ERCIM "ALAIN BENSOUSSAN"
FELLOWSHIP PROGRAMME

Scientific Report

First name / Family name	Jia-Chen Hua
Nationality	China
Name of the *Host Organisation*	NTNU
First Name / family name of the *Scientific Coordinator*	Ole Morten Aamo
Period of the fellowship	01/04/2018 to 30/09/2018 (anticipated departure due to resignation)

I – SCIENTIFIC ACTIVITY DURING YOUR FELLOWSHIP

During my fellowship, the main research activity focused on the continuation and development of technical ideas originated during the last several weeks when I was in University of Luxembourg - right before I moved to NTNU to start my fellowship. The ideas were sufficiently developed to a novel theoretical framework that implements the Koopman-von Neumann (KvN) theory in reproducing kernel Hilbert space (RKHS) and generalizes it to nonlinear systems from being restricted to classical mechanics. Because of the connection between RKHS and Gaussian Processes for machine learning, this new theoretical framework has a statistical interpretation related to Gaussian Process regression, and it can be applied to spatio-temporal data analysis and modeling, time-series prediction, nonlinear system identification and control. It also has the potential to be utilized for classification, patterns recognition, and anomaly detection, when combined with other techniques in machine learning such as subspace learning and clustering.

The Koopman-von Neumann classical mechanics was originally introduced by Bernard Koopman and John von Neumann in 1930s as a reformulation of classical mechanics in terms of Hilbert space, in the same manner as formulating quantum mechanics. The idea was, however, not utilized and rarely investigated outside the scope of quantum physics, until 2004~2005 when Igor Mezić developed the modern theory of Koopman operator in the context of dynamical systems and functional analysis. Although it was a thorough theoretical investigation and further development of this idea, it differs from the original one of Koopman and von Neumann in that it deals with functions or observables of the system's state variables (and other theoretical aspects such as ergodicity), but it does not directly “lift” the system variables to a “state” in a manner similar to quantum mechanics as Koopman's and von Neumann's idea do with classical mechanics. And due to the limited computational power at that time, there was no numerical application of the modern Koopman operator theory, until in 2009 when an algorithm called Dynamic Mode Decomposition (DMD) was developed in fluid dynamics community for spatio-temporal data analysis, and was linked to the modern Koopman operator theory. However, DMD is effectively using the identity functions of each state variable (i.e., the most naïve and trivial basis functions) as the basis of the function spaces in modern Koopman operator theory. Hence, it is very restrictive and has numerical issues when applied both within and beyond the scope of fluid dynamics. Then in 2014~2015, the extended DMD algorithm (EDMD) was introduced and a kernel method based extension was implemented to use pre-defined and implicitly defined nonlinear basis functions, respectively. This was the first time when DMD and modern Koopman operator theory were related to techniques in machine learning.

The theoretical framework that I developed is a direct generalization of the original idea of Koopman and von Neumann lifting the system's state variables to a “quantum state”-like quantity, from being restricted to classical mechanics to being capable of describing nonlinear systems as the modern Koopman operator theory did in 2004~2005. Associated with this novel theoretical framework is the related numerical algorithms that implement the theory in RKHS, and hence the theoretical framework is readily applicable in data sciences. Specifically, this novel theoretical framework and the related algorithms:
(1) implement unitary time evolution of a nonlinear system in RKHS, which keeps one of the original features of the idea of Koopman and von Neumann, unlike the modern theory of Koopman operator developed in 2004~2005;
(2) have a statistical interpretation related to Gaussian Process regression, and hence relate the Copenhagen interpretation of quantum mechanics to Bayesian interpretation of Gaussian Processes in machine learning;
(3) provide an alternative to DMD and its extensions and variants for spatio-temporal data analysis and modeling, within and beyond fluid dynamics;
(4) provide a novel methodology for time-series prediction alternative to the Kernel KMR, which I developed before (DOI: 10.1007/s11071-017-3764-y), and can be combined with and complement Kernel KMR to improve prediction performance;
(5) provide a better technique to estimate the time derivatives from time series data than the modern Koopman operator theory (e.g., arXiv:1709.02003), by implementing the Heisenberg picture of KvN theory in RKHS that can overcome the numerical issues in arXiv:1709.02003, and hence can improve the performance of time derivatives estimation which is arguably the most crucial step in nonlinear system identification;
(6) provide an alternative methodology to modern Koopman operator theory for nonlinear control using linear algorithms (e.g., DOI: 10.1016/j.automatica.2018.03.046): utilizing the eigenfunctions of the unitary time evolution operator of KvN theory in RKHS, both discrete time and continuous time control can be implemented with computational costs comparable to those of conventional linear techniques such as MPC and LQR.

Besides these implemented applications in data analysis, machine learning, system identification and control, this novel theoretical framework and the related algorithms also have the potential to be further utilized for time series classification, patterns and dynamical scenes recognition, and anomaly detection, when combined with other techniques in machine learning such as subspace learning and clustering, and/or more advanced mathematics such as Algebraic Topology and Persistent Homology. These promising potentials would have been explored and investigated if I could continue the fellowship without resignation and early termination.

II – PUBLICATION(S) DURING YOUR FELLOWSHIP

Book chapter:

Hua, J.-C., Noorian, F., Leong, P.H.W., Gunaratne, G.H., Gonçalves, J., 2018. Prediction of High-Dimensional Time Series with Exogenous Variables Using Generalized Koopman Operator Framework in Reproducing Kernel Hilbert Space, in: Time Series Analysis and Forecasting: Selected Contributions from ITISE 2017, Contributions to Statistics. Springer Berlin Heidelberg. ISBN: 978-3-319-96943-5.

Abstract: We propose a novel methodology to predict high-dimensional time series with exogenous variables using Koopman operator framework, by assuming that the time series are generated by some underlying unknown dynamical system with input as exogenous variables. In order to do that, we first generalize the definition of the original Koopman operator to allow for input to the underlying dynamical system. We then obtain a formulation of the generalized Koopman operator in reproducing kernel Hilbert space (RKHS) and a new derivation of its numerical approximation methods, namely, Extended Dynamic Mode Decomposition (EDMD) and its kernel-based version. We also obtain a statistical interpretation of kernel-based EDMD developed for deterministic Koopman operator by utilizing the connection between RKHS and Gaussian processes regression, and relate it to the stochastic Koopman and Perron-Frobenius operator. In applications, we found that the prediction performance of this methodology is promising in forecasting real world high-dimensional time series with exogenous variables, including financial markets data. We believe that this methodology will be of interest to the community of scientists and engineers working on quantitative finance, econometrics, system biology, neurosciences, meteorology, oceanography, system identification and control, data mining, machine learning, computational intelligence, and many other fields involving high-dimensional time series and spatio-temporal data.

Journal paper in preparation:

Hua, J.-C., et al., Koopman-von Neumann theory in reproducing kernel Hilbert space, with applications to data analysis, machine learning, nonlinear system identification and control.

III – ATTENDED SEMINARS, WORKHOPS, CONFERENCES

Planned attendance at ERNSI Workshop 2018 on System Identification to present my work on Koopman-von Neumann theory in RKHS, but unfortunately not undertaken due to severe delay of UK visa approval.

IV – RESEARCH EXCHANGE PROGRAMME (REP)

Research exchange was planned for a visit to INRIA to study topological data analysis but unfortunately not undertaken due to resignation and early termination of the fellowship.