# A Dynamical Systems Approach to Behavioral Modeling

Nicholas Tufillaro
Integrated Solutions Laboratory
HP Laboratories Palo Alto
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E-mail: nbt@hpl.hp.com

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This technical report describes the groundwork for our nonlinear modeling technologies. Future technical reports will go into detail about the specific solutions we are developing to build accurate models for nonlinear electronic devices from input-output measurements for possible use in CAD simulators such as currently sold by HP EESof.

# A dynamical systems approach to behavioral modeling

Nicholas B. Tufillaro
Measurement Information Department, HP Labs
1501 Page Mill Road, MS 4A-D, Palo Alto, CA 94303-1126
Email: *nbt@hpl.hp.com*

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## 0 Time series

A time series is a collection of observations made sequentially in time. Examples include a sequence of measurements showing the position of an oscillating pendulum, $\theta(t_n)$, the current, $i(t_n)$, or voltage, $v(t_n)$ in a circuit, or perhaps the daily rainfall in West Lake Village.

## 1 Introduction

A dynamical system is a system which changes in time according to some rule, law, or *evolution equation.* The two most commonly studied examples of dynamical systems are *flows* (or differential equations), and *maps* (or difference equations). In flows, time, $t$, is a continuous variable indexing the the state of the system, although measurements may occur at discrete times indexed by $t_n$.

An example of a *differentiable dynamical system*—that is, a dynamical system modeled by a set of differential equations—is the RLC circuit:

The RLC circuit is modeled by a second order linear differential equation:

$$\mathrm{CL}\frac{d^2i}{dt^2} + \mathrm{RC}\frac{di}{dt} + i = u(t), \qquad u(t) = -\omega \mathrm{CE}_0 \sin(\omega t) \tag{1}$$

One very useful characterization of a linear RLC circuit is given by its *Transfer Function*, which is (more or less) the frequency domain equivalent of the time domain *input-output* relation.[1] The causal relationship between the input (the voltage) and the output (the current), is emphasized by adopting the input-output terminology. Applying the Laplace transform to the time domain model

[1] Rolf Johansson, System Modeling and Identification, Prentice-Hall (1993).

and solving for the relationship between the input voltage and output current gives the transfer function:

$$G(s) = \frac{\mathcal{L}\{i(t)\}}{\mathcal{L}\{v(t)\}} = \frac{s\mathrm{C}}{s^2\mathrm{LC} + s\mathrm{RC} + 1} \tag{2}$$

The above transfer function might be called a "functional model" because the physical parameters—resistance, inductance, capacitance—are prominent in the transfer function and I can use this representation to design an RLC circuit to perform a desired "function" or task. This type of model is also commonly called a *parametric model.*

A *behavioral model*, on the other hand, can also be thought of as describing the input-output behavior of a system, but unlike a "functional model" we do not start from a detailed physical picture for the system. Rather I will start from a more general assumption, namely, *the device under test is modeled by a differential dynamical system*, i.e., a set of ordinary differential equations. Based on this assumption I will be interested in the following issues:

1. How do we design input signals to efficiently probe the differential structure governing the dynamical evolution of the device under test?

2. How can we construct a state space and dynamical models—based only on measured time series—for systems driven by deterministic sources (e.g., sine waves, or combinations of sine waves) and/or stochastic sources?

I will outline a general approach to this problem for "low dimensional" dynamical systems—that is, components whose dynamics are governed by a few differential equations. I would like to caution that this approach, although very attractive theoretically, might not be the most practical solution for a given set of problems. For instance, for "weakly nonlinear systems" a better practical solution might be a "describing function" approach or a "Volterra series" approach.[2]

In a nutshell, the dynamical systems approach goes as follows, from the measured input-output time series I will attempt to

(i) construct a minimal deterministic "state space" for the device under test, and

(ii) attempt to estimate a "vector field" determining the evolution equations for the reconstructed state space.

[2]The term weakly nonlinear is not very clear from a mathematical perspective, roughly it seems to mean that the nonlinear terms in the governing equations are small, *and* that the systems asymptotic behavior (the attractor) is close before and after the nonlinear term is turned on. See footnote [1] for a brief introduction to describing functions and Volterra series.

In the second half of this paper I will tell you one way to go about "reconstructing" a state space and dynamical equations from measured time series. The fact that such an approach is at all feasible might be startling at first, but it is based on a mathematical theorem due to Whitney, with major contributions by Takens, Packard et. al., Ruelle, and Sauer et. al. among others, usually called the *embedding theorem*.[3] However, to really get some understanding for this approach, and to see how it differs from what we do for linear systems (i.e., working in frequency space and using transfer functions), I would like to backup a bit to discuss the following topics with some examples:

- General solution of linear ordinary differential equations (ODE's), or why we can characterize linear devices,
- General properties of nonlinear systems from a "geometric" perspective,
- Why it might be sensible to try to estimate a state space and vector field for the test and measurement of nonlinear components,
- Embedology, or how to reconstruct a state space model from measured time series,
- Vector Field Estimation, or one approach to estimating the dynamical rules,
- Possible extensions of current research to parameter dependent multiple input-output systems.

## 2 Linear networks of circuit components

The connection between networks of circuit elements and differential equations is almost immediate. Most circuit elements and networks, by design, are governed by "lumped finite systems" which, in a low noise environment, are governed by a vector of ordinary differential equations,

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), t), \qquad \mathbf{x}(t_0) = \mathbf{x}_0 \tag{3}$$

where

$\mathbf{x}$ is the state vector in d-dimensions,[4]

$\mathbf{u}$ is the vector of inputs and,

[3] Tim Sauer et. al., Embedology, J. Stat. Phys. Vol 65 (3/4), 579-616 (1991); Tim Sauer and James Yorke, How many delay coordinates do you need?, Int. J. of Bif. and Chaos. Vol 3 (3) 737-744 (1993).

[4] As usual, we are going to confuse the basis vectors $x$ with the solution set. The "solution" is better written as $\varphi(\mathbf{x})$.

$\mathbf{x}_0$ is the initial (internal) state of the network or components.

To be complete I should also consider a (possibly nonlinear) measurement function

$$\mathbf{y}(t) = \mathbf{g}(\mathbf{x}(t), \mathbf{u}(t), t) \tag{4}$$

which formally at least gives us our outputs, $\mathbf{y}(t)$, in terms of our $\mathbf{u}(t)$ inputs. In the case when the network of elements is governed by Kirchoff's law, and all the individual components are linear, the above equations can be written in a standard matrix form:

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \tag{5}$$

$$\dot{\mathbf{y}} = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t) \tag{6}$$

for matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$.

The "linearity" of the above circuit network has two sources. First, the components are assumed to be linear, but more importantly—it follows from Kirchoff's laws—that the network's topology is "linear." Indeed, by a nonlinear circuit we usually mean that the network's topology remains linear, but a few individual components exhibit nonlinear behavior.[5]

My point here is just to emphasize that under normal test and measurement circumstances the behavior of the circuit network is captured by some set of ODE's.[6]. The somewhat abstract ideas we are about to embark on are very relevant to modeling circuit behavior. When studying linear ODE's we need tools and techniques dealing with linear spaces (linear algebra), when studying nonlinear problems we need tools and techniques intrinsic to curved spaces (like differential geometry).

# 3 A simple and sophisticated look at linear ODE's

Consider a low pass filter which is governed by the first order differential equation

$$\mathrm{RC}\frac{dv}{dt} + v = u(t) \tag{7}$$

Let's begin by considering the homogeneous equation ($u(t) = 0$):

$$\mathrm{RC}\frac{dv}{dt} + v = 0 \tag{8}$$

[5]Ronald A. Rohrer, Circuit Theory: An introduction to state variable approach, McGraw-Hill (1970); Martin Hasler and Jacques Neirynck, Nonlinear circuits, Artech House (1986)

[6]In a high frequency regime where "parasitic" wave effects come into play, it is possible that an effective ODE model exists, but how well an empirical ODE model will work in this regime is a question of current research.

Let $A \equiv 1/RC$, by simple integration we find

$$\begin{aligned} \frac{dv}{dt} &= -Av && (9) \\ \ln(v(t))|_{t_0}^{t} &= v(t) - v(t_0) = -A(t - t_0) && (10) \\ v(t) &= e^{-A(t-t_0)} v(t_0) && (11) \end{aligned}$$

Let $g_{t_0}^t \equiv e^{-A(t-t_0)}$, then

$$v(t) = \left[g_{t_0}^t\right](v_0) \tag{12}$$

$g_{t_0}^t$ is called the "evolution operator" since it carries a collection of initial states "$v_0$" into the final state $v(t)$. $t$. The form of our solution for the initial value problem (IVP) consists of the application of the evolution operator on the initial state producing the final state.

The notion of the solution of the IVP for a differential equation in terms of an evolution operator is really at the heart of the theory of ODE's—linear or nonlinear. The evolution operator has the following properties:

$$\begin{aligned} (g_{t_1}^t \cdot g_{t_0}^{t_1}) &= g_{t_0}^t && (13) \\ g_t^{t_0} &= \left(g_{t_0}^t\right)^{-1} && (14) \end{aligned}$$

These properties formalize our notion of a two-sided deterministic process. Assume that at the start, $t_0$, the device is in a state $x_0$. Then at another moment the device is in another state $x(t) = g_{t_0}^t x_0$. By determinacy we mean that the present state uniquely defines both the past and future. In addition, the new states depend "smoothly" on both arguments $t$ and $x_0$. This last property is formalized by saying the mapping is a "diffeomorphism" (both the space, and functions on the space are differentiable).

Now consider the nonhomogeneous RC equation

$$A\frac{dv}{dt} + v = u(t) \tag{15}$$

To get a quick solution to this multiply by the integrating factor $e^{At}$,

$$Ae^{At}\frac{dv}{dt} + e^{At}v = e^{At}u(t) \tag{16}$$

and notice that the left hand side is now a perfect differential:

$$\begin{aligned} \frac{d}{dt}(e^{At}v) &= e^{At}u(t) && (17) \\ \int_{t_0}^{t} \frac{d}{d\tau}(e^{A\tau}v)d\tau &= \int_{t_0}^{t} e^{A\tau}u(\tau)d\tau && (18) \\ e^{At}v(t) - e^{At}v(t_0) &= \int_{t_0}^{t} e^{A\tau}u(\tau)d\tau && (19) \end{aligned}$$

$$e^{At}v(t) = e^{At}v(t_0) + \int_{t_0}^{t} e^{A\tau}u(\tau)d\tau \quad (20)$$

$$v(t) = e^{-A(t-t_0)}v(t_0) + e^{-At}\int_{t_0}^{t} e^{A\tau}u(\tau)d\tau \quad (21)$$

The last equation can be rewritten in a couple of ways. First, let's try to identify $g^t_{t_0} = e^{-A(t-t_0)}$ in the above equation, then I get,

$$v(t) = e^{-A(t-t_0)}v(t_0) + e^{-A(t-t_0)}\int_{t_0}^{t} e^{A(t-t_0)}u(\tau)d\tau \quad (22)$$

or,

$$v(t) = g^t_{t_0}v(t_0) + g^t_{t_0}\int_{t_0}^{t} (g^\tau_{t_0})^{-1}u(\tau)d\tau \quad (23)$$

I won't prove it here, but equation (24) is a formal solution not just to the RC problem with arbitrary inputs, but also—and this is a bit of a leap—for all linear inhomogeneous systems of ODE's. Specifically, if we consider a vector differential equation,

$$\dot{\mathbf{x}} = \mathbf{A}(t)\mathbf{x}(t) + \mathbf{u}(t), \qquad \mathbf{v} \in \mathbf{R}^n \quad (24)$$

then it has a formal solution

$$\mathbf{x}(t) = g^t_{t_0}\left(\mathbf{x}_0 + \int_{t_0}^{t} (g^\tau)^{-1}\mathbf{u}(\tau)d\tau\right) \quad (25)$$

which for the homogeneous part can again be viewed as an evolution operator acting on the vector of initial conditions. For the n-dimensional linear problem $\mathbf{A}$ is now a matrix, and the flow operator, $e^{\mathbf{A}t}$, is the exponential matrix.

What does this have to do with the characterization of linear devices?

Let's go back to our first question—how to design inputs to effectively probe the dynamics of the system. When the system is linear, equation

$$\mathbf{x}(t) = g^t_{t_0}\mathbf{x}(t_0) + g^t_{t_0}\int_{t_0}^{t} (g^\tau_{t_0})^{-1}\mathbf{u}(\tau)d\tau \quad (26)$$

is very helpful in answering this question. The first term $g^t_{t_0}\mathbf{x}(t_0)$ is called (in Control Theory) the *zero input response* term since it is the solution for the unforced ($u(t) = 0$) case. The second term is called the *zero state response* ($x_0 = 0$) term. This decomposition of the dynamics of a system into transient behavior (independent of forcing) and forced behavior (independent of initial state) is generally not true for a nonlinear system. More to the point, equation (27) really captures the essential features of an "input-output" theory of *linear* systems. To "characterize" the system we need to design inputs that allow us to solve or approximate the evolution operator. Well, for a linear system, there at lots of ways to do this.

For instance, I could turn off all inputs, and just measure the systems response from a nonequilibrium state. By repeating this sort of measurement many times from many different states I can approximate the evolution operator since ($u(t) = 0$ in eq. (27)),

$$\text{(output)} \quad v(t) = g_{t_0}^{t} v(t_0) \quad \text{(input initial state)} \tag{27}$$

This procedure is sometimes called *initial condition response.* Additionally I can wait for the system to settle down to its final state ($v(t_0) = 0$) and then "ding" the system with a unit impulse, i.e., a delta function, then the output is ($v(t_0) = 0$ in eq. (27)),

$$\begin{aligned} v(t) &= g_{t_0}^{t} \int_{t_0}^{t} (g_{t_0}^{\tau})^{-1} \delta(\tau - t_0) d\tau && (28) \\ &= g_{t_0}^{t} (g_{t_0}^{t_0})^{-1} d\tau && (29) \\ &= g_{t_0}^{t} && (30) \end{aligned}$$

This is usually called *impulse response analysis.* Both techniques usually fall under the heading of *transient response analysis.*

In the engineering world, this approach is extended in several significant ways. First, a Laplace transform is used to work not in the time domain but the frequency domain. For linear systems, this is exactly the right thing to do because a (complex) exponential (the inputs) passes right through the system (the outputs) with only its amplitude and phase modified, but not its fundamental frequency. Second, the theory of the Transfer Function (Laplace transform on the zero response state) is built which effectively allows us to hide the underlying state space model and deal only with the inputs and outputs of the device in practical terms. Third, in non-ideal environments, when, for instance, issues of noise come into play, it is very useful to try to estimate the evolution operator from the cross-correlation of the inputs and outputs for a wider class of input signals (collections of sines or stochastic). The important point to keep in mind, though, is that in the linear theory it is usually possible to relate the input-output signals back to the evolution operator in a direct fashion. This is why issues of test and measurement are (at least at the theoretical level) usually doable for linear systems.

Put another way, *a priori* structural information about *linear* systems can be incorporated into a theory of test and measurement of linear devices in a direct and useful way.

These issues are commonly discussed in a slightly different fashion. Namely, linear characterization is seen as a problem in the estimation of the "kernel of an integral operator." Very quickly, another way to view the above solution of IVP problem for linear ODE's is via a Green's Function which in the present example is,

$$G(t,\tau) = e^{-\mathbf{A}(t-\tau)} \tag{31}$$

Rewriting equation (27) in terms of its Green's function shows

$$\mathbf{x}(t) = G(t,t_0)\mathbf{x}(t_0) + \int_{t_0}^{t} G(t,\tau)\mathbf{u}(\tau)d\tau \tag{32}$$

The above formula is an integral equation with Kernel $G(t,\tau)$. Thus, the characterization problem in this context is one of designing inputs $(u(t))$ and measuring outputs $(x(t))$ in order to estimate $G(t,\tau)$. This problem is called system *identification.*

# 4 Vector Fields

A vector field is a rule that assigns to each point in phase space a unique vector in a smooth manner. It is an ordinary differential equation from a geometrical perspective. Consider, again, the example

$$A\frac{dv}{dt} + v = u(t) \tag{33}$$

We first observe that when $u(t)$ is described by a differential equation itself (sines, or combination of sines are the simplest examples), then the above "forced" equation can be rewritten as an autonomous equation. For instance, if

$$u(t) = B\sin(\omega t) \tag{34}$$

then let $(\dot{u} = \varsigma, \ddot{u} = \dot{\varsigma})$

$$\dot{u} = \varsigma \tag{35}$$
$$\dot{\varsigma} = -\omega^2 u \tag{36}$$

so the periodically forced first-order system becomes a third-order autonomous system,

$$\dot{\varsigma} = -B\omega^2 u \tag{37}$$
$$\dot{u} = \varsigma \tag{38}$$
$$\dot{v} = \frac{1}{A}(u - v) \tag{39}$$
$$\tag{40}$$

In matrix form the linear system is

$$\begin{pmatrix} \dot{\varsigma} \\ \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & -Bu^2 & 0 \\ 1 & 0 & 0 \\ 0 & \frac{1}{A} & \frac{-1}{A} \end{pmatrix} \begin{pmatrix} \varsigma \\ u \\ v \end{pmatrix} \tag{41}$$

or, $\dot{\mathbf{x}} = \mathbf{f}\mathbf{x}$. The matrix $\mathbf{f}$ assigns a unique vector to each point $(\varsigma, u, v)$ of the phase space. The vector field at the plane defined by $u = 0$—$(\dot{\varsigma}, \dot{u}, \dot{v}) = (0, 1, -1/A)$. The vector field tells the flow (locally) to go that-a-way. Knowing the vector field is knowing the equations of motion.

In this example $\mathbf{f}$ is linear. This picture provides us with a quick explanation as to why "linear filters" preserve periodic motions. Since $\mathbf{f}$ is linear, it follows that the transformation induced by $\mathbf{f}$ on phase space is also linear—that is by $g^t_{t_0}$. Let us consider the image of $u(t)$ under $g^t_{t_0}$ in the autonomous phase space.[7] $g^t_{t_0}u(t)$ undergoes a (3-dimensional) linear distortion, but the period and topology of the original orbit is preserved under all such linear transformations. The "output," $v(t)$, is the projection of the 3-dimensional phase trajectory onto the $v$-axis. Thus, the output is a periodic orbit with the same period as the input orbit, but with a shape distortion. The transfer function is just one way to characterize this shape distortion.

# 5 Embedology

Nonlinear systems differ from linear systems in several fundamental ways. For a linear system we can speak of "the" solution since the system settles down to a unique solution after the transient dies out. Nonlinear systems, on the other hand, can have many different coexisting solutions depending on the initial state. These asymptotic states (what's left after the transient dies out) are called *attractors*. There are four basic types of attractors: equilibrium states, periodic orbits, quasi-periodic solutions (tori), and chaotic attractors. This classification scheme is based on the topology of the attractor.

In order to construct a nonlinear behavioral model we need to estimate either (directly or indirectly) the evolution operator. One (simple minded?) approach is to try to estimate a vector field directly from the observed input-output time-series data. To build such a behavioral model will require the collection and analysis of a good deal of data, but handling large amounts of data is now a realistic possibility because of computer automation.

The techniques we describe for creating an (empirical) state space model and estimating its dynamics have been applied to the attracting states of nonlinear systems for several years. For engineering applications, they need to be extended to handle transient solutions (approaches to attractors) and multiple collections of input-output time series obtained under a range of operating parameters. We will suggest some ways of handing these issues at the end of this paper. Here we will focus on the basic ideas and techniques.

A procedure for creating an empirical model of the state space is straightforward. Assume that the device under test is governed by an $d$-dimensional differential dynamical system. Consider a scaler time series generated by the

[7] In this particular example, the parametric form of the image is $(q, u, v) = (\omega B \cos \omega t, B \sin \omega t, \frac{B}{A^2+\omega^2}(A \sin \omega t - \omega \cos \omega t) + e^{-At} v_0)$.

device under test. The idea behind embedology is to change this scaler measurement back into a vector measurement. There are lots of ways to do this.[8] One useful way to accomplish this is to consider a *time delay coordinate* vector formed by

$$\mathbf{x} = (x_t, x_{t-\tau}, ..., x_{t-(m-1)\tau}) \tag{42}$$

There are now several related issues.

What properties do I want my reconstructed dynamical system to preserve from the original system? For behavioral modeling, I want a *one-to-one* correspondence between the original system and the reconstructed system. That is, I want to be able to uniquely predict future states from past states in the reconstructed system. It turns out, at least in the ideal case of infinite noise free data, that if the original space has $d$ dimensions, then it is possible to establish a one-to-one correspondence if the reconstructed space has $m$ dimensions, where $m > 2d$ (see Footnote [3]). Moreover, the trajectory in this reconstructed state space preserves not only predictability, but also the "local differential structure," i.e., tangent vectors—the stuff vector fields are made of. I won't dwell on why this is so here, rather I will focus on the the practical procedures used in uncovering both a state space model and it's vector field from time-series data.

In the nonideal case we will use a more pragmatic procedure. We will simply go ahead and create both a state space and an empirical model, and then test the model on (untrained) data sets. In numerical test cases the dimension of the reconstructed phase space varies between $d$ and $2d$, so we can often get by with a dimension less than that suggested by the embedding theorem.

How do I calculate $m$, the *embedding dimension*, and $\tau_1$, the *time delay* from scalar time series data? Let us assume we have sampled a trajectory from the system which is not an equilibrium solution but is an attractor (i.e., away from a transient solution). Then, it is likely the trajectory exhibits some degree of recurrence.

If the trajectory is periodic (or if a fundamental period can be estimated from the data), then a good rule of thumb is to take $\tau_1$ to be some fraction, say one fourth, of its fundamental period. Other, more sophisticated, rules of thumb have also been suggested.

For instance, an estimate of $\tau_1$ is provided by the first zero of the *autocorrelation function* (normalized to unity for zero delay),

$$R(\tau) = \frac{< x(t)I(t+\tau) - < x(t) >^2}{< x(t)^2 - x(t) >^2}. \tag{43}$$

[8] I could, for instance, take (numerical) derivatives of the original time series to create a vector. In practice this would not work well since numerical differentiation amplifies noise. When working with experimental data, though, differential and integral (e.g., Hilbert Transforms) filters of the original data often provide a useful alternative to straight time-delay. The "engineering issues" associated with different embedding techniques would be an area of profitable inquiry.

The procedure I use is based on calculating the *mutual information* of the time series with itself.[9] The average amount of information between two variables is quantified by the mutual information,

$$I(x;y) = H(x) + H(y) - H(x,y),$$
$$H(x) = -\int p_x(x)\log(p_x(x))dx,$$
$$H(x,y) = -\int\int p_{x,y}(x,y)\log(p_{x,y}(x,y))dxdy$$

which is the difference between their joint entropy and the sum of their scalar entropies. To determine $\tau_1$, let the time series for $y$ (of size N) be a lagged version of the original time series:

$$I(\tau) = -\sum_{x_t=1}^{N} p_1(x_t)\log_2 p_1(x_t) - \sum_{x_{t-\tau}=1}^{N} p_1(x_{t-\tau}\log_2 p_1(x_{t-\tau}) + \sum_{x_t=1}^{N}\sum_{x_{t-\tau}=1}^{N} p_2(x_t, x_{t-\tau})\log_2 p_2(x_t, x_{t-\tau}).$$

If the $x_t$ and $x_{t-\tau}$ are independent, then $I = 0$. On the other hand, if $x_t$ completely determines $x_{t-\tau}$, then the mutual information equals the scalar entropy.

To calculate the embedding dimension, $m$, I simply create a trajectory vector that is big enough to be consistent with a deterministic description. I can check this with a number of statistics, in practice I find it sufficient to check for *false neighbors* and false tangent vectors.[10] Consider a piece of the trajectory embedded in an $m-1$ dimensional space. If the embedding dimension is not big enough, some points—false neighbors—will appear close in $m-1$ dimensions which fail to be close in $m$ dimensions. As soon as $m$ is big enough, the number of false neighbors should be close to zero. In addition, we can check for false tangents—points close in the reconstructed phase space should have tangents that are close. Again, to ensure determinism we need to increase the size of the embedding space until there are no false tangents—thus ensuring that a estimate of the tangent vector at point of phase space is at least possible. More details with examples are found in the footnote.[11]

Our next goal is to try to estimate a vector field from reconstructed deterministic data.

[9] A. M. Fraser and H. L. Swinney, Independent coordinates for strange attractors from mutual information, Phys. Rev. A **33**, 1134-1140 (1986); A. S. Weigend and N. A. Gershenfeld editors, Time Series Prediction, Addison-Wesley (1994).

[10] M. B. Kennel, R. Brown, and H. Abarbanel, Determining minimum embedding dimension using a geometrical construction, Phys. Rev. A 45, 3111-3118 (1992)

[11] N. B. Tufillaro et. al., Topological time series analysis of a string experiment and its synchronized model, Phys. Rev. E 51 (1), 164-174 (1995); N. B. Tufillaro et. al., An experimental approach to nonlinear dynamics and chaos, Addison-Wesley (1992).

## 6 Vector field estimation

In considering the problem of vector field estimation it is helpful to think of a simple Euler estimation for the numerical solution of the initial value problem. One way to estimate (for small $t$) the next state is to start at the current state and move in the direction of the tangent vector. There are two simple ways to calculate the final state, via an *explicit Euler integration* scheme,

$$\mathbf{x}(n+1) = \mathbf{x}(n) + \Delta t \mathbf{f}(\mathbf{x}(n)) \tag{44}$$

or, an *implicit* scheme,

$$\mathbf{x}(n+1) = \mathbf{x}(n) + \Delta t \mathbf{f}(\mathbf{x}(n+1)). \tag{45}$$

Unlike the numerical problem, in our case $\mathbf{x}(n+1)$ and $\mathbf{x}(n)$ is given, and the task is to estimate $\mathbf{f}$. If we know the form of $\mathbf{f}$ then a least squares estimation will usually suffice in fitting the parameters. However, in the case of our reconstructed state space we do not know the form of the vector field, and the best we can hope for is to expand $\mathbf{f}$ is some basis,

$$\mathbf{f}(\mathbf{z}) = \sum_{\mathbf{I}=0}^{\mathbf{N}_p} \mathbf{p}^{(\mathbf{I})} \pi^{(\mathbf{I})}(\mathbf{z}) \tag{46}$$

In this equation $\pi^{(\mathbf{I})}(\mathbf{z})$ denotes the set of basis functions and the $\mathbf{p}^{(\mathbf{I})}$ are the parameters whose values must be determined by the modeling procedure. $\mathbf{I}$ is a vector index used to identify a particular parameter or basis function.

In practice we are confronted with number of problems. How do we go about picking a basis set for the vector field expansion? How do we go about truncating any basis set we pick, and how do we fit both the basis set parameters and numerical integration parameters? For that matter, what numerical integration should we try to fit to? How do we test the goodness of fit of the model we generate? And, are there any nice algorithms for answering some or all of these questions?

We will briefly cover one approach to these issues described by R. Brown for the case of chaotic attractors.[12] We are currently working to extend these techniques to include state space and vector field estimates based on multiple time

[12] See, Reggie Brown, Nikolai F. Rulkov, and Eugene R. Tracy, Modeling and synchronizing chaotic systems from time-series data, Phys. Rev. E 49 (5), 3784-3800 (1994), for a much more extensive coverage of this issues. Some additional papers of interest are: M. Giona, Functional reconstruction and local prediction of chaotic time series, Phys. Rev. A 44 (6), 3496-3502 (1991); R. Brown, V. In, E. Tracy, Parameter uncertainties in models of equivariant dynamical systems (preprint, 1995); R. Brown and R. Rulkov, Synchronization of chaotic systems: transverse stability of trajectories in invariant manifolds (preprint, 1996); R. Brown, N. Rulkov, and N. Tufillaro, Synchronization of chaotic systems: the effects of additive noise and drift in the dynamics of the driving, Phys. Rev. E 50 (6), 4488-4508 (1994); U. Parlitz et. al., Reconstructing physical variables and parameters from dynamical systems, Int. J. Bif. and Chaos 4 (6), 1715-1719 (1994).

series taken over a range of internal parameters in order to construct a behavioral model. This class of models and fitting problems is studied in the control literature where it is called *structure identification of linear-in-parameters nonlinear dynamic models.*[13] The issues of model fitting and optimal model truncation can be handled with ideas from statistical inference, namely, the methods of maximum likelihood (ML), and minimum description length (MDL), respectively.

The choice of the basis set depends on the specific problem. For instance, if the dynamics on the attractor are of interest (i.e., no transients), then Brown argues that a basis set orthonormal on the natural measure (which is relatively straight-forward to construct by Gram-Schmidt orthongonalization) is a good choice based on considerations of numerical stability. Other authors report using (perhaps nonorthogonal) polynomial or trigonometric bases.[14]

Given a basis set for the vector field $\mathbf{f}$, one possible method of integration is the Adams predictor-corrector method (which should provide better fits for less data than a straight Euler method),

$$\mathbf{x}(n+1) = \mathbf{x}(n) + \Delta t \sum_{j=0}^{M} a_j^{(M)} \mathbf{f}(\mathbf{x}(n+1-j)) \tag{47}$$

where $a_j^{(M)}$ are the implicit Adams predictor-corrector coefficients, and $M$ is the order of the method. In our case, we keep the standard predictor-corrector coefficients, we are given the $\mathbf{x}(n)$, and our task is to find $\mathbf{f}$.

Brown shows that the maximum likelihood method (which is just least squares in this instance) gives a fitting function of the form (see footnote [12] for more details),

$$\chi_{ML}^2 = \frac{1}{2N\sigma^2} \sum_{n=1}^{N} \left| \mathbf{x}(n+1) - \mathbf{x}(n) - \Delta t \sum_{j=0}^{M} a_j^{(M)} \sum_{I=0}^{N_p} \mathbf{p}^{(\mathbf{I})} \pi^{(\mathbf{I})}(\mathbf{x}(n+1-j)) \right|^2 . \tag{48}$$

The fitting equation leads to a unique solution once the order of the polynomial and the order of the Adams method is specified. Clearly, by taking both of these parameters to be large, a good fit can be achieved, but the number of parameters could easily be as large as the original data set. What we would like is an objective way of truncating the models. One answer to this kind of question is provided by the minimum description length principle, which is an extension of the maximum likelihood principle.

[13] R. Harber and H. Unbehauen, Structure identification of nonlinear dynamic systems—A survey on input/output approaches, Automatica 26 (4), 651-677 (1990)

[14] T. Eisenhammer et. al., Modeling experimental time series with ordinary differential equations, Biol. Cybern. 65, 107-112 (1991).

Let $\mathcal{X}$ denote the entire data set, and $\Theta$ the parameter set. The ML principle selects a model by minimizing

$$\chi^2_{ML} = -\log_2 \left[ P(\mathcal{X}|\Theta) \right], \tag{49}$$

where $P(\mathcal{X}|\Theta)$ is the joint probability of obtaining $\mathcal{X}$ and $\Theta$. The size of the model is a given in ML. The MDL principle selects a model by minimizing

$$\chi^2_{MDL} = -\log_2 \left[ P(\mathcal{X}, \Theta) \right], \tag{50}$$

where $P(\mathcal{X}, \Theta) = P(\mathcal{X}|\Theta)P(\Theta)$ is the joint probability of obtaining $\mathcal{X}$ and $\Theta$, and $P(\Theta)$ is the probability of obtaining $\Theta$, which uses the joint probability for obtaining the optimal size of a model. Roughly, the MDL principle tries to find the smallest encoding of the data *and* the vector field. Brown shows that this leads to a modified fitting functional of the form

$$\chi^2_{MDL} = \chi^2_{ML} + \frac{M_p}{2N} \left[ \ln(2\pi e N/M_p) + \ln(\|\Theta\|^2) \right]. \tag{51}$$

The new term is a penalty function for the size of the model. Rissanen has shown that this type of MDL fitting function has a unique minimum, thus (assuming the numerics can be evaluated) we can uniquely select a truncated model to encode the data.

The modeling procedure just outlined has successfully been applied to a number of experimental systems including the string experiment, chemical reactions, and discrete nonlinear circuits.

Empirical models constructed by these methods can be validate by a number of conventional (i.e., model error and residual analysis) and novel (synchronization and topological organization) methods. For instance, if the accuracy of the models for short term prediction is of interest, the relative prediction error,

$$\chi_E = \left| \frac{1}{N} \sum_{n=1}^{N} \frac{\left| \mathbf{x}(n+1) - \mathbf{x}(n) - \Delta t \sum_{j=1}^{M} a_j^{(M)} \mathbf{f}(\mathbf{x}(n+1-j)) \right|^2}{|\mathbf{x}(n+1) - \mathbf{x}(n)|^2} \right|^{1/2} \tag{52}$$

is calculated. This is the difference between the measured and model prediction normalized by the jump size taken by the integration step.

# 7 Current Research

To extend these techniques to behavioral modeling a number of technical and practical problems must be addressed. Here, I will mention the problems and pathways toward solutions.

1. How to handle multiple input signals?

If the input signals are generated by a deterministic process, then consider a higher-dimensional equivalent autonomous system. As a practical matter, the most straightforward way to proceed is to sample the input signals and create an embedded version of the input signals. Then tack this input space onto our model for the output space. This should create a deterministic model of the combined input-output space. A similar procedure should also be useful when the input signal is stochastic.[15]

2. How to handle (internal) parameter dependence?
Again, "parameter" dependent systems can be viewed as parameter free systems at the cost of higher dimensionality. Parameters become variables for training purposes. There are (difficult?) technical issues associated with efficiently training these larger dimensional models.

3. How to train on multiple data sets including transients?
The ML and MDL fitting functions can be modified to handle multiple data sets. Same problem as before, evaluating the new fitting function efficiently. Is there any "natural" choice for a basis set here?

4. How to design "optimal" input signals?
Currently, the procedure is to over sample the state space and "interpolate." One approach to designing a more efficient procedure would begin by considering the Fisher information matrix $M$,

$$M = \mathcal{E}\left(\frac{\partial \log P(\mathcal{X}|\Theta)}{\partial\Theta}\left(\frac{\partial \log P(\mathcal{X}|\Theta)}{\partial\Theta}\right)^T\right) \tag{53}$$

and to choose the experimental input $\mathcal{U}$ so that the Cramer-Rao lower bound $M^{-1}$ is minimized under the input constraints.

5. Can these procedures be automated?
Yes. The real question is, does the class of problems solved justify the expense of automation? For components modeled by a few ($< 7$?) ODE's, automation would represent a "nonlinear network analyzer." The success of a linear network analyzer, from an engineering point is view, is based, in a large measure, to the degree to which it buries the state space description. Can a similar theory/procedures be developed for this class of models? Probably not. But we can incorporated more analysis and functionality into instruments to bury the theoretical elements of these state space procedures.

Daniel Usikov and coworkers have recently developed a program that demos the automation of some of these modeling techniques.

[15] M. Casdagli, A dynamical systems approach to modeling input-output systems, in Nonlinear modeling and forecasting, edited by M. Casdagli and S. Eubank (Addison-Wesley, 1992).

6. Are there other alternatives?
Certainly, however for systems that can be accurately modeled by (almost stationary, low noise, low dimensional) differentiable dynamical systems, this marriage of dynamical systems theory and statistical inference theory would seem to be a good framework for addressing both the theoretical and practical questions associated with building nonlinear models.

This technical report describes the ground work for our nonlinear modeling technologies. Future technical reports will go into detail about the specific solutions we are developing to build accurate models for nonlinear (electronic) systems directly from input-output measurements.