A Quantum Mechanical Approach for Data Assimilation in Climate Dynamics

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Abstract

A framework for data assimilation in climate dynamics is presented, combining aspects of quantum mechanics, Koopman operator theory, and kernel methods for machine learning. This approach adapts the formalism of quantum dynamics and measurement to perform data assimilation (filtering), using the Koopman operator governing the evolution of observables as an analog of the Heisenberg operator in quantum mechanics, and a quantum mechanical density operator as an analog of probability distributions in Bayesian data assimilation. The framework is implemented in a fully empirical, data-driven manner by representing the evolution and measurement operators via matrices in a basis of kernel eigenfunctions learned from time-ordered observations. We discuss applications to data assimilation of Indo-Pacific SST and probabilistic forecasting of the Nino 3.4 index.

A Quantum Mechanical Approach for Data Assimilation in Climate Dynamics

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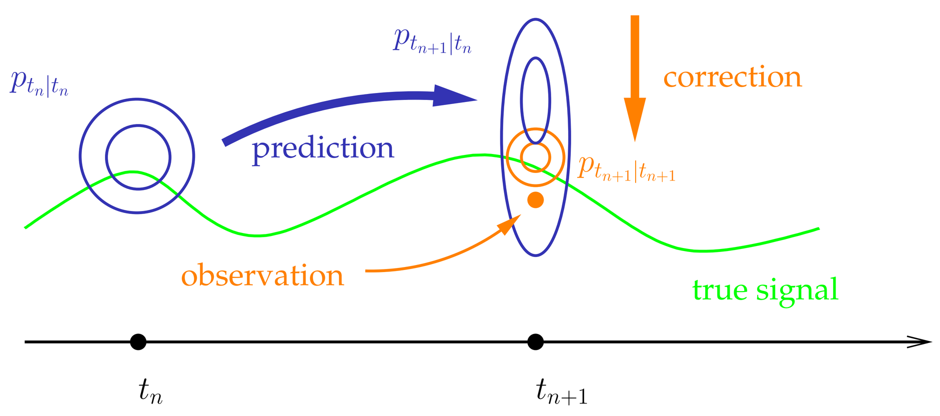
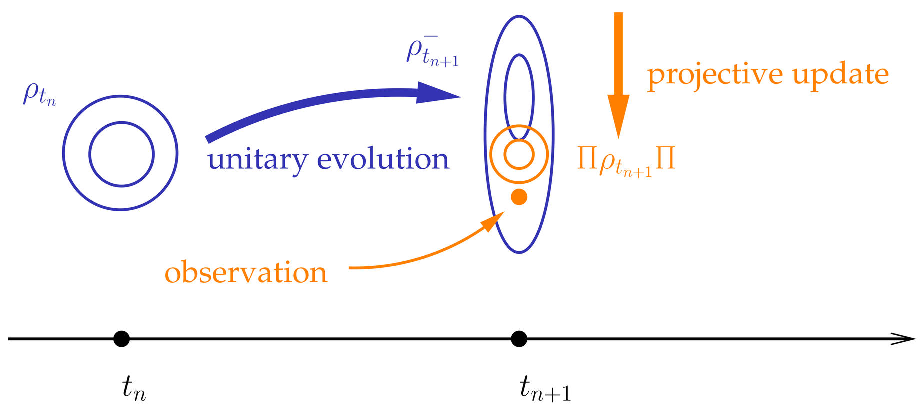
Motivation & Main Achievements

- **Sequential data assimilation** (a.k.a. **filtering**) is a predictor–corrector approach for state estimation and prediction of observables of dynamical systems. Among many applications, it is an integral part of **weather** and **climate forecasting systems**[1].
- Theoretical "gold standard" for filtering is computation of the **Bayesian posterior distribution**, given the full history of past observations of the system. However, this is oftentimes intractable, necessitating the use of *ad hoc* approximations, such as Gaussianity assumptions.
- We propose a new method[2,3] to address these issues, inspired from a conceptual similarity between data assimilation and **quantum mechanics**. Namely, both are inherently statistical theories, alternating between **evolutionary dynamics** between measurements, and **projective dynamics** during measurements.

Data assimilation



Quantum mechanics



- The **quantum mechanical data assimilation** (**QMDA**) framework is realized by mapping the assimilated dynamical system into a quantum system using **Koopman operator techniques**.
- A **data-driven formulation** is also constructed using **kernel methods** for machine learning, enabling data assimilation without prior knowledge of the equations of motion.

QMDA Framework

- We consider a dynamical system $\Phi^t : M \to M$ on a (unknown) state space M, preserving a probability measure μ (climatology). The system is observed at an interval Δt through a function $h : M \to \mathbb{R}$.
- The goal is to infer the probability distribution for future values of $v(t) = h(\Phi^t(x))$, given past measurements $v(t_n)$, $t_n = n\,\Delta t$.
- Associated with the dynamical system is the **Hilbert space of observables** (functions of the state) $L^2(\mu)$ and a group of unitary **Koopman evolution operators**[4]

$$U^t : L^2(\mu) \to L^2(\mu), \quad U^t f(x) = f(\Phi^t(x)).$$

- Following the quantum mechanical formalism, we represent the statistical state of the data assimilation system at time t by a **density operator** ρ_t on $L^2(\mu)$, such that

$$\rho_t \geq 0, \quad \operatorname{tr} \rho_t = 1.$$

This generalizes the notion of a probability distribution in Bayesian statistics.
- We represent the assimilated observable h by a self-adjoint **multiplication operator** T on $L^2(\mu)$, such that $Tf = hf$. This operator can be decomposed in terms of an **operator-valued measure** E, which generalizes the notion of a spectral measure in time series analysis, viz.

$$T = \int_{\mathbb{R}} \omega \, dE(\omega).$$

- Between measurements, $t_n \leq t < t_{n+1}$, the state ρ_t evolves by **unitary dynamics** under the action of the Koopman operator,

$$\rho_t = U^{\tau *} \rho_{t_n} U^\tau, \quad \tau = t - t_n.$$

The **probability distribution** for $v(t)$ to take values in a set $\Omega \subseteq \mathbb{R}$ is then given by

$$P_t(\Omega) = \operatorname{tr}(\rho_t E(\Omega)).$$

- If the measurement $v(t_{n+1})$ is found to lie in a set $\Xi \subseteq \mathbb{R}$, and the state immediately prior to t_{n+1} is $\rho^-_{t_{n+1}}$, the state $\rho_{t_{n+1}}$ immediately after the measurement is given by

$$\rho_{t_{n+1}} = \frac{E(\Xi)\rho^-_{t_{n+1}} E(\Xi)}{\operatorname{tr}(E(\Xi)\rho^-_{t_{n+1}} E(\Xi))}.$$

This **projection step** is analogous to the Bayesian update formula in classical statistics.

Data-Driven Approximation

- The scheme is implemented by **finite-rank approximation** (i.e., matrix representation) of all operators involved in a basis of $L^2(\mu)$ learned from training data using **kernel algorithms**[5,6].
- Given time-ordered training data $F(x_n)$ taken through a map $F : M \to \mathbb{R}^d$ on a dynamical trajectory $x_n = \Phi^{t_n}(x_0)$, we compute eigenfunctions $\phi_j(x_n)$ of a self-adjoint kernel integral operator $K : L^2(\mu) \to L^2(\mu)$,

$$Kf(x) = \int_M k(F(x), F(x')) f(x') \, d\mu(x'),$$

approximating integrals with respect to μ by **ergodic time averages**, i.e., $\int_M g(x)\, d\mu(x) \approx \sum_{n=0}^{N-1} g(x_n)/N$.
- Operators A on $L^2(\mu)$ are then represented by matrices,

$$A_{ij} = \langle \phi_i, A\phi_j \rangle_{L^2(\mu)} \approx \frac{1}{N} \sum_{n=0}^{N-1} \phi_i(x_n) A\phi_j(x_n).$$

The Koopman operator, in particular, is approximated by the **shift operator** for time series, $U^{q\,\Delta t}\phi_j(x_n) = \phi_j(x_{n+q})$.
- Given the corresponding values $v(t_n) = h(x_n)$ of the assimilated observable, we also approximate the spectral measure E by a **discrete measure** constructed through a histogram of the values of $v(t_n)$.

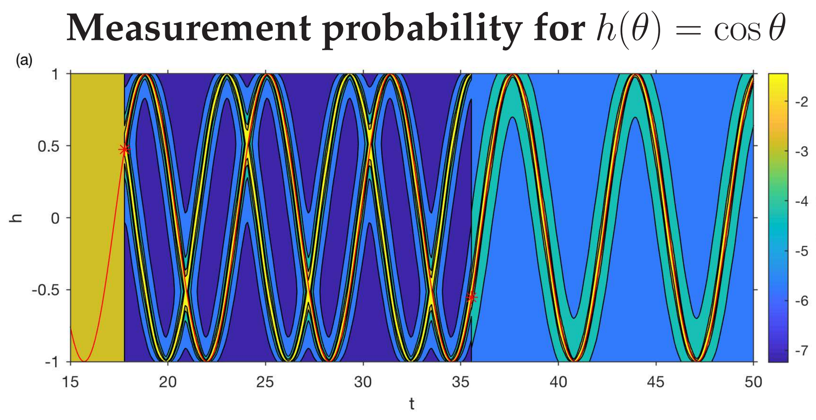
Comparison with Classical Methods

- By expressing data assimilation in terms of **intrinsically linear operators** for the dynamics (U^t), state (ρ_t), and measurement (T), QMDA avoids *ad hoc* approximations such as Gaussianity assumptions and diffusion regularization.
- The method outputs full probability distributions (P_t) in a nonparametric manner, as opposed to low-order moments (e.g., mean, covariance). The availability of P_t is useful for **risk assessment** and **uncertainty quantification**.
- Through basis projection, the cost of operator representation is decoupled from the ambient data space dimension and/or number of training samples.
- Unlike classical spectral approximation techniques, QMDA preserves sign and normalization of predicted probabilities.
- Rigorous **convergence results**[2] are obtained in a limit of infinite training data using techniques from linear operator theory in conjunction with spectral consistency results for kernel algorithms[7].

Periodic Dynamical System

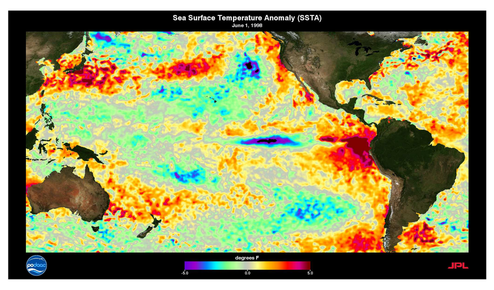
- Dynamical flow is a rotation on the circle $M = S^1$, $\Phi^t(\theta) = \theta + \nu t \mod 2\pi$.
- Assimilated observable is a trigonometric function, $h(\theta) = \cos\theta$.

Measurement probability for $h(\theta) = \cos\theta$



- QMDA starts from a stationary state ρ_0, corresponding to an uninformative (uniform) probability distribution P_0.
- When the first measurement is made, P_0 collapses to a **bimodal distribution**, consistent with the fact that $\cos\theta$ is a 2-to-1 function on the circle.
- When the second measurement is made, P_t collapses to a strongly peaked **unimodal distribution** that accurately tracks the true signal. This is consistent with the fact that two successive measurements of $\cos\theta$ are enough to uniquely infer θ.

El Niño Southern Oscillation



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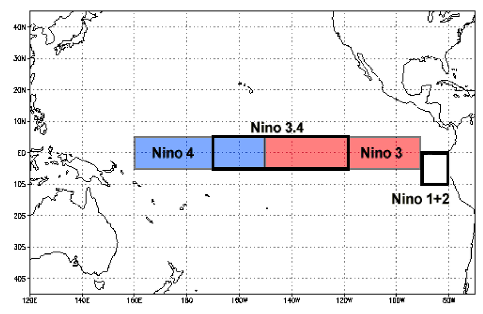
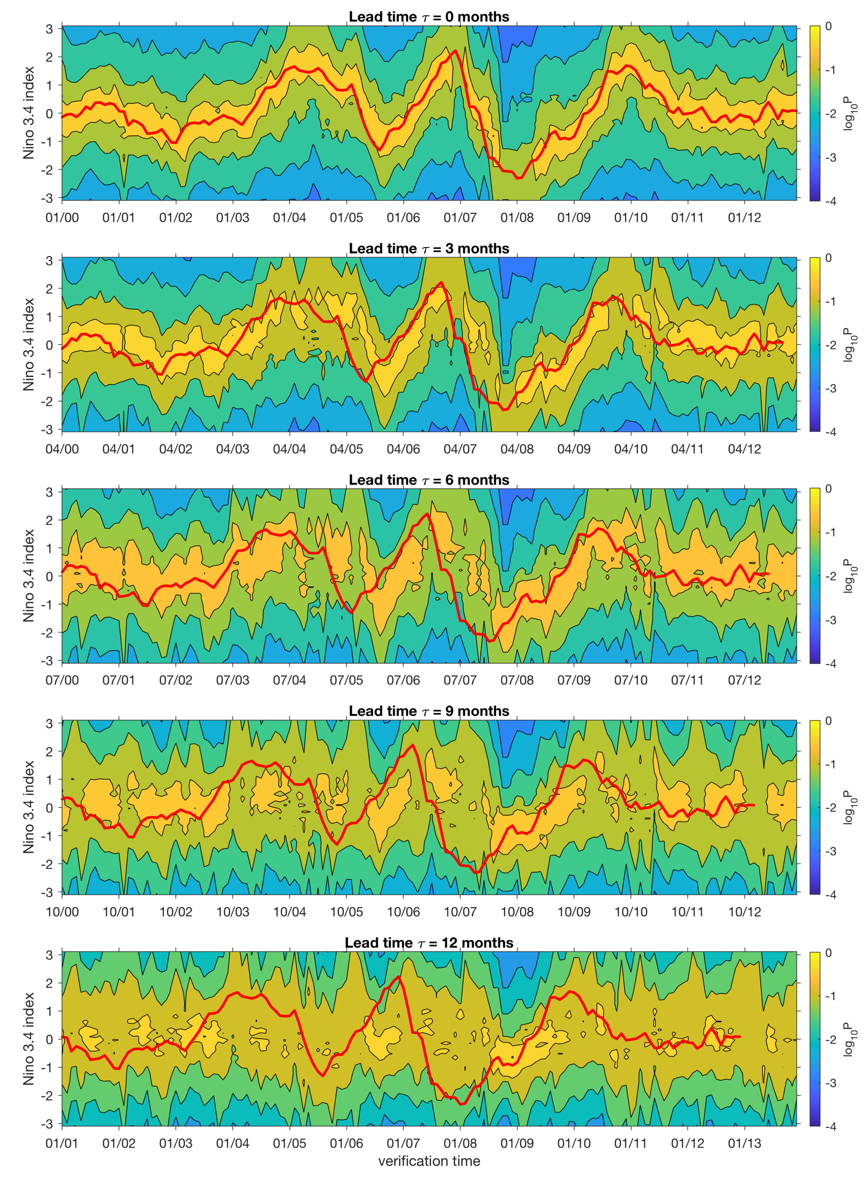


NOAA

- We apply QMDA to data assimilation of ENSO in the **Community Climate System Model Version 4 (CCSM4)**[8].
- Training data is 1200 years of monthly-averaged **Indo-Pacific SST** fields at 1° resolution ($d \simeq 10^4$ gridpoints).
- Verification data is the **Niño 3.4 index** over the last 100 years of the control integration.
- Assimilated observables (h) are the Niño 1+2, Niño 3, Niño 3.4, and Niño 4 indices, observed monthly.

Probability density P_t for Niño 3.4 index



- Starting from an uninformative (climatogological) distribution, the Niño 3.4 distribution P_t output by QMDA is seen to track the true signal.
- In addition to point forecasts (e.g., through the mean), P_t provides meaningful **uncertainty quantification**.
- **El Niño/ La Niña initiation** is oftentimes captured several months in advance. This suggests skillful **seasonal probabilistic ENSO prediction**.

Future Directions

- Extensions to high-dimensional observation functions using **multitask learning** techniques[9].
- Forecasting of ENSO impacts on the climate (e.g., **precipitation**, **sea ice**) and **socio-environmental systems**.
- Applications to closure and **stochastic subgrid-scale modeling** of unresolved dynamics.

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