FINAL REPORT PROGRAM LEFE

Program LEFE/ MANU	Project Title: ADOTSAD Learning ocean models dynamics by semi-group theory approaches for data assimilation	Years 2020 – 2021

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Context

Ensemble variational data assimilation methods aim at seeking for the initial condition of a model such that the estimated state corresponds at best to some sparse and noisy observations. The optimisation is based on an ensemble of solutions of the model, but it still requires to run the expensive model during the process.

Objectives / scientific questions

The objective is to learn dynamical trajectories, by embedding the system state in a time-dependent reproducing kernel Hilbert space (RKHS) manifold transported by the dynamics. This confers an interpolatory property to the ensemble, and allows to link estimations between different times through the Koopman operator defined in this RKHS.

Main results

We have demonstrated that in the RKHS manifold, an isometry between a given time and the initial conditions leads to the fact that the kernel evaluations (but not the kernel) are conserved along the whole trajectories. As a consequence, an estimated state defined as linear combinations of ensemble members conserves these linear combinations along time. This leads to very efficient and robust data assimilation strategies, since a 4D-Var problem is transformed into a 3D-Var-like problem applied on full trajectories. It allows to benefit from observations taken at other times to perform estimations. Limitations of the procedure are quantified based on Lyapunov times associated with each Koopman eigenfunctions, thus maximizing the information content thanks to the expansion into Koopman eigenfunctions for which we have an exact evaluation at the ensemble members.

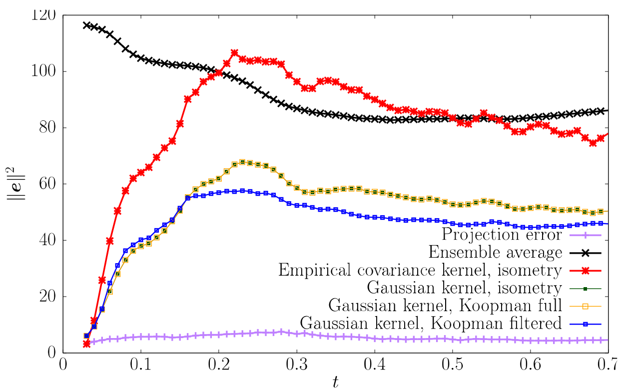

Fig. 1 : Prediction abilities of embedding a new initial condition in the RKHS manifold.

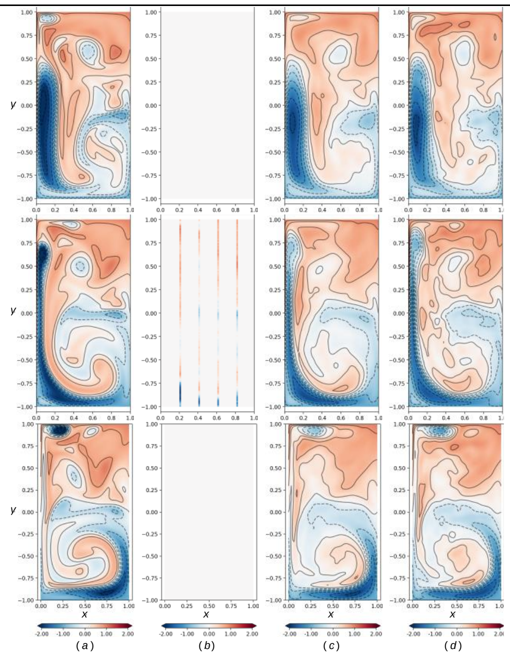

Fig.2: Data assimilation of barotropic quasi-geostrophic model. True state: a), observations: b), estimations: c) d).

The method has been tested with a barotropic quasi-geostrophic model of a double gyre typical of the north Atlantic large scale dynamics. With a simulated ensemble of trajectories (here 100 members), a kernel is built at the initial time, which measures in some sense the distances between the ensemble members. By isometry property, the kernel at later times is only known implicitly since its evaluations along the trajectories remains constant on the manifold. Once this space constructed, a new initial condition can be embedded in the RKHS at the initial time, thus defining a feature map. By construction, evaluations of this feature map at the ensemble members is directly inherited. As a consequence, an estimation of the whole trajectory is available, defined as linear combinations of ensemble members. Figure 1 shows estimation errors averaged over 100 new realisations. The projection error (violet), *i.e.* the best possible estimation, and the naïve estimation by the ensemble average (black) are reference bounds. We show that the use of a Gaussian kernel (yellow/green) leads to better performances than empirical covariance kernel (red). Moreover, we improve long-term predictions by filtering the estimation switching-off Koopman eigenfunction which have passed their Lyapunov predictability time (blue vs yellow curve). The method we propose allows to obtain estimations of a whole trajectory without having to run the numerical simulation.
Figure 2 shows data assimilation results based on estimations in the RKHS manifold. Panel a) is the true state to be estimated as a linear combination of the 100 ensemble members. Up to bottom figures are defined at times *t={0.04, 0.06, 0.08}* respectively. Panel b) are noisy sparse observations. Estimation knowing the observations only at time t=0.06 is shown in panel c), while having the observations at every time is shown in panel d). The data assimilation is very efficient since no direct-adjoint iterations are required because the times are linked between them through Koopman isometry, and only constant-in-time linear combination coefficients are sought. The optimization becomes robust since it strongly decreases the ratio between control parameters and observations. With this figure, we can show the consistency and the structuring behaviour of the built manifold, since estimations in panel c) are relevant even at times where no observation is available.

Future of the project :
We plan to apply the methodology to realistic numerical data. We are currently applying it to multi-layer quasi-geostrophic numerical simulations (Q-GCM) of a configuration similar to the north-Atlantic gulf-stream. The computational efficiency and the ability to take advantage of observations at different times makes it very attractive for improving optimal interpolation step in realistic configurations. Since the Koopman operator of the RKHS manifold associated with the dynamical system is learned locally in the phase space, it constitutes a strategy likely more adapted to realistic configurations than methods requiring the learning of the whole attractor of a system.

Publication :

- Bérenger Hug, Etienne Mémin and Gilles Tissot, *Ensemble forecasts in reproducing kernel Hilbert space manifold: dynamical systems in Wonderland* submitted to Journal of Computaional Physics (under review).

Conferences :

- Bérenger Hug, Etienne Mémin and Gilles Tissot, *Koopman eigenfunctions estimation from reproducing kernel Hilbert space manifold and ensemble forecasts: Dynamical systems in Wonderland.* Euromech colloquium Machine learning methods for prediction and control of separated turbulent flows, 16-18 June 2021, Paris, France

- Gilles Tissot, Etienne Mémin and Bérenger Hug, *Koopman eigenfunctions estimation from reproducing kernel Hilbert space manifold, and ensemble data assimilation*, European Geosciences Union (EGU) general assembly, Vienna, Austria, 23-27 May 2022