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A Schrödinger-type Formalism and Observable Wavefunctions in Dynamical Systems

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Abstract—There is recent interest in the use of Koopman (composition) operator theory for a wide range of problems in dynamical systems. In its dual, Perron-Frobenius theory, the use of invariant measures for understanding of statistical properties of dynamical systems is routine. A much less used concept is that of eigenmeasures [10]. We extend the theory related to eigenmeasures to introduce the notion of wavefunctions into dynamical systems theory. A wavefunction can be thought of as the density of a complex measure on the state space. It satisfies the common Perron-Frobenius equation. Using this, we derive a Shrödinger-type formalism for complex measure propagation on embeddings of dynamical system dynamics into the output space of an observable propagated by the Koopman operator. The resulting wavefunction is named an observable wavefunction (OW).

1. Introduction

Driven by success in operator-based framework in quantum theory, Bernard Koopman proposed in his 1931 paper [3] to treat classical mechanics in a similar way, using the spectral properties of an operator associated with the dynamical system evolution. Koopman extended this study in a joint work with von Neumann in [2]. Those works, restricted to Hamiltonian dynamical systems, did not attract much attention originally, as evidenced by the fact that between 1931 and 1963, the Koopman paper [3] was cited 25 times, according to Google Scholar. This can be attributed largely to the major success of the geometric picture of dynamical systems theory in its state-space realization advocated by Poincaré. In fact, with Lorenz's discovery of a strange attractor in 1963, the dynamical systems community turned to studying dissipative systems and much progress has been made since. Within the current research in dynamical systems, some of the crucial roadblocks are associated with high-dimensionality of the problems and necessity of understanding behavior globally (away from the attractors) in the state space. However, the weaknesses of the geometric approach are related exactly to its locality (it often relies on perturbative expansions around a known geometrical object) and low-dimensionality (it is hard to make progress in higher dimensional systems using geometry tools).

Out of today's 400+ citations of Koopman's original work, [3], 75% come from the last 20 years. Thus, it was only in the 1990's that potential for wider applications of the operator-theoretic approach has been realized [4, 7]. In this century the trend of applications of this approach has continued, as summarized in [1]. This is partially due to the fact that strong connections have been made between the spectral properties the Koopman operator for dissipative systems and the geometry of the state space. In fact, the hallmark of the work on the operator-theoretic approach in the last two decades is the linkage between geometrical properties of dynamical systems - whose study has been advocated and strongly developed by Poincaré and followers - with the geometrical properties of the level sets of Koopman eigenfunctions [7, 5, 6]. The operator-theoretic approach has been shown capable of detecting object of key importance in geometric study, such as invariant sets, but doing so globally, as opposed to locally as in the geometric approach. It also provides an opportunity for study of high-dimensional evolution equations in terms of dynamical systems concepts [8, 11] via a spectral decomposition, and links with associated numerical methods for such evolution equations [12].

In this paper we consider the propagation of observables under the Koopman operator and derive an equation for wavefunction evolution for such a propagation. We first define the notion of a wavefunction on the state-specе. Than we define a complex observable on the state space and consider the evolution of a complex measure associated with such an observable. The result is a Schrödinger-type formalism that couples the Koopman operator and the Peron-Frobenius operator state-space formalisms and extends them to embedding space of observable outputs. We pursue this in $1-D$ here, and will present the n-dimensional theory in a forthcoming paper.

2. Wavefunctions for Observable Evolution

Let $M = \mathbb{R}$ and $(x,t) \in R = \mathbb{R} \times \mathbb{R}$. Let v be a smooth vector field on $\mathbb{R}$. The wavefunction ρ (we will call it the true wavefunction or TW) satisfies

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0, \tag{1}$$

Let the observable $f : \mathbb{R} \to \mathbb{C}$ be defined by

$$f = e^{-iY}, \tag{2}$$

where $Y(x,t)$ is smooth (at least in C^2). This implies that the observable wavefunction (OW) ψ defined by

$$\psi = \frac{\rho}{i\frac{\partial Y}{\partial x} e^{iY}}. \tag{3}$$

is the density of a complex measure of the observable $f = e^{-iY}$ corresponding with the TW ρ, since

$$\frac{df}{dx} = i\frac{\partial Y}{\partial x} e^{iY}. \tag{4}$$

We proceed to derive an equation of evolution for ψ. We will denote partial derivatives with respect to t by $(\cdot)_t$ and partial derivatives with respect to x by $(\cdot)_x$.

We have

$$\begin{aligned} \psi_t &= \frac{\rho_t}{iY_x e^{iY}} + \rho\left(\frac{1}{iY_x e^{iY}}\right)_t \\ &= -\frac{v\rho_x}{iY_x e^{iY}} - \frac{v_x \rho}{iY_x e^{iY}} + \rho\left(\frac{1}{iY_x e^{iY}}\right)_t . \end{aligned} \tag{5}$$

From (3) we have

$$\rho_x = i\psi_x Y_x e^{iY} + i\psi Y_{xx} e^{iY} - \psi (Y_x)^2 e^{iY}, \tag{6}$$

and, as a consequence,

$$\frac{-v\rho_x}{iY_x e^{iY}} = -v\psi_x - \frac{v}{Y_x}\psi Y_{xx} - i\frac{v}{Y_x}\psi (Y_x)^2. \tag{7}$$

We also have

$$\begin{aligned} \left(\frac{1}{iY_x e^{iY}}\right)_t &= -\frac{1}{(iY_x e^{iY})^2}\left(iY_{xt}e^{iY} - Y_x Y_t e^{iY}\right) \\ &= -\left(\frac{Y_{xt}}{i(Y_x)^2 e^{iY}} + \frac{Y_t}{Y_x e^{iY}}\right), \end{aligned} \tag{8}$$

and thus

$$\begin{aligned} \rho\left(\frac{1}{iY_x e^{iY}}\right)_t &= -i\psi Y_x e^{iY}\left(\frac{Y_{xt}}{i(Y_x)^2 e^{iY}} + \frac{Y_t}{Y_x e^{iY}}\right) \\ &= -\psi\left(\frac{Y_{xt}}{Y_x} + iY_t\right). \end{aligned} \tag{9}$$

Collecting all of these, from (5) we get

$$\psi_t = -v\psi_x - \psi v_x - \frac{v}{Y_x} Y_{xx}\psi - \frac{Y_{xt}}{Y_x}\psi - i(Y_t + \frac{v}{Y_x}(Y_x)^2)\psi. \tag{10}$$

This is the equation that governs the observable wavefunction evolution. If the observable is real, with $Y = iK$, we get

$$\begin{aligned} \psi_t &= -v\psi_x - \psi v_x - \frac{v}{K_x}K_{xx}\psi - \frac{K_{xt}}{K_x}\psi + (K_t + \frac{v}{K_x}(K_x)^2)\psi \\ &= -v\psi_x - \psi v_x + (-\frac{v}{K_x}K_{xx} - \frac{K_{xt}}{K_x} + (K_t + \frac{v}{K_x}(K_x)^2))\psi \\ &= -v\psi_x - \psi v_x + (K_t - \frac{v}{K_x}(K_{xx} - K_x^2) - \frac{K_{xt}}{K_x})\psi. \end{aligned} \tag{11}$$

3. Conclusions

We have derived a wavefunction formalism for continuous-time dynamical systems in $1D$. The theory developed here leads to Schrödinger-type equations for evolution of constant speed on a 1-dimensional Riemannian manifolds [9]. It also admits generalization to higher dimensions. The formalism provides a coupling betweem Koopman operator theory - evolving observables - and Schrödinger operator theory - evolving densities - for embeddings of dynamical systems.

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