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A probabilistic foundation for dynamical systems: phenomenological reasoning and principal characteristics of probabilistic evolution

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Abstract This paper is the second in a series of two. The first paper has been devoted to the detailed explanation of the mathematical formulation of the underlying theoretical framework. Specifically, the first paper shows that it is possible to construct an infinite linear ODE set, which describes a probabilistic evolution. The evolution is probabilistic because the unknowns are expectations, with appropriate initial conditions. These equations, which we name, Probabilistic Evolution Equations (PEE) are linear at the level of ODEs and initial conditions. In this paper, we first focus on the phenomenological reasoning that lead us to the derivation of PEE. Second, the aspects of the PEE construction is revisited with a focus on the spectral nature of the probabilistic evolution. Finally, we postulate fruitful avenues of research in the fields of dynamical causal modeling in human neuroimaging and effective connectivity analysis. We believe that this final section is a prime example of how the rigorous methods developed in the context of mathematical chemistry can be influential in other fields and disciplines.

Keywords Dynamical systems · Probability · Expectation values · Ordinary differential equations · Quantum dynamics

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1 Introduction

In the first paper in this series, we show that an infinite set of ODEs with linear initial conditions can characterize the evolution of the expectation values for the elements in a set of basis operators [1]. We call these equations "Probabilistic Evolution Equations (PEE)". The first paper is focused on the comprehensive description of the construction of PEEs. We also incorporated the utility of considering mathematical fluctuations in the initial conditions that accompany the PEE.

Our intuition for the PEE is based on a number of insights that are part of widely researched areas such as quantum dynamics and nonequilibrium statistical dynamics as proposed and developed by Liouville. In our earlier works we have explored certain relationships that subtend the theoretical framework described in the first paper [2–6]. We will not go into the details of these items here, however we incorporate the intuition that guided our earlier work into the section of the paper where we discuss applications of this approach in the areas of dynamic causal modeling in neuroscience. In fact, we devote two sections to the PEE and its spectral nature as well as its potential applications in dynamical causal modeling in neuroscience.

This paper is organized as follows. The second section covers the phenomenological intuition underlying the work. The third section focuses on various practical and methodological issues in PEEs. The fourth section describes how PEE can be applied to dynamical causal modeling as it is used in neuroscience. The fifth section finalizes the paper with concluding remarks.

2 Phenomenological reasoning

One of our biggest sources of inspiration comes from the concept of measurement. Scientific discovery based on empirical research relies on information obtained from objects and events that take place in the world. Measurement gathers information by using two basic components: the device that measures the observables and the information carrying agent. The device often has a number of limitations. Take the human visual system for instance. An electron is too small for the resolution with which the human eye obtains information from the world. On the other hand, the spherical shape of the earth is also not noticable by the human that is not sufficiently elevated from the earth's surface. In this sense, the sensitivity of the human visual system can be characterized by an interval ranging from milimeter to tens of kilometers. Extending this analogy, it can be intuitively said that a device is capable of capturing representative information only if the observables can be distinctly conceptualized and differentiated within its sensitivity interval. Otherwise, information loss is bound to happen. This loss of information will manifest itself as uncertainty. In fact, since there is no measurement device which has an infinite interval of sensitivity, uncertainty is bound to appear at some aspect of the measured information. The key issue is whether this uncertainty influences the process of scientific discovery and inference.

The device cannot gather information in isolation and by itself. It needs an information carrying agent. In the case of the human visual system, or any other visual device such as a microscope, the information is carried by light and therefore photons. In the case of the electron microscope and the radio telescope, the information carrying agent is the electron and the radio wave. It is easy to see that, the information carrying agent has a significant influence on the sensitivity of the measurement device that relies on it. It is important to emphasize that the information carrying agent can actually have more information than the device that relies on it. For instance, the photons that fall on the human retina might actually contain more information than what the human visual system makes of them. In this sense, the information transferred during the action of measurement depends on the interplay between the information carrying agent and the measurement device.

It is also important to consider the source of the information and the way in which it interacts with the measurement device and the information carrying agent. Let's take two hypothetical cases. In the first case, the information source generates the carrying agent. Following our analogy of the human visual system, it is easy to see that a light bulb is both a source of information and the generator of the information carrying agent when the individual is observing it. In the second case, the information carrying agent is generated by another source, but the measurement device is sensitive to how that particular agent interacts with the source of information. Following our example of the human visual system, this would be perception of a rock. The information carrying agents, in this case photons, are generated by the sun. The measurement device measures the way in which these photons reflect off the surface of the rock. We can extend this analogy further to give you an even better idea of the source of uncertainty. Consider a blind individual who is using braille in order to obtain information about the world surrounding him or her. In this case, every act of tactile sensation involves touching a particular object, therefore potentially changing its unperturbed state. It is easy to see how the uncertainty information depends on a number of factors. The important issue is the degree to which the observers and the agents interact with each other. Furthermore, if there is drastic size differences between the agents and the observers, the interactions might be too minute to be noticed. For instance a macro level observer might not be able to sensitively observe the interaction of two or more micro (at a level that cannot be perceived) systems. All measurements contain some level of uncertainty. The goal of strong inference in science is to advance theoretical development such that these uncertainties can be estimated.

The realm of quantum phenomena is rife with such examples of uncertainty. Let us itemize some of these below:

- 1. The position and momentum of an electron can not be precisely and simultaneously observed. This is due to the uncertainty principle of Heisenberg and minimum uncertainty is determined by Planck's universal constant.
- 2. The situation in (1) is not the only example. There are some property pairs whose values can not be precisely known at the same time instant. The pair of time and energy is one of the other examples to this.
- 3. There is a deviation in the expectation value of an observable square from the square of the expectation value of the same observable itself. This is fluctuation and does not exist in classical mechanics.
- 4. The deviation in (3) decreases as the physical dimension of the particle increases towards macro levels.

- 5. It is not possible to define a precise orbit for particles as done in classical mechanics. There is no simple trajectory for them. Instead, the probability of residing in some spatial region emerges. This description corresponds to a pulsing probability cloud.
- 6. Sufficiently small particles can produce interference patterns under certain appropriate conditions. This is due to wave-particle duality which dictates that the considered particle behaves as a wave or a solid structure depending on the nature of the event concerned.

It is also important to consider properties of systems that emerge from interactions between populations of subsystems. For example, it is very well known that a given amount of gas spontaneously and homogeneously fills a closed and empty vessel. In this case, the population is at the level of Avogadro number and makes the tracing of individual molecules impossible. Often this feature of the system leads to uncertainty. However, it is feasible to consider the whole system as a unitary object or a collection of a few objects by using statistical and probabilistic approaches. These kinds of events are called "Stochastic Processes" and the systems are named "Stochastic Systems" and rely heavily on probability theory. Another example of a stochastic process can be taken from physics. When an empty container is being filled with a gas, after a certain period of time, the same amount of pressure is exerted on all points of the container. This emergent equivalence can only be explained using probabilistic considerations.

Neuroscience is also rife with examples of such emergent processes. Take the example of the experience of emotion for instance. An experience of happiness might be subtended by a myriad of different activation patterns in the human brain [7]. In some cases, there is a focus on the pleasant scenery or scent that is perceived. In other cases, a subtle memory that is spontaneously recalled can bring our mind to a pleasant state. Experiences are constructed as multiple brain systems interact. One experience can be subtended by multiple brain states and a brain state can be associated with multiple experiences depending on the context in which they take place. For instance, simply hearing gossip about an individual is sufficient to change the basic way in which that individual's face is perceived [8]. In fact, dynamical causal modeling of interactions between brain systems have been used for investigating topics such as these.

3 Spectral and other important aspects of probabilistic evolution

Consider a dynamical system whose evolution can be given by the following ODEs and initial conditions

$$\dot{x}_i = f_i(x_1(t), \dots, x_n(t)), \quad x_i(0) = \overline{x}_i, \quad i = 1, 2, \dots, n$$
 (1)

The evolution operator (Hamiltonian) for this system is defined as follows

$$\widehat{E} = \sum_{j=1}^{n} \frac{1}{2} \left\{ f_j\left(\widehat{x}_1, \dots, \widehat{x}_n\right) \widehat{p}_j + \widehat{p}_j f_j\left(\widehat{x}_1, \dots, \widehat{x}_n\right) \right\}$$
(2)

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where \hat{x}_j and \hat{p}_j stand for the position and momentum operators respectively. The position operator (say \hat{x}_j) multiplies its operand by the relevant scalar independent variable (x_j) while the *j*th momentum operator is related to differentiation with respect to x_j as follows

$$\widehat{p}_j \equiv -i\frac{\partial}{\partial x_j}, \quad j = 1, 2, \dots n$$
(3)

We may define the $\xi_i(t)$ function as the expectation value of the operator \hat{x}_i as follows

$$\xi_i(t) \equiv \langle \widehat{x}_i \rangle (t) \equiv \int_{-\infty}^{\infty} dx_1 \dots \int_{-\infty}^{\infty} dx_n \psi^* (x_1, \dots, x_n, t) \, \widehat{x}_i \psi (x_1, \dots, x_n, t)$$

$$i = 1, 2, \dots, n$$
(4)

where ψ (x_1 , ..., x_n , t) stands for the wave function satisfying the following partial differential equation

$$i\frac{\partial\psi(x_1,\ldots,x_n,t)}{\partial t} = \widehat{E}\psi(x_1,\ldots,x_n,t)$$
(5)

Note that it is not necessary to solve this PDE because the wave function is never explicitly used in this framework. As we describe in the companion paper, the following equality can be written for the time derivative of $\xi(t)$ s

$$\dot{\xi}_j(t) = \left(\psi(t), \left\{ i \left[\widehat{E}\widehat{x}_j - \widehat{x}_j \widehat{E} \right] \right\} \psi(t) \right), \quad j = 1, 2, \dots, n$$
(6)

Now, by appropriately using (2) in this equality, it is not hard to see that the following equalities hold

$$\dot{\xi}_j(t) = \langle f_j(\widehat{x}_1, \dots, \widehat{x}_n) \rangle(t), \quad j = 1, 2, \dots, n$$
 (7)

If we consider the following Maclaurin expansion of f_i

$$f_{j}(\widehat{x}_{1},...,\widehat{x}_{n}) = \sum_{k_{1}=0}^{\infty} \cdots \sum_{k_{n}=0}^{\infty} f_{k_{1},...,k_{n}}^{(j)} \widehat{o}_{k_{1},...,k_{n}}, \quad \widehat{o}_{k_{1},...,k_{n}} \equiv \widehat{x}_{1}^{k_{1}} \widehat{x}_{2}^{k_{2}} \dots \widehat{x}_{n}^{k_{n}},$$

$$j = 1, 2, \dots, n$$
(8)

then, from (7), we can write

$$\dot{\xi}_{j}(t) = \sum_{k_{1}=0}^{\infty} \cdots \sum_{k_{n}=0}^{\infty} f_{k_{1},\dots,k_{n}}^{(j)} \eta_{k_{1},\dots,k_{n}}(t), \quad \eta_{k_{1},\dots,k_{n}}(t) \equiv \left\langle \widehat{o}_{k_{1},\dots,k_{n}} \right\rangle(t),$$

$$j = 1, 2, \dots, n \tag{9}$$

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which urges us to construct an ODE for $\eta_{k_1,...,k_n}(t)$. To this end we can trace the same route we have used above and get

$$\dot{\eta}_{k_1,\dots,k_n}(t) = \left\langle \tilde{f}_{k_1,\dots,k_n}(\widehat{x}_1,\dots,\widehat{x}_n) \right\rangle(t), \quad j = 1, 2, \dots, n$$
 (10)

where

$$\widetilde{f}_{k_1,\dots,k_n}(x_1,\dots,x_n) \equiv \sum_{j=1}^n k_j x_1^{k_1}\dots x_{j-1}^{k_{j-1}} x_j^{k_j-1} x_{j+1}^{k_{j+1}}\dots x_n^{k_n} f_j(x_1,\dots,x_n)$$
(11)

and we can use the following Maclaurin expansion

$$\widetilde{f}_{k_1,\dots,k_n}(x_1,\dots,x_n) = \sum_{\ell_1=0}^{\infty} \cdots \sum_{\ell_n=0}^{\infty} E_{k_1,\dots,k_n;\ell_1,\dots,\ell_n} x_1^{\ell_1} \dots x_n^{\ell_n}$$
(12)

which implies

$$\widetilde{f}_{k_1,\dots,k_n}\left(\widehat{x}_1,\dots,\widehat{x}_n\right) = \sum_{\ell_1=0}^{\infty}\cdots\sum_{\ell_n=0}^{\infty} E_{k_1,\dots,k_n;\ell_1,\dots,\ell_n}\widehat{o}_{\ell_1,\dots,\ell_n}$$
(13)

whose utilization in (10) gives

$$\dot{\eta}_{k_1,\dots,k_n}(t) = \sum_{\ell_1=0}^{\infty} \cdots \sum_{\ell_n=0}^{\infty} E_{k_1,\dots,k_n;\ell_1,\dots,\ell_n} \eta_{\ell_1,\dots,\ell_n}(t)$$
(14)

and the initial conditions

$$\eta_{k_1,\dots,k_n}(0) = \overline{x}_1^{k_1}\dots\overline{x}_n^{k_n}, \quad k_1,\dots,k_n = 0, 1, 2,\dots$$
(15)

 $E_{k_1,...,k_n;\ell_1,...,\ell_n}$ coefficients can be generated from the $f_{k_1,...,k_n}^{(j)}$ coefficients through (11) and (8) by using the Cauchy product formula for series multiplications. (14) and (15) describe the initial value problem of the infinite linear ODE we call "Probabilistic Evolution Equation (PEE)". $\eta_{k_1,...,k_n}(t)$ stands for an *n*-way array (multilinear array). Its indices play the role of the column index of an ordinary linear algebraic vector. It is possible to convert it to a one-index array, or in other words, a vector, by using "Unfolding". This urges us to call $\eta_{k_1,...,k_n}(t)$ "Folded Vector" simply "Folvec". Its time dependence urges us to use a more appropriate terminology and we can say "Folvec Valued Function". We are going to denote this folvec by $\eta(t)$ in shorthand notation as we do for vectors and matrices in ordinary linear algebra.

We can analogously call the multilinear array $E_{k_1,...,k_n;\ell_1,...,\ell_n}$ "Folmat" since its $k_1, ..., k_n$ and $\ell_1, ..., \ell_n$ indices respectively play the role of row and column indices of a matrix in ordinary linear algebra. We denote this folmat by **E**.

We are going to use $\eta(t)$ and **E** to refer to folded and unfolded forms depending on our needs. Now we can write the PEE as follows

$$\dot{\boldsymbol{\eta}}(t) = \mathbf{E}\boldsymbol{\eta}(t), \quad \boldsymbol{\eta}(0) = \overline{\mathbf{x}}$$
(16)

where the folvec $\bar{\mathbf{x}}$ is composed of given initial values. (16) can be conceptualized via matrices and vectors of ordinary linear algebra. It can also be considered in terms of folmats and folvecs or under a more general multilinear algebraic name "Folarr"s (Folded Arrays, Multilinear Arrays). In each case slightly different but parallel interpretations can be made. We call the linear algebraic case discussions "Ordinary Interpretation" while the other case will be called "Folarr Interpretation".

Let us focus on the ordinary interpretation for this portion. It is better to use finite truncations of (16) from left uppermost part to efficiently handle infinity. We can write

$$\dot{\boldsymbol{\eta}}_m(t) = \mathbf{E}_m \boldsymbol{\eta}_m(t), \quad \boldsymbol{\eta}_m(0) = \overline{\mathbf{x}}_m \tag{17}$$

where the nonnegative integer m stands for the truncation order. If the algebraic and geometric multiplicities of all eigenvalues are the same, then the following spectral decomposition for \mathbf{E}_m can be written.

$$\mathbf{E}_m = \sum_{i=1}^m \varphi_i \mathbf{r}_i \mathbf{l}_i^{\dagger}$$
(18)

where φ s, **l**s and **r**s represent the eigenvalues, left and right eigenvectors respectively. There are as many eigenvalues as their multiplicities. Each pair of eigenvectors is mutually normalized to make the corresponding outer product a projection matrix. Hence $\mathbf{r}_i^{\dagger} \mathbf{l}_i = 1$ The dagger symbol stands for the Hermitian conjugation operation. In the case where certain multiple eigenvalues' algebraic and geometric multiplicities differ, sufficiently many Jordan blocks should be added to the right hand side of (18).

Now the solution of (17) can be written as follows

$$\boldsymbol{\eta}_m(t) = \mathrm{e}^{t\mathbf{E}_m} \bar{\mathbf{x}}_m = \sum_{i=1}^m \left(\mathbf{l}_i^{\dagger} \bar{\mathbf{x}}_m \right) \mathrm{e}^{\varphi_i t} \mathbf{r}_i \tag{19}$$

which corresponds to the case where Jordan blocks do not exist. The form that contains Jordan blocks has a similar structure but it also includes some terms which include exponential times t powers. This is an explicit result in terms of spectral entities. We call the set φ s "Probabilistic Spectrum" of the dynamical system under consideration while the left and right eigenvectors of \mathbf{E}_m are named "Evolutionary Basis Vectors " of the same dynamical system. Within this philosophy we call \mathbf{E} and \mathbf{E}_m "Evolution Matrix" and "Truncated Evolution Matrix" of the considered dynamical system. What we have presented above has been in fact the spectral properties of the Truncated Evolution Matrix. It is possible to analyze the stability of this probabilistic evolution, however considering the well established nature of theory on linear ODE sets, we will be skipping it here. The PEE in (16) is unique for the starting functional structure of the original ODE set defined through f functions. However it is always possible to convert x variables to some other coordinates as long as the conversion's Jacobian Matrix remains nonsingular. A different PEE appears for the new coordinates such that the Evolution Folmat has a more appropriate structure to handle the equations for numerical purposes. The effect of such a coordinate transformation on the spectrum of the evolution folmat is an important issue worth investigation. We may expect that this spectrum remains unchanged under such transformations.

One other important issue here is the case where m goes to infinity. As long as the spectrum remains discrete, everything seems to be nonproblematic. However it is a strong possibility that some of the eigenvalues can densely populate on certain curves or even on some regions in the complex plane of the eigenvalue parameter depending on the dynamical system under consideration. If this happens then continuous spectra can arise. The analysis then becomes more cumbersome, and, more careful and rigorous analyses may be needed. We will not focus on this within this paper. It is one avenue of research we intend to pursue in the future.

Second important point is about the initial values. The solution vector $\eta(t)$'s elements are related to each other by power relations over the operators whose expectations are under consideration. Thus we can expect to see similar relations amongst their initial values. Whether this relationship will exist depends on the initial conditions and existence of similar relationships between elements of at least one eigenvector. It is possible that at least one eigenvector possesses such a property. If the initial value vectors are in the subspace of such eigenvectors, then the problem under consideration is fluctuation free. Otherwise a mathematical fluctuation analysis should be conducted. There is seminal work on this topic by the research group of the second author of this paper [9–12].

Another striking property is the number of the independent parameters in the Maclaurin series coefficients. Of course, finite and small number of parameters will facilitate the analysis. This happens when the f functions are restricted to multinomials and especially second degree multinomials. A couple of papers [13, 14] by the second author of current paper put light on this issue. It is shown that all first order sets of ODEs can be converted to first order sets of ODEs but this time with the second degree multinomial right hand side functions.

In the case of folarr interpretation, the situation is different. Although there have been many important developments [15–20], generally, all efforts are focused on getting a multilinear singular value decomposition (SVD). This is primarily because of the utility of traditional SVD in ordinary linear algebra and well known methods such as principal component analysis. While this framework is useful, it is important to consider novel decomposition approaches that are more appropriate for the discussion at hand. These approaches are lead by the group of the second author and are based on High Dimensional Model Representation and Enhanced Multivariance Product Representation [21–26].

For the current section, we do not intend to go beyond this level of information about probabilistic evolution.

4 Application possibilities for dynamical causal modeling of neuroscience

This work is largely motivated by questions of connectivity and causality as they are conceptualized in neuroscience. In this field, one of the most prominent approaches is Dynamic Causal Modelling [27,28]. In this framework, the main goal is to estimate model parameters and use these parameters to describe and compare the temporal causality in the system. These quantitative findings are used to make qualitative inferences about human brain function and organization. In fact, the first two authors of this paper have been developing efficient algorithms for estimation within this framework [29,30]. In this section, we expand upon this previous work and consider the possibility of stability analysis in the context of Dynamic Causal Modeling.

We focus on the quadratic dynamic causal modeling as being the simplest nonlinear form in vector format

$$\dot{\mathbf{z}}(t) = \left(\mathbf{A} + \sum_{i=1}^{m_1} u_i(t) \mathbf{B}_i + \sum_{j=1}^{m_2} z_j(t) \mathbf{C}_j\right) \mathbf{z}(t) + \mathbf{R}\mathbf{u}(t)$$
(20)

where $\mathbf{z}(t)$ denotes an n_1 -element vector and characterizes the considered system's state while $\mathbf{u}(t)$ stands for an n_2 -element temporally varying vector and reflects the influence of external agents on the system. **A**, **B**_i s, and **C**_is are all square matrices of $n_1 \times n_1$ type. On the other hand **R** denotes an $n_1 \times n_2$ type rectangular matrix. These matrices are not derived based on theory, in that sense they are exploratory. These matrices are to be estimated by using data obtained from certain experimentations. We are not going to focus on how those entities are estimated here. However, interested readers can read the proceedings papers of first two authors that describe the estimation procedure [29, 30].

We can now consider the probabilistic evolution underlying the system defined by (20). The ODEs in this set of equations are quadratic with respect to the unknown vector. This feature makes the Evolution Matrix rather simple. However, the presence of a temporal function structure by $\mathbf{u}(t)$ makes the equations nonautonomous. This lack of autonomy can be removed via increasing the number of unknowns. However, this possibly brings high level nonlinearity to the $\mathbf{u}(t)$ dependent terms. The convergence of the truncations in probabilistic evolution may be negatively influenced from this.

On the other hand, we can divide the evolution's time interval to appropriately chosen subintervals and then approximate $\mathbf{u}(t)$ by lower degree splines. This is followed by autonomization of the equations for each subinterval and then what we have told in the previous section can be applied on the resulting equations. This enormously decreases the number of parameters in the probabilistic evolution and very high level of convergence can be achieved. It also becomes possible to make an efficient stability analysis enabling us for better characterization of the system under consideration. We believe that certain applications of these ideas will be attempted pretty soon.

The concept of stability in neuroscience is in fact quite elusive. One of the primary reasons for this is that there is no functional description of human brain function which is universal. The absence of such a representation makes it impossible to have a meaningful and canonical analysis of the overall stability of the system that is generalizable.

Furthermore, since brain function is heavily situated and dependent on the context in which it operates, the equations that characterize the functioning of the system become nonautonomous making it impossible to use traditional linear algebraic approaches to analysis of the system's stability. As it is described in the previous paragraph, the framework described in this and the companion paper makes it possible to analyze the stability of the nonautonomous dynamical systems that are often used to characterize causality and effective connectivity in the human brain.

5 Concluding remarks

This paper is the final portion of the theoretical framework that we propose and describe. Specifically, in this paper, we emphasized the underlying phenomenological intuition and provided a meaningful description of the characteristics of probabilistic evolutions.

The most important contribution seems to be that all explicit ODEs with initial conditions have infinite linear representations which we named probabilistic evolution equations (PEE). We believe that this is a stunning finding and opens a field rife with potential for exploration. Furthermore, this framework can be used to explain theoretical puzzles in multiple disciplines, therefore casting fruitful bridges for the interdisciplinary cross pollination of ideas, principles and methods. We will continue this line of work investigating ways in which one can reach similar conclusions to those introduced in this paper using nonprobabilistic tools. It is ironic that intuitions and methods developed to study extremely micro level phenomena can inform and guide investigations of macro level phenomena as human brain function and experience. We believe that a number of important developments using this theoretical framework are at the horizon.

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