

A Quantum Mechanical Approach for Data Assimilation in Climate Dynamics

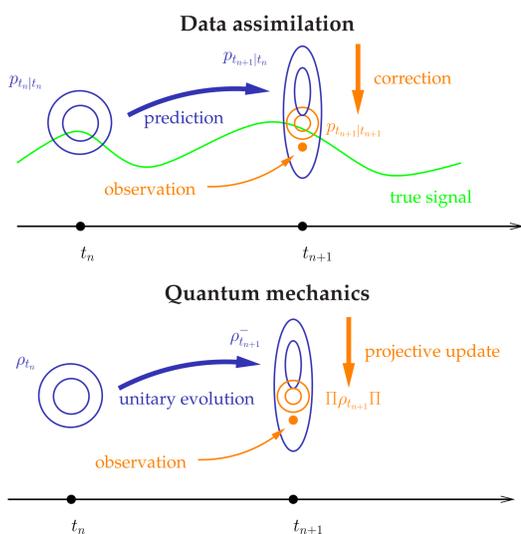
Joanna Slawinska,^{1,*} Abbas Ourmazd,^{1,†} Dimitrios Giannakis^{2,‡}

¹Department of Physics, U Wisconsin-Milwaukee, ²Courant Institute of Mathematical Sciences, NYU

*slawinsk@uwm.edu, †ourmazd@uwm.edu, ‡dimitris@cims.nyu.edu

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.



- 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 $\Phi^t : M \rightarrow M$ on a (unknown) state space M , preserving a probability measure μ . The system is observed at an interval Δt through a function $h : M \rightarrow \mathbb{R}$.
- 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

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

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

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

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

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

- If the measurement $v(t_{n+1})$ is found to lie in a set $\Omega' \subseteq \mathbb{R}$, 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

$$\rho_{t_{n+1}} = \frac{E(\Omega') \rho_{t_{n+1}}^- E(\Omega')}{\text{tr}(E(\Omega') \rho_{t_{n+1}}^- E(\Omega'))}.$$

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

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 $F : M \rightarrow \mathbb{R}^d$ 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 $K : L^2(\mu) \rightarrow L^2(\mu)$,

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

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, $U^q \Delta^t \phi_j(x_n) = \phi_j(x_{n+q})$.

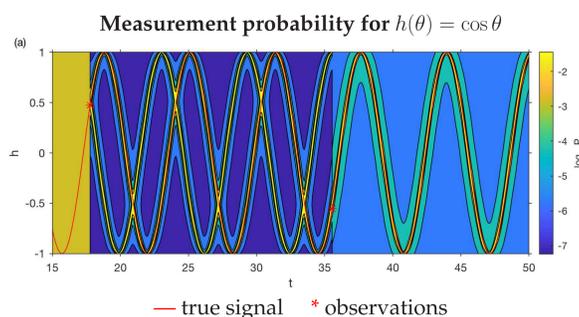
- Given the corresponding values $v(t_n) = h(x_n)$ of the assimilated observable, we also approximate the spectral measure E by a **discrete measure** constructed through a histogram of the values of $v(t_n)$.

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.
- 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 algorithms⁷.

Periodic Dynamical System

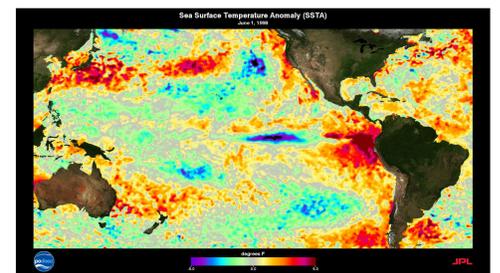
- Dynamical flow is a translation on the circle $M = S^1$, $\Phi^t(\theta) = \theta + \nu t \pmod{2\pi}$.
- Assimilated observable is a trigonometric function, $h(\theta) = \cos \theta$.



- 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 .

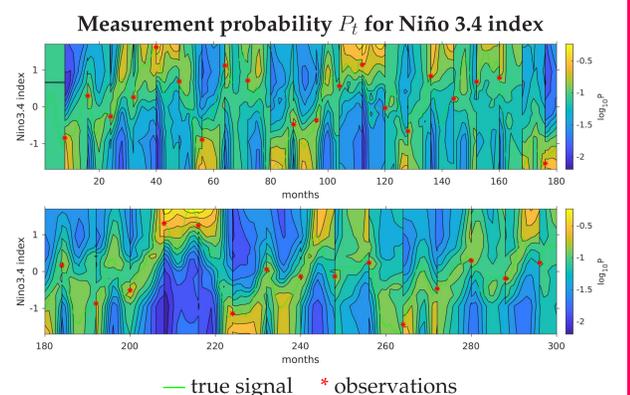
El Niño Southern Oscillation

- The **El Niño Southern Oscillation (ENSO)** is the dominant mode of variability of the Earth’s climate system on interannual (3–5 year) timescales⁸.
- It is manifested by an oscillation of sea surface temperature (SST) anomalies in the eastern equatorial Pacific, whose warm and cold phases are called **El Niño** and **La Niña** events, respectively.
- The occurrence of these events affects global weather patterns, as well as longer-term climate trends, causing considerable **socioeconomic impacts**.



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- We apply QMDA to simulated data from a 1200 year control integration the **Community Climate System Model Version 4 (CCSM4)**⁹.
- Training data is 1200 years of monthly-averaged **Indo-Pacific SST fields** at 1° resolution ($d \approx 10^4$ gridpoints).
- Verification data is the **Niño 3.4 index** (a standard proxy for ENSO activity) over the last 100 years of the control integration.



- Data assimilation of the Niño 3.4 index is performed at an interval of $\Delta t = 8$ months.
- Starting from an uninformative (uniform) probability distribution, QMDA progressively refines its predicted probability, accurately tracking the true signal.
- **El Niño/ La Niña initiation** is oftentimes captured several months in advance. This suggests skillful **seasonal probabilistic ENSO prediction**.

Future Directions

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

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