Omega$, and each partition carries unique symbol $a \in \mathcal{A}$

$\{\omega_0, \omega_1, \omega_2, \dots\}$ becomes $\{a_0, a_1, a_2, \dots\} = \{G_{\mathbb{P}}(\omega_0), G_{\mathbb{P}}(\Phi(\omega_0)), G_{\mathbb{P}}(\Phi^2(\omega_0)), \dots\}$.

NONLINEAR MODELING AND SYMBOLIC PROCESSES

$G_{\mathbb{P}} \circ \Phi$ induces partition $\Phi^{-1}\mathbb{P}$ over Ω ; $(\Phi^{-1}\mathbb{P})_i$ is set of all $\omega \in \Omega$ s.t. $G_{\mathbb{P}}(\Phi(\omega)) \in \mathbb{P}_i$

each time step induces new $\Phi^{-n}\mathbb{P}$ whose elements are $\omega \in \Omega$ s.t. $G_{\mathbb{P}}(\Phi^n(\omega)) \in \mathbb{P}_i$

partition refinement $\mathbb{P} \vee \mathbb{Q} = \{\mathbb{P}_i \cap \mathbb{Q}_j : \mathbb{P}_i \in \mathbb{P} \text{ and } \mathbb{Q}_j \in \mathbb{Q}\}$ also a partition

first *dynamical refinement* of \mathbb{P} under Φ is $\mathbb{P} \vee \Phi^{-1}\mathbb{P}$,

maps point $\omega \in \Omega$ to two-symbols $a_0a_1 \in \mathcal{A} \times \mathcal{A}$

the *full dynamical refinement* of \mathbb{P} under Φ is $\mathbb{P} \vee \Phi^{-1}\mathbb{P} \vee \Phi^{-2}\mathbb{P} \vee \Phi^{-3}\mathbb{P} \dots$,

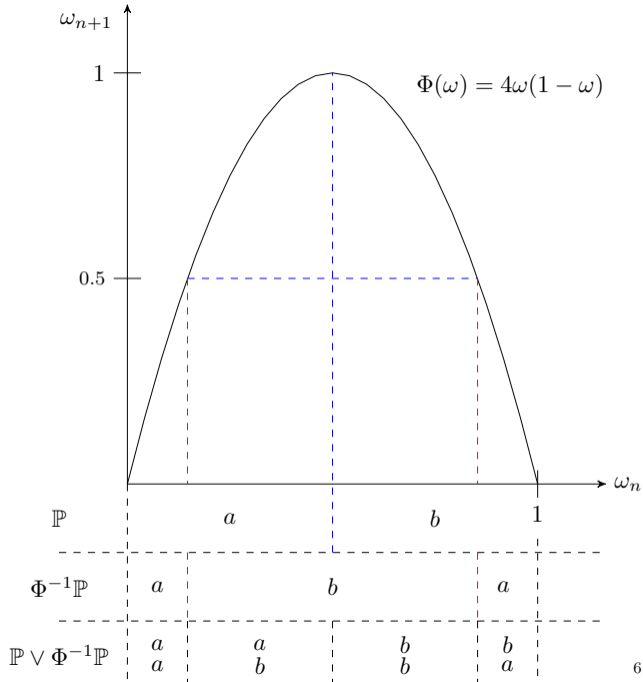
maps point $\omega \in \Omega$ to infinite-length symbol sequence $\mathcal{A} \times \mathcal{A} \times \mathcal{A} \times \dots$

a *generating partition* is a partition \mathbb{P} s.t. the full dynamical refinement is a.e. one-to-one between points $\omega \in \Omega$ and infinite-length symbol sequences—volume of partition elements goes to 0 for full dynamical refinement

A.N. Kolmogorov, Russian Academy of Sciences (1959), Y.G. Sinai Russian Academy of Sciences (1959)

Generating Partition of
Logistic Map

$$G_{\mathbb{P}}(x) = \begin{cases} a & 0 \leq \omega \leq 0.5 \\ b & 0.5 \leq \omega \leq 1 \end{cases}$$



KOLMOGOROV-SINAI ENTROPY: RANDOMNESS FROM CHAOS

entropy of partition (in terms of invariant distribution over partition elements)

$$H(\mathbb{P}) = - \sum_i \Pr(\mathbb{P}_i) \log \Pr(\mathbb{P}_i)$$

entropy rate

$$h_\nu(\Phi, \mathbb{P}) = \lim_{N \rightarrow \infty} \frac{1}{N} H\left(\bigvee_{n=0}^N \Phi^{-n}\mathbb{P}\right)$$

Kolmogorov-Sinai (metric) entropy

$$h_\nu(\Phi) = \sup_{\mathbb{P}} h_\nu(\Phi, \mathbb{P})$$

achieved for generating partitions—provides variational principle for approximation

(asymptotic distribution over \mathbb{P}_i limits to invariant density f^* of Φ for generating \mathbb{P})

Pesin's theorem: relation to positive Lyapunov exponents

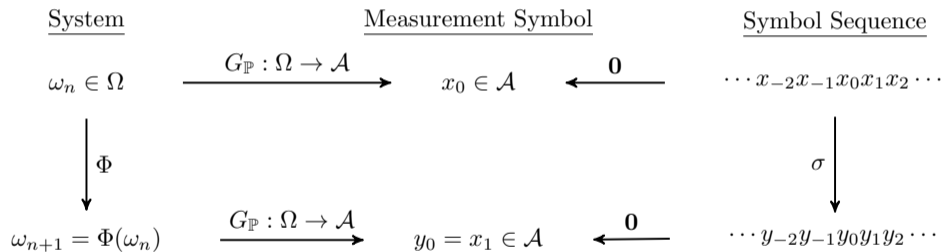
$$h_\nu(\Phi) \leq \sum_{\lambda_i > 0} \lambda_i$$

NONLINEAR MODELING AND SYMBOLIC PROCESSES

Symbolic process is a *shift dynamical system* $(\mathcal{A}^{\mathbb{Z}}, \sigma)$ under *shift operator*

for two symbol sequence $x, y \in \mathcal{A}^{\mathbb{Z}}$, $y = \sigma(x) \iff y_i = x_{i+1}$ for all $i \in \mathbb{Z}$,

i.e. σ advances observation time index forward



Converted nonlinear dynamical system into (symbolic) measurement process governed by **linear**, *infinite-dimensional operator* σ that advances observation time

SYSTEMS, DATA, AND MODELS

Advantages of nonlinear modeling:

- ▶ symbolic processes allow for discrete information and computation theory
- ▶ clean and rigorous framework for information storage, generation, and processing
- ▶ interpretability of system structure and organization through ϵ -machines

Challenges:

- ▶ even for idealized systems, generating partitions hard to find (e.g. Henon map)
- ▶ for a given physical system, don't have full control of system measurements
- ▶ scalability of inference and interpretability for large alphabets

generalize to continuum setting using Koopman and Perron-Frobenius Operators

A. Lasota and M. C. Mackey (2013). Chaos, Fractals, and Noise: Stochastic Aspects of Dynamics. Springer

System: $\omega_0 \in \Omega$

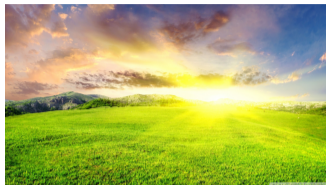


Φ^t



Credit: NASA-Apollo 17 crew

Observations: $x_0 = X(\omega_0)$



$X : \Omega \rightarrow \mathcal{X}$

$X_t : \Omega \rightarrow \mathcal{X} = U^t X$

$= X \circ \Phi^t$

U^t

$X : \Omega \rightarrow \mathcal{X}$



SYSTEMS AND DATA

The “true” physical system described by dynamical system $(\Omega, \Sigma_\Omega, \nu, \Phi)$:

- ▶ phase space Ω is complete metric space (typically \mathbb{R}^d or d-dimensional manifold)
- ▶ Σ_Ω a σ -algebra (Borel sets)
- ▶ ν a reference measure (Borel or Lebesgue)—phase space volume
- ▶ Φ the generator of (semi)group of measurable flow maps $\{\Phi^t : \Omega \rightarrow \Omega\}$

$$\Phi = \lim_{\tau \rightarrow 0} \frac{1}{\tau} (\Phi^t(\omega) - \Phi^{t+\tau}(\omega))$$

- ▶ orbits $\{\omega(t) : t \in \mathbb{R}_{(\geq 0)}\}$ continuous in time
- ▶ discrete intervals are bounded $\|\Phi^{t+\delta}(\omega_0) - \Phi^t(\omega_0)\| < \epsilon$

SYSTEMS AND DATA

The “observed” or “measured” system is measurable space $(\mathcal{X}, \Sigma_{\mathcal{X}})$

Observable $x \in \mathcal{X}$ generated by the dynamical system under the measurable mapping $X : \Omega \rightarrow \mathcal{X}$ so that $x_t = X(\omega_t)$

Generally interested in *partially-observable systems*, for which X is *not invertible*:
knowledge of x insufficient for determining state ω of the true system
 \implies there are “unobservable” or “immeasurable” degrees of freedom in ω

Will later consider a second set of observables $(\mathcal{Y}, \Sigma_{\mathcal{Y}})$ that are also given as a (generally non-invertible) measurable map $Y : \Omega \rightarrow \mathcal{Y}$ s.t. $y_t = Y(\omega_t)$.

X (and Y) represent “windows” through which we can view true physical system, but can never have a full view with $\mathcal{X} = \Omega$

Asymptotic behavior of ω may be reconstructable from x : *delay-coordinate embedding*

KOOPMAN OPERATORS

system “observable” $f : \Omega \rightarrow \mathbb{C}$, element of a function space (typically $L^\infty(\Omega, \nu)$ or $L^2(\Omega, \nu)$)

Koopman operators $\{U^t : \mathcal{F} \rightarrow \mathcal{F}\}$ evolve observables through composition with Φ^t

$$U^t f = f \circ \Phi^t$$
$$f_t(\omega) \equiv f(\Phi^t(\omega)) = U^t f(\omega)$$

linear, infinite-dimensional operators whose action on observable $f \in \mathcal{F}$ gives the time shifted observable (function) $f_t = U^t f$

Inherits (semi)group structure of $\{\Phi^t\}$ s.t. $U^t \circ U^{\Delta t} = U^{t+\Delta t}$ and generated by

$$Uf = \lim_{t \rightarrow 0} \frac{1}{t} (U^t f - f)$$

X (and Y) vector-valued observables, i.e. $X_i = f$, evolved by product operator U^t

DYNAMICAL PROCESSES

observables may be collected in a *time series* $\{x_0, x_1, \dots, x_{T-1}\}$ —a time-ordered sequences of “measurements” of x taken at uniform time intervals.

a *dynamical process* is bi-infinite time series of observables $\{\dots, x_{-2}, x_{-1}, x_0, x_1, x_2, \dots\}$

* for non-invertible dynamics, index is “observation time”

in terms of Koopman operators:

$$x_t = X(\omega_t) = X(\Phi^t(\omega_0)) = X_t(\omega_0) = U^t X(\omega_0)$$

Goal of dynamical process modeling: infer or approximate action of U on observables X

$$\{x_0, x_1, x_2, x_3, \dots\} = \{U^0 X(\omega_0), U^1 X(\omega_0), U^2 X(\omega_0), U^3 X(\omega_0)\}$$

(finite) *reconstructability*: X in finite invariant subspace \mathbf{U} s.t. $U^t X \in \mathbf{U}$ for all t

PERRON-FROBENIUS OPERATORS

Rather than evolve observables, *Perron-Frobenius operators* $P^t : L^1(\Omega, \nu) \rightarrow L^1(\Omega, \nu)$ evolve *densities* $f \in L^1(\Omega, \nu)$: $f \geq 0$ and $\|f\| = 1$.

$$f_t = P^t f$$
$$\int_S P^t f d\nu = \int_{(\Phi^t)^{-1}(S)} f d\nu \quad \text{for } S \in \Sigma_\Omega$$

May also consider P^t evolving $L^2(\Omega, \nu)$ measures μ : $\mu_t = P^t \mu$
relation to densities through Radon-Nikodym:

$$\mu^f(S) = \int_S f d\nu \quad \text{and} \quad f = \frac{d\mu^f}{d\nu}$$

$P^t : L^1 \rightarrow L^1$ adjoint of $U^t : L^\infty \rightarrow L^\infty$ and $P^t : L^2 \rightarrow L^2$ adjoint of $U^t : L^2 \rightarrow L^2$

$$\langle P^t f, g \rangle = \langle f, U^t g \rangle$$

STOCHASTIC PROCESSES

Can now formulate *continuous stochastic processes* generated by dynamical systems

- ▶ dynamical system $(\Omega, \Sigma_\Omega, \nu, \Phi)$ with initial probability density (ensemble) f_0
- ▶ density at time t is $f_t = P^t f_0 \implies$ probability measure $\mu_t(S) = \int_S f_t d\nu$
- ▶ at time t have probability space $(\Omega, \Sigma_\Omega, \mu_t) \implies$ observable map $X : \omega_t \mapsto x_t$ now defines random variable X_t
- ▶ X_t distributed according via pushforward $\mu_t^X(S_{\mathcal{X}}) = \mu_t(X^{-1}(S_{\mathcal{X}}))$ for $S_{\mathcal{X}} \in \Sigma_{\mathcal{X}}$

$$\text{pr}(X_t \in S_{\mathcal{X}}) = \int_{S_{\mathcal{X}}} d\mu_t^X = \int_{X^{-1}(S_{\mathcal{X}})} d\mu_t = \int_{X^{-1}(S_{\mathcal{X}})} f_t d\nu = \int_{X^{-1}(S_{\mathcal{X}})} P^t f_0 d\nu$$

Therefore, an initial density f_0 on a dynamical system $(\Omega, \Sigma_\Omega, \nu, \Phi)$ produces continuous stochastic process $\{X_0, X_1, X_2, \dots\}$

random variables are actually $X(t, \omega)$; for fixed ω a *sample path* given by $t \mapsto X(t, \omega)$, here are (continuous) dynamical processes $\{x_0, x_1, x_2, \dots\}$

CONNECTION TO SYMBOLIC PROCESSES: KOOPMAN

symbolic process:

$$\{\omega_0, \omega_1, \omega_2, \dots\} \rightarrow \{a_0, a_1, a_2, \dots\} = \{G_{\mathbb{P}}(\omega_0), G_{\mathbb{P}}(\Phi(\omega_0)), G_{\mathbb{P}}(\Phi^2(\omega_0)), \dots\}$$

dynamical process:

$$\{\omega_0, \omega_1, \omega_2, \dots\} \rightarrow \{x_0, x_1, x_2, \dots\} = \{U^0 X(\omega_0), U^1 X(\omega_0), U^2 X(\omega_0), \dots\}$$

Logistic map:

Partition isomorphic to generating partition given by

$$G_{\mathbb{P}}(x) = \begin{cases} 0 & 0 \leq x \leq 0.5 \\ 1 & 0.5 \leq x \leq 1 \end{cases}$$

$G_{\mathbb{P}}(x)$ generally given as sum of labeled indicator functions for partition elements \mathbb{P}_i :

$$G_{\mathbb{P}}(x) = \sum_{i=0}^{N-1} i \mathbb{1}_{\mathbb{P}_i}, \quad N = \|\mathbb{P}\|$$

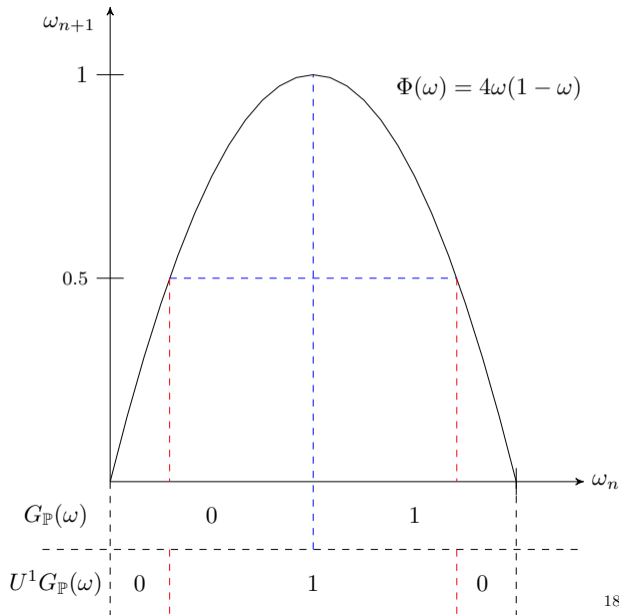
$$\mathbb{1}_{\mathbb{P}_i} = \begin{cases} 1 & x \in \mathbb{P}_i \\ 0 & x \notin \mathbb{P}_i \end{cases}$$

CONNECTION TO SYMBOLIC PROCESSES: KOOPMAN

$$G_{\mathbb{P}}(\omega) = \begin{cases} 0 & 0 \leq \omega \leq 0.5 \\ 1 & 0.5 \leq \omega \leq 1 \end{cases}$$

$$U^1 G_{\mathbb{P}}(\omega) = G_{\mathbb{P}}(\Phi(\omega)) = \Phi^{-1} \mathbb{P}$$

$$U^1 G_{\mathbb{P}}(\omega) = \begin{cases} 1 & \frac{1-\sqrt{\frac{1}{2}}}{2} \leq \omega \leq \frac{1+\sqrt{\frac{1}{2}}}{2} \\ 0 & \text{otherwise} \end{cases}$$



CONNECTION TO SYMBOLIC PROCESSES: PERRON-FROBENIUS

REFERENCE MEASURE VS INVARIANT MEASURE

if reference measure is invariant, constant density $f = 1$ is stationary: $P^t 1 = 1$

for logistic map with Borel / Lebesgue reference measure:

$$P^1 1 = \frac{1}{2\sqrt{1-\omega}}$$

\implies Borel measure not invariant

invariant measure μ^* found from solving $P^1 f^* = f^*$:

$$\mu^*(S) = \int_S f^* d\omega = \int_S \frac{d\omega}{\pi\sqrt{\omega(1-\omega)}}$$

Ulam and von Neumann (1947)

CONNECTION TO SYMBOLIC PROCESSES: PERRON-FROBENIUS

REFERENCE MEASURE VS INVARIANT MEASURE

consider uniform density on \mathbb{P}_1 ($\Pr(a_0 = 1) = 1$) and its evolved density

$$f(\omega) = \begin{cases} 0 & 0 \leq \omega \leq 0.5 \\ 2 & 0.5 \leq \omega \leq 1 \end{cases} \quad P^1 f(\omega) = \frac{1}{2\sqrt{1-\omega}}$$

with Borel reference measure:

$$\Pr(a_1 = 1) = 2 \int_{\frac{1}{2}}^{\frac{1+\sqrt{\frac{1}{2}}}{2}} d\omega = \int_{\frac{1}{2}}^1 \frac{d\omega}{2\sqrt{1-\omega}} = \sqrt{\frac{1}{2}}$$

with invariant reference measure:

$$\Pr(a_1 = 1) = 2 \int_{\frac{1}{2}}^{\frac{1+\sqrt{\frac{1}{2}}}{2}} d\mu^* = 2 \int_{\frac{1}{2}}^{\frac{1+\sqrt{\frac{1}{2}}}{2}} \frac{d\omega}{\pi\sqrt{\omega(1-\omega)}} = \frac{1}{2}$$

ERGODICITY

Typical to consider *measure-preserving* dynamical system $(\Omega, \Sigma_\Omega, \nu, \Phi)$ with $\Phi\nu = \nu$

Assumes a *stationary* stochastic process: $\text{pr}(X_t \in S_{\mathcal{X}}) = \text{pr}(X_0 \in S_{\mathcal{X}})$ for all t

This corresponds to dynamics on an *attractor*, but want to consider more general dynamics that include transient relaxation to the attractor

We do this using *ergodic components*, which correspond to *basins of attraction* (including the attractor itself)

A dynamical system $(\Omega, \Sigma_\Omega, \nu, \Phi)$ is *ergodic* if $\nu(S) = 0$ or $\nu(S) = 1$ for every *invariant set* $S : \Phi^{-1}(S) = S$

\implies all invariant sets are trivial subsets of Ω and we must study Φ on the entire space Ω

*** Note ergodicity is independent of measure preservation—but they are often assumed together

ATTRACTORS AND BASINS

invariant set : $\Phi^{-1}(S) = S$

forward-invariant set : $\omega_0 \in S \implies \Phi^t(\omega_0) \in S$ for all t

an invariant set is necessarily forward-invariant, but converse not true

An *attractor* of $(\Omega, \Sigma_\Omega, \nu, \Phi)$ is a set $A \in \Sigma_\Omega$ with

- ▶ A is a forward-invariant set of Ω under Φ
- ▶ there exists an open set $B \supset A$, call the *basin of attraction* of A , s.t. for every $\omega \in B$
 $\lim_{t \rightarrow \infty} \Phi^t(\omega) \in A$, and
- ▶ there is no proper subset of A with the first two properties

Attractors are *not* Φ -invariant, but *basins are Φ -invariant*

Can define basins as limit of pre-images of attractor: $B = \lim_{t \rightarrow \infty} (\Phi^t)^{-1} A$

ATTRACTOR BASINS AS ERGODIC COMPONENTS

Multi-stable dynamical systems with multiple attractors can be partitioned: each basin may be treated independently since, by definition, orbits never cross basin boundaries

Without loss of generality, will from here out consider systems that either:

- ▶ have one attractor with Ω as basin
- ▶ independently consider *ergodic components*: reduced systems with $\Omega = B$

System $(\Omega, \Sigma_\Omega, \nu, \Phi)$ considered this way is thus *ergodic*

Asymptotic behavior on the attractor:

- ▶ ergodicity guarantees P^t has unique invariant density $f^* : P^t f^* = f^*$
- ▶ this defines *asymptotic invariant measure* $\mu^*(S) = \int_S f^* d\nu$
- ▶ ergodic theorem: time averages equal phase space averages

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} f(\Phi^k(\omega)) = \frac{1}{\mu^*(\Omega)} \int_{\Omega} f(\omega) d\mu^*$$

THE PREDICTION PROBLEM

We set up a general prediction problem for dynamical processes as follows:

For a physical system $(\Omega, \Sigma_\Omega, \nu, \Phi)$ let the observable $X : \Omega \rightarrow \mathcal{X}$ represent the collection of all possible measurements that can be made of the system.

Let $Y : \Omega \rightarrow \mathcal{Y}$ represent “variables of interest”

* typically $\mathcal{Y} \subseteq \mathcal{X}$, but variables of interest may not be adequately measurable, in which case $\mathcal{Y} \not\subseteq \mathcal{X}$

* variables in \mathcal{X} that are not in \mathcal{Y} are sometimes called *exogeneous*

From definitions / assumptions, the physical system $(\Omega, \Sigma_\Omega, \nu, \Phi)$ generates the *true* dynamical processes (indices again correspond to observation time)

$$\begin{aligned} & \{ \dots, x_{-2}, x_{-1}, x_0, x_1, x_2, \dots \} \\ & \{ \dots, y_{-2}, y_{-1}, y_0, y_1, y_2, \dots \} \end{aligned}$$

THE PREDICTION PROBLEM

Denote *past* random variable $\overleftarrow{X} = \{\dots, X_{-2}, X_{-1}, X_0\}$ with realizations $\overleftarrow{x} = \{\dots, x_{-2}, x_{-1}, x_0\}$ represent observed series of measurements up to present time t_0

Similarly denote *future* random variable $\overrightarrow{Y}_\tau = \{Y_1, Y_2, Y_3, \dots, y_\tau\}$ with realizations $\overrightarrow{y}_\tau = \{y_1, y_2, y_3, \dots, y_\tau\}$ represent future values of variables of interest to lead time τ

deterministic prediction problem: find *target function* \mathcal{T}_τ that maps \overleftarrow{x} to \overrightarrow{y}_τ

$$\text{minimize } \|\mathcal{T}_\tau \circ \overleftarrow{x} - U^\tau Y\|_{L^2(\nu)}$$

R. Alexander and D. Giannakis, *Physica D: Nonlinear Phenomena* (2020)

probabilistic prediction problem: find *conditional distribution* $\text{pr}(\overrightarrow{Y}_\tau | \overleftarrow{X} = \overleftarrow{x})$

PREDICTIVE MODELS OF DYNAMICAL PROCESSES

Model dichotomy:

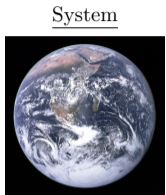
myopic models—learn target functions for finite τ (and finite-length pasts)

- ▶ (N)ARIMA(X)
- ▶ Analogue forecasting
- ▶ Neural networks (e.g. LSTM, TCN, RC, etc.)

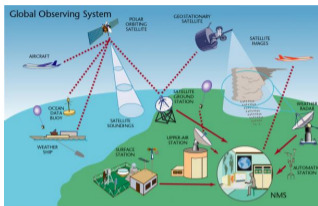
process models—generative models that approximate U (i.e. $\lim \tau \rightarrow \infty$)

- ▶ approximate action of U with surrogate dynamical system $\tilde{\Phi}_\alpha : \mathcal{X} \rightarrow \mathcal{X}$
- ▶ numerical simulations with discretization X and approximation scheme α
- ▶ complex physics simulations with analysis/assimilation \tilde{X} from measurements X with parameterizations α
- ▶ reduced-order models (ROMS)
- ▶ (generalized) Galerkin approximations of U

EXAMPLE: EARTH SYSTEM

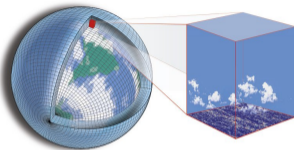


$$X : \Omega \rightarrow \mathcal{X}$$



(analysis / assimilation)

Simulation

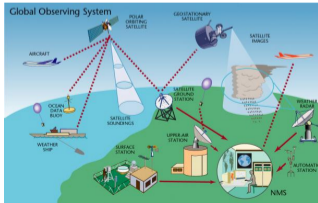


“data image”

Φ^t

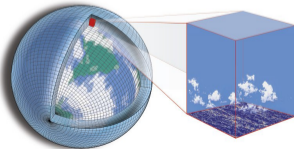


$$X : \Omega \rightarrow \mathcal{X}$$



$$\tilde{X}$$

$\tilde{\Phi}_\alpha^t$



$$\tilde{X}$$

$$X_t = U^t X$$

U^t

Credit: NASA-Apollo 17 crew

Credit: WMO

Credit: Tapio Schneider/Kyle Pressel/Momme Hell/Caltech

GALERKIN APPROXIMATIONS

EDMD: project U^t onto finite subspace spanned by dictionary $\Psi = [\psi^1, \dots, \psi^k]^T$

