The State Space Approach to Evolution

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Abstract
Mathematical models of dynamical systems typically employed in modern science are based on a very simple paradigm: the system has a state and an environment, and the time rate of change of the state is a function of the state and the environment. This function is a known mathematical function, and the system evolution if possible is studied under the assumption that the environment stays constant.

This paradigm, derived originally from Newton's Second Law, is one of the greatest achievements of science. It has been used with overwhelming success to describe a vast range of phenomena in nature. However, its apparent simplicity belies its true nature.

The paradigm serves to unify extremely diverse conceptual structures, subjecting them to mathematical treatment in a common language while scarcely limiting their reach. In this paper we illustrate this fact by offering examples of the paradigm of different types, showing how widely it has been used, and how little restriction it imposes on nature. We also propose some generalizations that have rarely been seen outside pure mathematics. Finally we note that the essential value in this paradigm is to be found in both its malleability and its relation to mathematics and quantity.
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1 Introduction

Here we investigate various notions of state in the sciences, focusing on the protean character of these notions, on their capacity to embrace manifold possibilities and to metamorphose into new forms that encompass new phenomena.

Aristotle said that each object in nature has its own natural path. Any other path is unnatural and is known to be such by its difference from the natural one and hence by the constraints and forces that necessitate it. The modern form of Aristotle's idea is that of a path in state space.

2 The Notion of State

The point of view to be examined and expanded upon here is most simply illustrated by

Malthus' law:

$$\frac{dx(t)}{dt} = \lambda x(t) \tag{1}$$

The state is population size x and the law asserts that the time rate of change of the state equals the net growth rate times the current state. The net growth rate λ is typically equal to b - d where b and d respectively are the net birth and death rates of the population (possibly including immigration and emigration). The parameter λ represents the total influence of the environment. Here "environment" refers to all aspects of the Universe not under direct scrutiny (including not only spatially separate aspects but aspects representing a different level of detail - for example, the properties of individual members of the species and how they interact with each other and their surroundings as opposed to their number alone). The object of study is a system whose state is changing in time according to an evolutionary law. The evolutionary law describes the rate of change in terms of the state and in terms of the environment.

The state of a system is generally taken to be a collection of observable quantities characterized by certain properties. One property is independence - e. g., x and x^2 are both observables, but they are not independent. The state variables should be independent so that no one of them can be determined from the others if the latter are known. Another property is completeness. The state variables should form a maximal independent set. Any observable not included among them should be a mathematical function of them. Thus energy, position, and momentum are not all needed to characterize the state of a Newtonian particle since the energy is a function of the position and the momentum (in a closed conservative system), and we would expect any other observable besides energy to be a function of the particle position and momentum (and other fixed parameters such as the mass). One other property of the state is that the time rate of change of each state variable should itself be a mathematical function of the state variables. Thus the evolutionary law is of the form:

$$\frac{dx(t)}{dt} = F(x(t)) \tag{2}$$

The function F and other observables may depend on other quantities besides the state x but these quantities are to be thought of as outside the system and are typically represented by constants or given functions of time.

The Universe is thus divided mentally into two parts: the system and its environment. The state describes the system, and its evolution depends on itself and the environment. This is a program for modeling systems. Let a system be thought of as any aspect of the Universe on which we wish to focus attention. Then we collect, or contemplate collecting, observables related to this aspect, aiming for independence and completeness. At each stage we must decide whether a variable is part of the system or outside of it, and we thus clarify our notion of the system with respect to desired generality, level of detail, elements considered, and elements ruled out. Although our original idea of what the system is may be somewhat vague, our model-building forces us to make decisions and move toward exact if idealized conceptions.

For this discussion we accept time as a fundamental concept and do not offer an analysis of it. A system that does not persist for some duration of time is of no interest since truly unique events are not the proper object of science. Time need not be absolute time, just the experimenter's clock time. We shall also ignore the relativistic perspective since it does not substantially alter the points to be made here. (Indeed by a familiar device time can be included as a state variable s satisfying the evolutionary law ds/dt = 1.) Time measurements shall be treated as lying in the continuum and the methods of calculus shall be assumed. If one prefers discrete time, just substitute differences for derivatives throughout.

Calculus leads us, in connection with evolutionary laws, to consider time rates of change of observables as new observables (*derived* observables). Either these derived observables are expressible in terms of other observables or else we must add them to the list of state variables. Thus by a combination of observation and logic we can arrive at evolutionary laws of Newtonian type:

$$\frac{dx}{dt} = v, \frac{dv}{dt} = \frac{1}{m} f(x, v) \tag{3}$$

Here the time rate of change of the state (x,v), namely (dx/dt, dv/dt), depends on the state (and the parameter m). Mathematically there is no barrier to repeating such a process indefinitely. Thus given a variable x_1, its successive time derivatives might be called x_2, x_3, ..., x_n , and can be added to the state until one is found that is empirically expressible in terms of the previous ones. The evolutionary law is then:

$$\frac{dx_1}{dt} = x_2, \frac{dx_2}{dt} = x_3, \ldots, \frac{dx_n}{dt} = f(x_1, \ldots, x_n) \tag{4}$$

This evolutionary law describes how x_1, x_2, ..., x_n evolve as a function of x_1, x_2, ..., x_n.

Of course new observables are also generated in other ways than by taking derivatives. We would expect to have a finite number of basic variables and then take derived variables until we obtain the "closure" that an evolutionary law gives. Newtonian (and Galilean) mechanics gives closure at the second derivative.

Note that state variables are not unique. A population x might be described just as well by x^3 as by x (or by x^2 if we assume nonnegativity). Newtonian mechanics can be expressed in terms of position x and velocity v or in terms of position x and momentum p = mv, and thus by the evolutionary law:

$$\frac{dx}{dt} = \frac{p}{m}, \frac{dp}{dt} = f(x, \frac{p}{m}) \tag{5}$$

This is a matter merely of recoordinatization. The state is thus an abstract notion that can be expressed in terms of different sets of quantities, different coordinates. It has alternative numerical representations depending on which observables are taken as basic and which units of measurement are adopted. The evolutionary law singles out paths in state space, a unique one through each state, but the equations describing these paths will vary with the coordinate system. See Mackey (1963) for discussion of these issues, and motivation for many of the ideas in this article.

Yet we should acknowledge an anomaly. By allowing derived variables, we have subtly enlarged the notion of state. If the state represents the system at an epoch of time, then it should be a snapshot of the system. Time derivatives, though, require comparing the value of an observable at two nearby times. Such observables are not really instant, but have tendency and multiple times built into them. Once one allows tendency there is no telling where one will stop. The idealized instant is of limited value even in so basic a theory as Newtonian mechanics. One needs to know more about the system than merely its status, or standing, at an instant in time.

In fact, many systems have closure at the first derivative. Population models, linear and nonlinear, for single or multiple populations (e.g., predator-prey), do; the differential equations describing a system of chemical reactions do (the state variables being the concentrations of the reactants); models of epidemics do. So do compartment models that describe the contents (or one type of content) of a compartment with immigration and emigration taking place. Such models have a special place in biology where they are used, for example, to describe the amount of medication in body organs.

The logical progression of ideas just developed permits indefinite iteration. As we study the system, we may, even without benefit of derivatives, discover an infinite number of independent variables. Or when we take successive time derivatives, we may never arrive at closure. In practice closure is usually encountered by the second, third, or fourth derivative if it is encountered at all.

Suppose closure fails under differentiation. Then x_2 can be defined to be dx_1/dt, x_3 can be defined to be dx_2/dt, etc. Formally we may write the infinite-dimensional vector equation:

$$\frac{d(x_1, x_2, \ldots)}{dt} = (x_2, x_3, \ldots) \qquad (6)$$

Eq. 6 can be regarded as an evolutionary law. Indeed it is even possible to write down a formal solution expressing the state at time t_2 in terms of the state at time t_1: $X(t_2) = \exp\{(t_2 - t_1)S\}X(t_1) = X(t_1) + (t_2 - t_1)S(X(t_1)) + ((t_2 - t_1)^2/2)S^2(X(t_1)) + \ldots$ where S is an infinite matrix with ones on the first superdiagonal and zeroes elsewhere. Whether the solution makes sense depends on whether X(t) can be regarded as analytic in t and whether the components of the initial state $X(t_1)$ converge to zero with sufficient rapidity so that the sum is finite. If the i-th component of X(t) is bounded by a constant independent of i and independent of t for short time intervals, convergence does occur. Note that the evolutionary law is linear.

The formal solution of eq. 6 raises as many questions as it answers. In particular, its practicality is in doubt since determining a state, say the initial state, may be beyond human powers. Indeed, humans prefer finitary measurements and computations. We like to think about a finite number of things or about a finite number of types of things.

3 Fields

The notion of field comes to our rescue. Examining a piece of string tied between two points in a vertical plane, if the displacement is not so extreme that the string can curve back or forth over itself, we can imagine a unique string height at each horizontal location from one end to the other. We have one kind of variable "height," but it is evaluated at infinitely many horizontal positions, giving us a profile of the string at a particular time. The continuous structure of space is taken for granted here, including the remarkable construct of the real numbers to represent spatial coordinates (as well as the time coordinate). We now have an infinite number of observables, namely, string height $u(x)$ at horizontal position x for x varying from one end of the string to the other. Letting x remain abstract, we can specify a height function $u(\cdot)$. This is called a scalar field, and this function is part of the state. Permissible functions might be polynomials and the like represented by formulas or functions piecewise representable by formulas, but we may impose other requirements such as continuity (so that the string is unbroken). With this field as part of the state, we have many observables implicitly included. Thus if u is assumed to be differentiable with respect to x, then $\partial u(x)/\partial x$, $\partial^2 u(x)/\partial x^2$ are available (if space is taken to be discrete, differences or second differences of u at various locations can be taken instead). None of these observable is independent of $u(\cdot)$. They can be aggregated into fields themselves such as $\partial u(\cdot)/\partial x$, $\partial^2 u(\cdot)/\partial x^2$, and various operations such as applying functions or integrating can be performed on them to yield real-valued observables, all dependent on the original field $u(\cdot)$.

Evolutionary laws can now be developed of partial differential equation type:

$$\frac{\partial u(\cdot,t)}{\partial t} = F(u(\cdot,t)) \tag{7}$$

to describe the field $u(\cdot, t)$ at time t. This equation is usually local, i. e., it is interpreted pointwise in x with u and any spatial derivatives evaluated at each x. Examples include: the heat equation where u is a temperature field and $F(u(\cdot,t)) = k\, \partial^2 u(\cdot,t)/\partial x^2$, or the reaction-diffusion equation where u represents the concentration of a chemical throughout a region and $F(u(\cdot,t)) = au(\cdot,t)^b + k\, \partial^2 u(\cdot,t)/\partial x^2$.

The evolutionary law need not be interpreted pointwise, though. Indeed the state u at least in principle need not be differentiable and neither u nor $\partial u/\partial t$ need exist as point functions. The y can be equivalence classes of measurable functions in the Lebesgue theory, or distributions in the sense of Dirac and Laurent Schwartz. Think of them as mathematical limits of sequences of familiar functions. What is important is that suitably concatenated with other entities at hand, they yield real numbers, i.e., values of observables.

If $\partial u(\cdot,t)/\partial t$ is not a function of $u(\cdot,t)$, we can take another time derivative and treat $\partial u(\cdot,t)/\partial t$ as part of the state. Thus we might obtain:

$$\frac{\partial u(\cdot,t)}{\partial t} = v(\cdot,t), \frac{\partial v(\cdot,t)}{\partial t} = F(u(\cdot,t), v(\cdot,t)) \tag{8}$$

or

$$\frac{\partial^2 u(\cdot,t)}{\partial t^2} = F(u(\cdot,t), \frac{\partial u(\cdot,t)}{\partial t}) \tag{9}$$

Laws of this type include the wave equations for sound and water waves, for pressure and displacement. Remember that the mathematical function F can perform operations such as spatial differentiation and many others.

The state space of fields $u(\cdot)$ or pairs of fields $(u(\cdot),\partial u(\cdot)/\partial t)$ can be taken to satisfy certain constraints such as differentiability or having fixed values for certain observables so long as these constraints are compatible with the evolutionary law. In many cases the constraints are specific boundary values - either behavior at spatial infinity or behavior at the boundary of a finite region. In the latter case the system is spatially internal to that region and the boundary values represents a stipulated interaction with the environment. That environment may include the same variable, e.g., temperature evaluated outside the region of interest.

Other classical examples where fields arise include the Navier-Stokes equations, where the state may consist of a fluid density field together with a fluid velocity field defined at each point occupied by the fluid. Maxwell's equations are of the same type with the state being the six-component electromagnetic field. The two vector equations are the evolutionary law and the scalar equations are constraints compatible with the evolutionary law. In the simplest case charge density and current density are givens in the environment satisfying a charge conservation law. The Navier-Stokes equations, it should be noted, are still the subject of major research: no one has managed to show or disprove existence, uniqueness, or well-behavedness of solutions to these equations in the general case (Clay Mathematics Institute, 2000).

4 Probability

It may happen that the state x is defined and an evolutionary law dx/dt = F(x) exists, but for one reason or another it is more convenient to treat the probability density function $\rho(x,t)$ of the states. For a region A in the original state space $\int_A \rho(x,t)\, dx$ is the probability that at time t the state x is in the region A. Then Liouville's equation, derived from the original evolutionary law, describes the evolution of probabilities:

$$\frac{\partial \rho(x,t)}{\partial t} = -\nabla_x(\rho(x,t)F(x)) \tag{10}$$

The quantity ∇_x is the gradient with respect to the original state variables. Eq. (10) is linear in $\rho(., t)$ and can be solved explicitly provided the original evolutionary law can be.

Probability in this way affords the opportunity for another expansion of the notion of state. The original state x has its own "deterministic" evolution, and is called the deterministic state, while a probability distribution $\rho(\cdot,t)$ is called the probabilistic state. This is a generalization of the former since a distribution concentrated at a single point x corresponds to the original state. Probabilistic observables are the probabilities that the original observables will take values in arbitrarily prescribed regions. Instead of asking for g(x(t)), we ask for $P(g(x(t)) \in B) = \int \rho(x,t)\, dx$ where the integration is over the region $\{x : g(x) \in B\}$. We can also ask for the expected value of g(x), i.e., $E(g(x)) = \int g(x)\rho(x,t)\, dx$ where integration is over the deterministic state space. The new observables, based on the probability distribution $\rho(\cdot,t)$, are not even potentially observable in the sense that deterministic variables are. One needs to make repeated observations of systems with a given probability distribution to verify probabilities or expected values.

Opening this door permits us to consider probabilistic models in which the evolutionary law is not obtained from a deterministic counterpart. Examples include the Fokker-Planck-Kolmogorov equation used in statistical mechanics and genetics and the Sewall Wright equation in genetics. Stochastic differential equations may be regarded in the same light. Although they are often regarded as arising from a probability measure on the space of all classical trajectories (world lines), they can be reformulated to represent evolution in time of a probabilistic state at each given time.

Probability may be introduced because we lack true knowledge of the deterministic state, but it also serves us when no deterministic evolutionary law can be discerned and the only regularity is the evolution of probabilities.

5 The Quantum State

The most unusual extension of the notion of state in common use is that of the quantum state. Observables are probabilities and expected values corresponding to (repeated) measurements performed on a quantum system. The measurement protocols are linked by semiclassical and ad hoc reasoning to self-adjoint operators on a Hilbert space. This Hilbert space, in general, is isomorphic to the set of equivalence classes of square-integrable complex-valued functions defined on the product of the spectra of a complete and independent set of these operators (where complete and independent are used in senses similar to our earlier usage). Thus in the simplest case the Hilbert space is $L^2(R^{3n})$ where the observables are the three position coordinates of n spinless particles, each coordinate operator having spectrum equal to the entire real number system R. The quantum state is a unit vector in this Hilbert space, also called a wave function, two such being regarded as equivalent if they differ by a scalar of the form $e^{i\lambda}$, λ a real number. The number λ has no physical significance in general and is like a constant added to a classical potential. The quantum state evolves according to the Schrödinger equation or one of its relativistic counterpart, the Klein-Gordon equation or the Dirac equation.

What is most bizarre about the quantum theory is not only that states are probabilistic entities describing ensembles of systems rather than a single system, but also that, although classical observables are present, there is no classical state underlying the quantum state. There appears to be no determinate reality beyond that of the evolving probabilities. Measurement of the state, as in conventional probability theory, results in new statistics, but these statistics are incompatible with proposed classical states. Collapse of the wave function occurs at a measurement, and the state jumps into one of a set of orthogonal states associated with the type of measurement. This jump substitutes for the old probabilities new ones and constitutes an irreducible interaction with the environment. For example, a relatively precise measurement of a position coordinate, according to the Uncertainty Principle, leads to a situation where the conjugate momentum probabilities are dispersed over a wide range of momenta.

6 Other Exotica

In addition to deterministic states, probabilistic states, and quantum states, many other avenues for expansion of the notion of state have been pursued.

Control theory arose with the advent of self-regulating machinery and has been applied to chemical, biological, and social systems. The basic notion is that some aspect of the state is fed back into the system and used to update the state or restore it to a desired region. This falls under traditional notions of evolution except in the case when *delay* occurs.

Imagine a system with conventional state x(t) that is updated on the basis of the values of x(t), $x(t - h_1)$, $x(t - h_2)$, ..., $x(t - h_n)$ where $0 < h_1 < h_2 < ... < h_n = D$. The evolutionary law takes the form:

$$\frac{dx(t)}{dt} = F(x(t), x(t-h_1), \ldots, x(t-h_n)) \tag{11}$$

To accommodate this form, the notion of state can be expanded further. The state is no longer taken to be instant or with the infinitesimal delay of a time derivative, but is taken to be a *time profile* of the former state over a time interval of length D. Thus the state is a portion of the time trajectory of the original state. The evolutionary law can now be used to update this trajectory. Given x(t) for $0 \geq T \geq -D$, we find x(t) for $T \geq t \geq T - D$ at any time $T > 0$. The former is the state at time 0 and the latter is the state at time T. The state includes a memory of the recent past.

The state notion can be generalized further still to include an *infinite memory*, with the new notion of state at time t consisting of the original state trajectory for the entire past, i.e., the state at time T is the entire set of readings x(t) for $T \geq t \geq -\infty$. The evolutionary law may now draw on all quantities obtainable from the past or present, e.g, values of x at any past time, integrals of x over past time intervals, time derivatives of x at past times, et cetera. The original state x before this generalization may already be a field. Hence the evolutionary law may be a partial integro-differential delay equation.

A system of particular interest is a family of charged particles interacting electromagnetically and relativistically. The acceleration of a particle at the space-time point P is a function of the electromagnetic fields generated at P by the other particles. The values of these fields can be expressed in terms of the positions and velocities of the other particle at the times when they were on the past light cone of P, i.e., events that can send a signal to P at the speed of light. To understand the interaction of the system, positions and momenta of all particles in some Lorentz frame must be given over a range of times, and then one must show how the evolutionary law predicts what will happen over an equally large range of times. A multi-time state seems to be inherent in this case.

When an evolutionary law is incomplete or is given by a multi-valued "function," another adjustment of the state notion can be contemplated. Suppose the evolutionary law for a conventional state is of the form:

$$\frac{dx(t)}{dt} \in F(x(t)) \tag{12}$$

where F(x(t)) denotes a state-dependent set of values and $\in$ denotes membership. Then the future state lies on any trajectory compatible with the relation (12).

Such a situation may be handled by probabilistic methods or one may introduce another new notion of state, namely any *set* of conventional states. If $S(t_1)$ denotes a set of conventional states at time t_1, then $S(t_2)$ denotes the set of all conventional states reachable at time t_2 along a conventional trajectory satisfying relation (12) for $t_1 \leq t \leq t_2$ and beginning in $S(t_1)$ at time t_1. Thus sets of states evolve. Although this notion may seem far-fetched, it sometimes yields results for sets of points that are comparable to those for deterministic evolution along point trajectories. For example, Barnsley et al. (1988) have shown that fractals arise as the equilibrium sets in a discrete form of relation (12) (with x updated each time period by applying one of a finite number of contractions). More general forms than relation (12) can also be accommodated. Indeed, if any aspect of the future can be predicted, it can be used to define an evolution of sets of states to sets of states. Fuzzy sets can also be substituted for ordinary sets.

Category theory can also be used to extend the reach of the notion of state. (I am indebted to Paul Kainen for reminding me of this point). If an evolutionary operator T(t) takes the state space X to itself, updating the state by a time interval t, then a functor $\mathfrak{J}$ can induce $\mathfrak{J}$(T(t)) taking $\mathfrak{J}$(X) to $\mathfrak{J}$(X). The object $\mathfrak{J}$(X) may contain X as a subobject or may contain all important structures in X. Examples already given fall under this rubric.

Also worthy of mention is the notion of a *superstate*. If trajectories in state space intersect, it is sometimes appropriate to regard these trajectories as projections or shadows of non-intersecting trajectories in a higher-dimensional space, a space of superstates. The superstates will involve additional variables that may or may not have physical significance but do permit a deterministic evolution. The opposite case may hold as well, namely, the trajectories in the state space down below, the base space, are deterministic, but there are multiple trajectories in the superstate space, the total space, all of which project down to the visible trajectory. Both types of space, hypothesized for mathematical convenience or speculative adventure, have played generally constructive roles in theoretical physics - in hidden variable theories, gauge theories, and string theories.

7 Conclusion

The repertoire of the system modeler thus includes: additional independent variables, derived variables, fields, probabilistic and quantum states, states with finite or infinite memory, sets of states, category-theoretic states, and superstates. This litany perhaps suggests a decline in the importance of physical observables and an increase in the importance of nominal prediction. However, the more advanced notions of states generally have earlier notions embedded in them so that traditional observables are represented.

Nonetheless, we are a long way from Aristotle's natural paths. The malleability of the notion of state, as it becomes more remote from simple observation, threatens to deprive it of meaning. In reality, though, the state approach is a sturdy one and only changes in the face of stubborn facts. It has successfully survived its greatest challenge to date, namely, the quantum theory. Its essence is a framework to express temporal pattern and mathematical lawfulness.

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