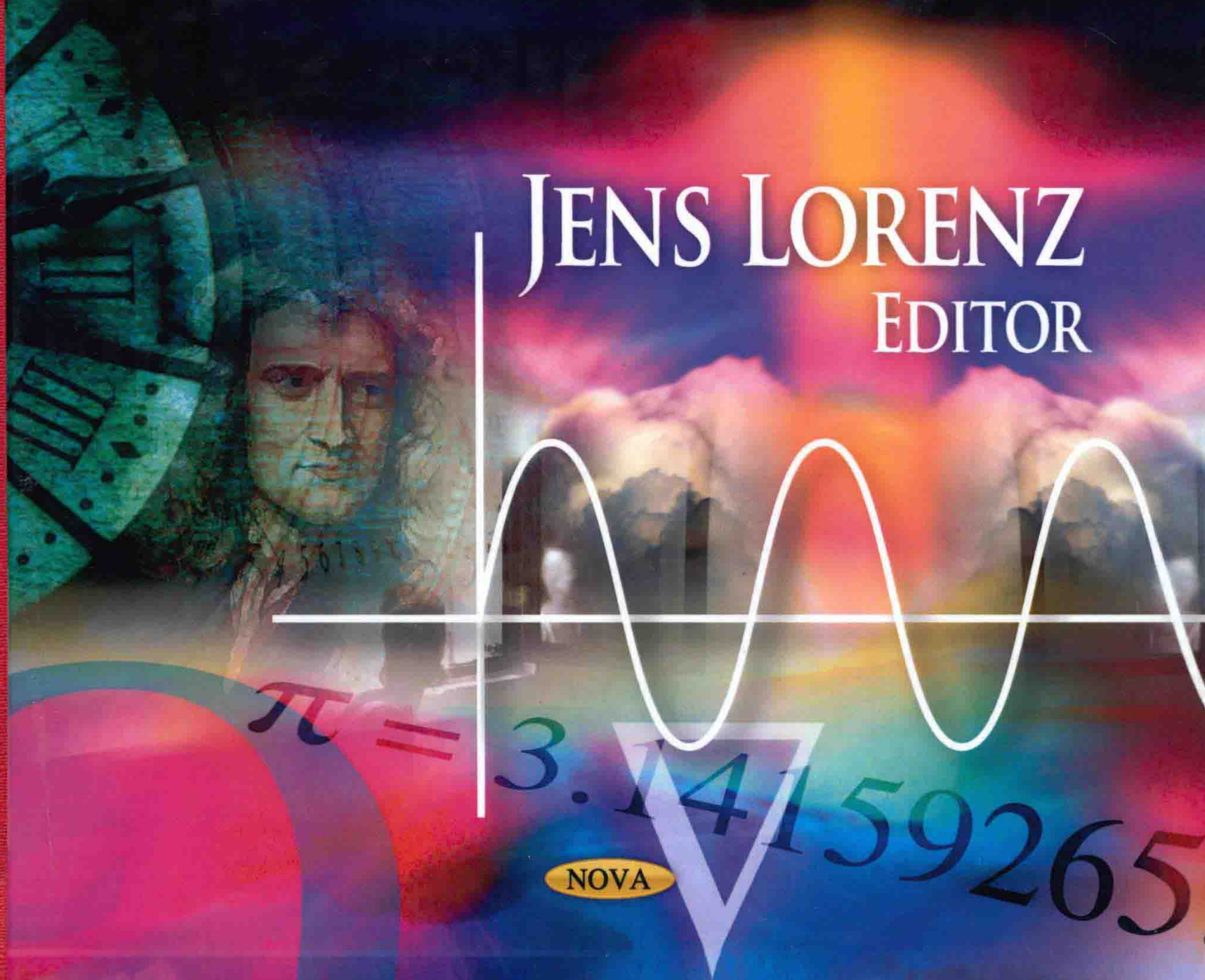
Mathematics Research Developments

Deterministic and Random Evolution

Jens Lorenz
Editor



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DETERMINISTIC AND RANDOM EVOLUTION

JENS LORENZ
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Mathematics is sharpening of common sense.

Preface

The first notes for this text were written during the summers of 2008–2010 when I taught a short course on mathematical modeling at the University of New Mexico. The audience consisted mostly of undergraduate mathematics students, and an aim of the course was to interest them in math at the graduate level.

The students had some basic knowledge of ordinary differential equations and numerics. I tried to build on this foundation, but instead of increasing the technical skills of the studen   I tried to lead them to more fundamental questions. What can one model with differential equations? What is determinism? If the universe evolves deterministically, what about free will and responsibility? Does it help if there are elements of randomness in the laws of evolution?

Of course, these are deep questions, and in this text we can only scratch the surface in our discussion. Nevertheless, mathematics — even at a rather elementary level — may help to clarify what is at stake. Throughout, I try to put the discussion into historical context. For example, the text contains a rather detailed description of the derivation of Kepler's laws of planetary motion using ordinary differential equations. After all, Newton's great success in deriving these laws were an important starting point of the scientific revolution and a deterministic world view. It made classical mechanics a model for all sciences.

Even if a deterministic description of an evolution is possible, there are often practical limitations of predictability because of the exponential growth in time of any uncertainty in the initial condition. Iteration with the logistic map gives an example. However, even if the accurate determination of future states is impractical, the *average behavior* of a system may still be very robustly determined. The logistic map again serves as an example. Do we have a similar situation for weather and climate? We cannot predict the weather two weeks in advance, but it may still be possible to determine the average weather 30 years from now.

There are similarities to random evolution. When throwing a fair coin, we cannot predict the outcome of the n–th throw, but we can be rather certain to have between 450 and 550 heads in a thousand throws. If you do not want to compute the exact probability for this claim and also do not want to throw a coin many thousand times, you can test the claim using a Matlab code and Matlab's random number generator. Some simple Matlab codes are provided in the text. They may encourage the readers to get their own experience with models for deterministic or random evolution.

The mathematical level of the text corresponds to the ability and experience of undergraduate mathematics students making the critical transition to graduate work. The text is accessible if you had an undergraduate course on ordinary differential equations and numerical methods. For some parts, it is good to be familiar with elementary concepts of probability and statistics, though the concepts will be reviewed in the text.

The course was part of an MCTP program, *Mentoring through Critical Transition Points*, supported by the NSF. It is a pleasant task to acknowledge the support by the NSF and to thank the PIs of the grant, Prof. Cristina Pereyra and Prof. Monika Nitsche, for their tireless work on all the details of the MCTP program. I also like to thank Katherine and Randy Ott, David Phillips, and Olumuyiwa Oluwasami for proof reading the text, for making figures, and for managing Latex.

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Contents

Chapter 1

Introduction

Summary: First we briefly introduce three classes of models, two of them are deterministic, namely initial value problems for ordinary differential and difference equations. The third class of models is random evolution in discrete time.

We then comment on three subjects that will be developed further in the text:

1. Newton's derivation of Kepler's laws and the resulting deterministic world view.

2. For sensitive deterministic systems, it is practically impossible to predict individual solutions, but *averages* may still be robustly determined. Is the weather/climate system an example?

3. Kinetic theory as an example relating micro and macro models.

Evolution is the change over time. In this text we introduce the reader to three classes of models that are used to describe evolutionary processes:

a) initial value problems for ordinary differential equations:

$$\frac{du}{dt} = f(u), \quad u(0) = u_0 . \tag{1.1}$$

Here $u(t)$ is a vector that specifies the state of a system at time t. At time $t = 0$ the state vector is given by the initial condition $u(0) = u_0$, and the differential equation $\frac{du}{dt} = f(u)$ then determines how the state $u(t)$ evolves in time.

The function $f(u)$ in (1.1) often depends on a parameter λ, i.e., $f(u) = f(u, \lambda)$. If this is the case, bifurcations and hysteresis phenomena may occur. Using simple examples, we will introduce these subjects in Chapter 8.

b) difference equations:

$$u_{n+1} = \Phi(u_n), \quad n = 0, 1, 2, \ldots \tag{1.2}$$

The vector u_n specifies the state of the system at time $t = n$, and Φ is a map of the state space into itself, which is assumed to be known. Given an initial state u_0, the equation (1.2) determines the sequence of states

$$u_0, u_1, u_2, \dots$$

One calls $\{u_n\}_{n=0,1,2,\dots}$ the orbit with initial value, or seed, u_0.

Whereas time is a continuous variable in (1.1), it changes discretely in (1.2). Time discretization occurs, for example, if one applies numerical codes to solve (1.1).

In general, replacing continuous time by discrete time, changes the dynamics not only quantitatively but also qualitatively. We will discuss this change using the logistic differential equation and the delayed logistic map as examples in Chapter 8.

c) random evolution: We will consider processes of the form

$$u_n \to u_{n+1} \quad \text{with probability} \quad p = p(u_n, u_{n+1}), \quad n = 0, 1, 2 \dots \tag{1.3}$$

The gambler's ruin problem serves as an example for the process (1.3); see Chapters 11 and 12. Random evolution with continuous time will also be discussed. In Chapter 13 we illustrate this by a model for a stochastic growth process.

We will apply elementary concepts from probability theory to analyze random evolutions and then compare the analytical results with numerical simulations. Matlab's random number generator is a great tool for running such simulations.

Throughout the text, simple Matlab codes are provided. They were not written to emphasize speed of execution or elegance of coding. The only aim is to make them easy to read. This may encourage readers to modify the codes and develop their own experience in mathematical modeling of evolutionary processes.

An aim of the text is also to discuss the more fundamental, or philosophical, aspects of mathematical models for evolution. A key figure of the scientific revolution of the 17th century was Johannes Kepler (1571–1630) who formulated his three laws for planetary motion in 1609 (first and second law) and 1619 (third law). Almost a century later, Isaac Newton (1643–1727) was able to deduce Kepler's laws by applying the inverse square law of gravitation to the two–body problem. This tremendous success of Newton not only removed the last doubts about the heliocentric system, but also advanced the scientific revolution in general. Newton's equations for the two–body problem can be formulated as an initial value problem of the form (1.1), which is a *deterministic* system (under mild assumptions on the function $f(u)$). In fact, one may say that Newton's success was a main reason for a *deterministic world view*, a search for a set of universal laws that rule the evolution of the universe. Throughout the text we will comment further on such issues. Of course, we cannot settle the age–old controversies regarding determinism, free will, causality, predictability etc. Nevertheless, the three classes of mathematical models (1.1)–(1.3) may help to clarify what is at stake.

How one models a phenomenon depends on the *scale* one is interested in. A good, but difficult, example is given by weather and climate. Weather and climate are similar phenomena, but on different time and space scales. We know the equations governing the change of the weather well and, with the help of computers, can use the equations to rather reliably predict the weather for a few days.

However, the weather system is too sensitive to make accurate predictions for a month in advance. How, then, can we predict the climate 30 years from now? This is difficult, indeed. Between day and night, the temperature at any place may change by 20 degrees or more. It may also vary by 20 degrees within a distance of less than 50 miles. This, together with the sensitivity of the weather system, makes it hard to believe that we can indeed predict a rise of the average temperature by three degrees in the next 30 years.

To illustrate that such a prediction is not completely hopeless and absurd, we will consider the logistic map, an example of a difference equation (1.2); see Chapter 6. The example shows that it may be practically impossible to predict future states accurately, but that the *average behavior* of the evolution is nevertheless very well determined and predictable. It is an open question if the same applies to the weather/climate models currently in use.

Conceptually, the situation is similar but easier for micro and macro models of fluids and gases. It is easier since we have good experiments and equations on the micro and the macro scale. Nevertheless, it is by no means trivial to connect the micro and macro models. This is the subject of kinetic theory. In Chapter 14, we give an introduction to this vast subject. If we had a similar theory relating weather and climate, our current climate predictions would have a sounder scientific base.

It seems that we face somewhat similar mathematical difficulties in micro and macro economics. The models work on different scales, but it remains a challenge to connect them mathematically with statistical arguments. How do the actions of a 100 million people determine the dollar/euro exchange rate?

In kinetic theory, the historically first result is attributed to Daniel Bernoulli (1700–1782), who tried to explain Boyle's law ($pV = const$) from a particle point of view. Bernoulli's simplifying assumptions are certainly wrong, but are still a stroke of genius and made his derivation possible. We present his arguments in Section 2.. We also describe James Clark Maxwell's (1831–1879) derivation of his velocity distribution, which is based on plausible symmetry assumptions for the probability distribution function. Maxwell's distribution, dating back to 1860, is historically very important: The first introduction of probability into physics.

A third remarkable result goes back to Sadi Carnot (1796–1832). Around 1770, James Watt (1736–1819) greatly improved the steam engine, an important starting point of the industrial revolution. Watt's engineering work also led to fundamental scientific questions: How can heat be used to produce mechanical work? Is there a most efficient way to do this? These are, of course, still important topics of engineering today. Amazingly, Sadi Carnot described an *idealized heat engine* that had *optimal efficiency*. Carnot's insights are remarkable since at his time *conservation of energy*, i.e., the first law of thermodynamics, was not yet understood.

The dynamic interpretation of Carnot's ideas later led to various formulations of the second law of thermodynamics. Some of the related mathematical issues were first addressed by Ludwig Boltzmann (1844–1906) and are still an active research topic today. In the last chapter of the book we describe a random evolution which illustrates the transition from order to chaos, or the direction of time, in an elementary way.

Chapter 2

Basic Concepts

Summary: In this chapter we will give more details about the three classes of models, initial value problems for ODEs, difference equations, and discrete–time random evolution. The important concept of a Markov chain will be introduced. We also discuss the notion of randomness.

1. Initial Value Problems for ODEs

In this section we introduce some basic concepts for first order systems of ordinary differential equations (ODEs). More advanced concepts, like stability, bifurcation, different time scales, and sensitive dependence on initial conditions will be discussed later.

Let us start with a simple example of an initial value problem for a scalar ODE:

$$u'(t) = -u(t) + 1, \quad u(0) = 3 \ . \tag{2.1}$$

Here $u = u(t)$ is the unknown function. We will think of the independent variable t as time. As one learns in any introductory ODE course, the general solution of the differential equation $u' = -u + 1$ is $u(t) = 1 + ce^{-t}$ where c is a free constant. Imposing the initial condition $u(0) = 3$ leads to $c = 2$, i.e., the solution of the initial value problem (2.1) is

$$u(t) = 1 + 2e^{-t} \ .$$

For this simple example, the following is quite obvious: The general law of evolution, expressed by the differential equation $u' = -u + 1$, together with the initial condition $u(0) = 2$, determines the value of the solution $u(t)$ exactly at any other time t. The future $(t > 0)$ as well as the past $(t < 0)$ values of the solution are exactly determined by the initial condition and the general law of change. In other words, the initial value problem (2.1) gives a simple example of how to encode a deterministic evolution.

In more advanced courses on ODEs one learns how to generalize these simple observations. The function $u = u(t)$ may be vector valued, $u(t) \in \mathbb{R}^N$, where $\mathbb{R}^N$ is called the state space . The general law of evolution becomes a system of ODEs, $u' = f(u)$, where $f : \mathbb{R}^N \to \mathbb{R}^N$ maps the state space into itself. [1] If $u_0 \in \mathbb{R}^N$ is any fixed state, then the initial value problem

$$u'(t) = f(u(t)), \quad u(0) = u_0 \tag{2.2}$$

is a generalization of example (2.1). If the function f obeys some technical condition [2] then the initial value problem (2.2) can be shown to have a unique solution $u(t)$ defined for all time, $-\infty < t < \infty$. As in example (2.1), the state of the system, described by $u(t)$, is precisely determined by the general law of evolution $u' = f(u)$ and the state of the system at any particular time, for example by the initial condition $u(0) = u_0$.

The clear distinction between a general law of change, like $u' = f(u)$, and the specification of the state of a system at a particular time, $u(0) = u_0$, appears to be due to Isaac Newton. Some people have called this Newton's greatest discovery. [3] One of Newton's important contributions to science is the solution of Kepler's problem. Based on observations by Tycho Brahe (1546–1601), Kepler formulated his three laws of planetary motion : (1) Every planet travels around the sun in an elliptical orbit with the sun at one focus; (2) The line joining the sun to the planet sweeps out equal areas in equal times; (3) If T is the time of revolution around the sum and a is the major semi–axis of the planets orbit, then $T^2 = const \cdot a^3$ where the constant is the same for all planets.

Newton succeeded in deriving Kepler's laws from the inverse square law of gravity and Newton's second law, *force = mass times acceleration*. Newton's success was very influential for the history of science. Classical mechanics became a model for all sciences. For example, numerous (unsuccessful) attempts were made to explain light and electro–magnetic phenomena in terms of mechanics.

Remark: The result that the initial value problem (2.2) has a unique solution if f is Lipschitz continuous can be shown by a contraction argument applied to Picard's iteration:

$$u^{n+1}(t) = u_0 + \int_0^t f(u^n(s))\, ds, \quad n = 0, 1, 2, \ldots$$

with $u^0(t) \equiv u_0$. In general, if the vector function $f(u)$ is nonlinear, one cannot obtain an explicit formula for the solution $u(t)$, however.

[1] One can also allow $f = f(u,t)$ to depend explicitly on time, i.e., the law of change may change in time.

[2] A sufficient condition is Lipschitz continuity of f, i.e., there is a constant L so that the estimate $\|f(u) - f(v)\| \le L\|u - v\|$ holds for all $u, v \in \mathbb{R}^N$. Here $\|\cdot\|$ is any norm on the state space $\mathbb{R}^N$.

[3] This distinction has proved to be very useful in many areas of science. An exception is the cosmology of the early universe where the distinction between the initial state and the general law of evolution gets blurred.