

# 1 Part 1: CS 28501 (Topics in Scientific Computing)

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## 1.1 Part 1a: Introduction to Dynamical Systems, Numerical Methods and Programming

The emphasis in Part 1a is on defining basic concepts and presenting examples that help provide a foundation for understanding the more general development given in Part 2.

### 1.1.1 Lecture 1: Discrete dynamical systems I

What is a dynamical system. How do they arise in problems in physical science, biology, chemistry, and economics.

Derivation of the discrete logistic equation as a population growth problem

$$x_{n+1} = x_n + gx_n\left(1 - \frac{x_n}{C}\right) \quad (1)$$

$C$  is the *carrying capacity*. The population stops growing, and begins dying off, if the carrying capacity is exceeded. The equation can be reduced to the following standard form

$$x_{n+1} = ax_n(1 - x_n) \quad (2)$$

This is an instance of a general class of dynamical systems, consisting of iterated maps on  $\mathbb{R}$ . The general problem is  $x_{n+1} = f(x_n, \lambda)$  where  $\lambda$  is a parameter or vector of parameters.

We now define some basic concepts.

A fixed point is a point such that  $f(x) = x$

Stability of fixed points. Definition of stability. Definition of asymptotic stability. Not all stable systems are asymptotically stable. Example:  $f(x) = -x$ .

Linearization about a fixed point. Stability criterion. The amplifying factor  $\gamma$  ( $x'_{n+1} = \gamma x'_n$ ). Growth rate  $\kappa = \ln \gamma$  ( $x'_n = x'_0 \exp(\kappa n)$ )

Nonlinear stability. Global asymptotic stability. Linear asymptotic stability guarantees nonlinear stability, but linear neutral stability does not. Example:  $f(x) = -x \pm x^3$

Proof of nonlinear stability: Suppose that  $x_0$  is a fixed point,  $|f'(x_0)| < 1$ , and  $f'$  is continuous in an open neighborhood of  $x_0$ . Then, the mean value theorem implies that  $|f(x_1) - f(x_0)| = |f'(x_m)||x_1 - x_0|$  for some  $x_m$  in the interval. Continuity of  $f'$  implies that we can make  $|f'(x)| < |f'(x_m)| + \epsilon < 1$  by making the interval small enough. Let  $M = |f'(x_m)| + \epsilon$ . Then we have  $|f(x_1) - x_0| = |f(x_1) - f(x_0)| < M|x_1 - x_0|$ , which proves the assertion, since the  $n^{\text{th}}$  iterate of any  $x$  in the interval will satisfy  $|x_n - x_0| < M^n|x_1 - x_0|$ , which can be made arbitrarily small.

Point out that the above is an example of a *Lipschitz* condition. A function need not be continuously differentiable to have a Lipschitz property.

Now we return to the specific case of the discrete logistic map.

Show sketch of the map. Graphical iteration.

**Proposition 1:** If  $a \leq 4$ , the map maps the unit interval into itself.

**Proposition 2:** If  $a < 2$  the map takes the unit interval into  $[0, b]$ , with  $b < .5$ . The map is expanding near the origin, though ( $|f'| > 1$ ). The origin is a *repellor*. (or "source"). (We'll see soon that the map is contracting in a suitably defined subinterval).

**Proposition 3:** If  $a < 1$  the map is contracting everywhere,  $|f'| < 1$ . It is a *contraction map*, and everything is *attracted* to the origin regardless of its initial position in the unit interval. (This is an example of a type of *fixed point theorem*).

Definition: *Invariant set*. Fixed points are an invariant set. In fact, any orbit forms an invariant set. Proposition: For  $2 < a \leq 4$ , the interval  $[0, a/4]$  is an invariant set. However, there are smaller invariant sets. Once orbits leave the vicinity of the origin, they have no way of getting back. We will return to this point later when we discuss limit sets and attractors. The left hand boundary is  $f(a/4)$  as can be verified by graphical integration. This does approach zero as  $a \rightarrow 4$ .

The fixed points of the logistic map, and their stability. Dependence of results on  $a$ :

- Fixed point at  $x = 0$ . Stable if  $a < 1$ , otherwise unstable.
- Fixed point at  $x = 1 - 1/a$  if  $a > 1$
- For the second fixed point,  $\gamma = 2 - a$ , so it is stable without oscillations for  $1 < a < 2$ , and stable with oscillations for  $2 < a < 3$ . It is unstable for  $a > 3$ .

Bifurcation diagram. The bifurcation criterion: bifurcations occur only where  $f'(x, a) = 1$ .

Illustrate repulsion from unstable fixed point, attraction to stable fixed point, and transition from non-oscillatory to oscillatory behavior by numerical simulation.

### 1.1.2 Lecture 2: Discrete dynamical systems II

Definition of periodic orbit. Bifurcation from an unstable fixed point to a periodic orbit. Periodic orbits are fixed points of  $n$ -times composition of  $f$ . Show plots illustrating this point, and bifurcation from unstable fixed point in the logistic map.

Linear stability of periodic orbits.

Definition of  $\alpha$  and  $\omega$  limit sets. Definition of an attractor, and basin of attraction.

Bifurcation of periodic orbits as they cross stability threshold. Application of bifurcation criterion to  $n$ -times composition. Period doubling bifurcations.

(Note on using mapExplorer to compute stability of periodic orbits: The growth rate is very sensitive to the initial position. All the growth rates for members of a cycle should be identical, but at low resolution (e.g. 1000 points in the interval), the error in the orbit position throws this off. At 10000 points, it's much better. At some point, I'll add a bisection refinement step to the periodic orbit finder, to improve this).

The numerically generated orbit bifurcation diagram for the logistic map. Chaotic behavior. Goes chaotic at around  $a = 3.6$ . Some properties of chaos:

- Sensitive dependence on initial conditions. Lyapunov exponents as a measure of sensitivity. Alternate definition of sensitivity (HSD p. 341). Illustrate both with numerical simulation
- Unstable periodic orbits are dense. Illustrate.
- Transitivity.

Other 1D maps (Tent map. Bernoulli map.). We will define these maps, but leave exploration of behavior to problem set.

**Definition:** Conjugacy of chaotic systems. Maps  $f$  and  $g$  are conjugate on an interval if there is a bijective continuous map  $h$  such that  $h \circ f = g \circ h$ . Note that  $h$  need not be a diffeomorphism.

**Proposition:** Conjugacy preserves periodic orbits. Therefore if one map in a conjugate pair has a dense set of periodic orbits, the other map does as well.

**Proposition:** Conjugacy preserves sensitive dependence to initial conditions. (HSD p 341). Define "sensitivity" constant, and distinguish from Lyapunov exponent. Conjugacy does not preserve stability properties of fixed points and periodic orbits.

**Number theory meets dynamical systems: the  $3n + 1$  conjecture.** This is a nonlinear map on  $\mathbb{Z}^+$ , defined by the following procedure. Take an integer  $n$ . Form a new integer  $3n + 1$ . If the result is even, divide by 2 repeatedly until you are left with an odd integer. The conjecture: No matter what initial  $n$  you take this procedure inevitably terminates at 1 after a finite number of iterations. Powers of 2 are "drains," or strongly contracting points. Proposition: Rate of growth is bounded by  $2(3/2)^M - 2$ . (results from the fact that  $3n + 1$  is even if  $n$  is odd, so we divide by 2 at least once, yielding  $(3/2)n + 1/2$ . Result follows by iteration, and using formula for geometric series. Note that we can construct short cycles for arbitrarily large numbers. suppose  $3j + 1 = 2^m$ . This can be satisfied with integer  $j$  when  $2^m \equiv 1 \pmod{3}$ , i.e. when  $m$  is even. Then  $j = (2^{2n} - 1)/3$  gives a cycle of length 2. Can we construct arbitrarily long cycles?

*Optional:* A brief discussion of maps on the plane. The sin-sin map. Special consequences of being area preserving.

### 1.1.3 Lectures 3 and 4: Python

Analysis of 1D dynamical systems will be used throughout these lectures to illustrate the use of Python in exploratory numerical work.

Logging on to the server. How to get an xterm. `ssh -X -l<username> seine.local` or `ssh -X -l<username> 192.168.0.9` or (from outside the Paris center ) `ssh -X -l<username> 81.255.59.189`.

Basics of programming in Python: Variables, lists,modules,functions, loops, conditionals. Uses of list comprehension and list methods. Using the Python development environment to write and edit programs.

Objects and object-oriented programming;Basic use of objects; simple examples. Use of the `mapExplorer` object.

Anatomy of the `mapExplorer` object, used in exploring the logistic map.

The `Numeric` array module. Example: Use of array arithmetic to compute the growth of the log of the distance between two orbits, and test convergence of the Lyapunov exponent. For a reprise of what was done in class, look at the module `lyapPlot`.

Overloading operators (use  $\mathbb{Z}[\sqrt{5}]$  as example). The the examples in the module `ObjectExamples`.

Use of the simple plotting package;Writing out your results to a file. See Python notes, and also look at examples of how plotting is done in the `mapExplorer` class and in the function `ezplot` contained in the `map1D` module. Saving a plot as postscript. Converting to pdf (`pstopdf` on OSX, but `ps2pdf` may also be available).

#### 1.1.4 Lecture 5 and 6: Introduction to ODEs

Definition of an ordinary differential equation;Differential equations defined in terms of a map on function spaces; Linear vs. nonlinear maps, and why linear is easier (superposition); One should think of solution of O.D.E. as a matter of substituting in a function and see if it maps to zero, not primarily in terms of "sniffing out" the solution from a starting point.

Example of non-uniqueness:  $dy/dx = y^{2/3}$ .  $dy/dx = y/x$ .

ODE's have *families* of solutions, and auxiliary (e.g. initial) conditions must be specified to pick out which one we want. Examples of solution families (see BR Chapter 1). Specify a family of functions, and find what ODE it satisfies.  $y = \sqrt{C + x}$ . Generalization to normal-curve families  $y = f(x, c)$ ,  $f$  continuously differentiable with respect to both arguments, which can be solved for  $c(x, y)$  having  $\partial_y c \neq 0$ .

For  $dy/dx = f(x)$  or  $dy/dx = f(y)$  the problem reduces to quadrature (integration).

Solution methods for first order equation initial value problems. Separation of variables. Integrating factors. General solution to the first order linear ODE.

Scientific examples:

- Radiative cooling of an object.  $\frac{dT}{dt} = -aT^4$
- Logistic equation (example of growth and saturation).  $\frac{dC}{dt} = (1 - C)C$ . This also provides an example of solution by partial fractions.

- Finite time blowup. Condorcet's equation.  $\frac{dC}{dt} = (1 + C)C$ . Condorcet's philosophy (the anti-Malthus), and his sad fate.
- Ocean mixed layer, Newtonian cooling, forced by oscillating heat source. Use of complex exponentials in solution.

Lipschitz conditions.

Lemma on exponential bound of solution to D.E.

Separation theorem, and proof of uniqueness (Existence proof in Part 2)

Comparison theorem.

### 1.1.5 Lectures 7 and 8: Linear ODEs

This is the section in which we develop the notion that linear ODE's are basically an extension of finite dimensional linear algebra.

General discussion of linear, second-order differential equations with nonconstant coefficients: Linear operators,  $d/dx$  is not a continuous operator, linear independence, bases, Wronskian, uniqueness (i.e. is there anything nontrivial in the kernel?); the variation-of-constants method for the inhomogeneous problem and the influence (or Green's) function; Introduction to idea of "weak solution", and theory of distributions; the system formulation; Poincaré phase plane.

Oscillation theorems.

Examples. The Harmonic oscillator. Phase portrait for the harmonic oscillator. Green's function for the damped harmonic oscillator initial value problem.

#### Derivation of the Green's function

We wish to solve

$$\frac{d^2y}{dx^2} + p(x)\frac{dy}{dx} + q(x)y = r(x) \quad (3)$$

with  $r(x) = 0$  for some  $x < x_a$  and subject to the initial condition  $y(x) = y'(x) = 0$  at  $x = x_a$ . (Note: The condition on  $r$  can be relaxed somewhat, and the problem can be generalized to cases where  $r$  vanishes sufficiently rapidly at  $-\infty$ .) We solve the problem by constructing the Green's function  $G(x, x_1)$ , which satisfies the equation

$$\frac{d^2}{dx^2}G(x, x_1) + p(x)\frac{d}{dx}G(x, x_1) + q(x)G(x, x_1) = \delta(x - x_1) \quad (4)$$

where the symbol  $\delta$  represents an entity with the property that  $\delta(\zeta) = 0$  for  $\zeta \neq 0$  and

$$\int_{-\infty}^{\infty} \delta(\zeta)d\zeta = 1 \quad (5)$$

Of course, there is no such function with this property, but as discussed in class it is possible to make sense of this symbol as a "weak limit" of a sequence of ever-sharper functions, or as a linear map from a suitably defined function space to the reals. It is an example of what is called a *distribution*. A consequence of the definition of  $\delta$  is that its integral is unity over any interval containing

the origin, however small. Similarly, the integral of  $f(\zeta)\delta(\zeta)$  over any interval containing the origin is  $f(0)$ .

If we multiply Eqn. 4 by  $r(x_1)$ , integrate with respect to  $x_1$ , and make use of linearity (on the left hand side) and the definition of  $\delta(\zeta)$  on the right hand side, we find immediately (well, almost) that the following is a solution to the homogeneous problem which satisfies the desired initial conditions:

$$y(x) = \int_{x_1=-\infty}^{\infty} G(x, x_1)r(x_1)dx_1 \quad (6)$$

Note that if you think of  $G$  as a sort of a matrix, but with real-valued rather than integer indices, this integral expresses a form of "matrix multiplication" extended to infinite, indeed continuous, dimensions. The Green's function is in fact the "matrix" expressing the inverse of the operator  $L = d^2/dx^2 + pd/dx + q$ .

Now we show how to construct  $G$  in terms of a solution basis of the *homogeneous* problem. First, we prove a few lemmas concerning the continuity properties of  $G$  at  $x_1$ . Using integration by parts, we find that for any function  $F(x)$ , the following relations hold in the limit  $\epsilon \rightarrow 0$ , provided  $|F|$  is bounded above near  $x_1$ :

$$\int_{x_1-\epsilon}^{x_1+\epsilon} F(x)dx = 0 \quad (7)$$

$$\int_{x_1-\epsilon}^{x_1+\epsilon} (x - x_1)F(x)dx = 0 \quad (8)$$

$$\int_{x_1-\epsilon}^{x_1+\epsilon} \frac{dF}{dx} dx = F(x_1 + \epsilon) - F(x_1 - \epsilon) \quad (9)$$

$$\int_{x_1-\epsilon}^{x_1+\epsilon} (x - x_1) \frac{dF}{dx} dx = 0 \quad (10)$$

$$\int_{x_1-\epsilon}^{x_1+\epsilon} (x - x_1) \frac{d^2F}{dx^2} dx = -(F(x_1 + \epsilon) - F(x_1 - \epsilon)) \quad (11)$$

So, we first multiply Eqn. 4 by  $(x - x_1)$  and integrate over a small interval, which, using the lemmas, tells us that  $G(x, x_1)$  is continuous at  $x = x_1$ , i.e.  $G(x_1 + \epsilon, x_1) = 0$ . Then, we integrate Eqn. 4 over the small interval, but this time *without* first multiplying by  $x - x_1$ . Using our previous continuity result and the definition of the  $\delta$ -function, we then find the jump condition:

$$G'(x_1 + \epsilon, x_1) - G'(x_1 - \epsilon, x_1) = 1 \quad (12)$$

where  $G'(x_1 + \epsilon, x_1)$  is shorthand for the derivative of  $G$  with respect to its first argument, evaluated at  $x = x_1 + \epsilon$ . Because  $G$  is identically zero for  $x < x_1$ , the second term on the left hand side vanishes for the initial value problem we are considering.

Now we can construct  $G$  given two independent solution of the *homogeneous* problem, which we will call  $y_1(x)$  and  $y_2(x)$ . The solution  $G = a \cdot$

$(y_1(x)y_2(x_1) - y_2(x)y_1(x_1))$  is a solution of the homogeneous problem, by superposition. It also satisfies the continuity equation that  $G(x + \epsilon, x_1) = 0$  as  $\epsilon$  approaches zero. Because the two solutions are linearly independent, we know that  $G$  is not identically zero. We are almost done now, since we only need to choose  $a$  so as to satisfy the jump condition on  $G'$ . This condition requires that  $a = 1/(y_1'(x_1)y_2(x_1) - y_2'(x_1)y_1(x_1))$ . The astute student will notice that  $a$  is just the reciprocal of the Wronskian of the two solutions, which is guaranteed to be nonzero whatever the value of  $x_1$  (since the two solutions are linearly independent). To summarize, the Green's function is

$$G(x, x_1) = \frac{1}{W[y_2, y_1](x_1)}(y_1(x)y_2(x_1) - y_2(x)y_1(x_1)) \quad (13)$$

*Example:* Let's find the Green's function that solves the problem

$$\frac{d^2y}{dx^2} + y = r(x) \quad (14)$$

The functions  $y_1 = \sin(x), y_2 = \cos(x)$  form a solution basis. Their Wronskian is constant, and has the value  $W = 1$  (There is a general class of problems for which the Wronskian will be constant. What is it?). Thus the Green's function is

$$G(x, x_1) = \sin(x)\cos(x_1) - \sin(x_1)\cos(x) = \sin(x - x_1) \quad (15)$$

Note that in this case, the Green's function turns out to be a function of  $x - x_1$ , i.e.  $G = G(x - x_1)$ . This is a (generalizable) consequence of the fact that we started with a constant-coefficient system.

### 1.1.6 Lecture 9: Equations with constant coefficients

Preliminary: Uniqueness for  $n$ th order linear equation with non-constant coefficients.

Linear differential equations with constant coefficients; the characteristic polynomial; Operator polynomials, factoring the characteristic polynomial, and use of commutativity of factors; multiple roots;

**Lemma**  $(d/dx - a)^n(x^m \exp(ax)) = 0$  for  $0 \leq m < n$ .

*Optional:* The method of undetermined coefficients for the inhomogeneous problem. Green's functions and transfer functions.

### 1.1.7 Lecture 10: Systems of equations

The reformulation of linear equations with constant coefficients as linear systems; system formulation of the general initial-value problem; Solution bases and the "resolvent" for general systems; Reduction of constant-coefficient case to matrix eigenvalue problem; A few remarks on repeated roots and Jordan canonical forms.

Autonomous, nonlinear systems and the stability of their equilibrium points; Possibility of algebraic instability in the case of repeated neutral eigenvalues.

"Autonomization" (turn N-d non-autonomous into (N+1)-d autonomous).  
*Foucault's Pendulum*

For small amplitude oscillations, the motion of the Foucault pendulum is described by the equations

$$\frac{d^2x}{dt^2} = -x + f \frac{dy}{dt}, \quad \frac{d^2y}{dt^2} = -y - f \frac{dx}{dt} \quad (16)$$

If  $f = 0$  this consists of two independent harmonic oscillators. The general solution can be built as a sum of solutions of the form

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} A \\ B \end{bmatrix} e^{-i\omega t} \quad (17)$$

Substituting into the differential equation yields the system

$$\begin{bmatrix} 1 - \omega^2 & i\omega f \\ -i\omega f & 1 - \omega^2 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = 0 \quad (18)$$

Taking the determinant and doing a little re-shuffling of terms yields the characteristic equation in the form:

$$(\omega^2 - 1)^2 - (\omega^2 - 1)f^2 - f^2 = 0 \quad (19)$$

whence

$$\omega^2 - 1 = \frac{f^2 \pm \sqrt{f^4 + 4f^2}}{2} \quad (20)$$

The solutions are  $\pm\omega_+$  and  $\pm\omega_-$ , where  $\omega_+$  and  $\omega_-$  are the two positive solutions of Eq. 20 obtained by taking the + or - sign on the right hand side, respectively. It can be shown that the "-" branch of the right hand side is never below -1, and asymptotes to -1 as  $f \rightarrow \infty$ . For the "+" branch, the right hand side is always positive. Hence,  $\omega$  is always real. It is easily seen that,  $\omega_-$  is  $1 - f/2$  at small  $f$ , and asymptotes to 0 at large  $f$ . Further  $\omega_+$  is  $1 + f/2$  at small  $f$  and asymptotes to  $f$  at large  $f$ . We find the corresponding  $A$  and  $B$  from Eq. 18, which can be satisfied by

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} i\omega f \\ \omega^2 - 1 \end{bmatrix} \quad (21)$$

The solution for the eigenvector is undetermined up to multiplication by a constant. We denote the solution corresponding to  $\omega_+$  by  $A_+$  and  $B_+$ , and so forth. Since the eigenvalues come in plus-minus pairs, solutions can be superposed to yield a real solution; this is guaranteed by the fact that the original equation had purely real coefficients. The general real solution is then

$$\begin{bmatrix} x \\ y \end{bmatrix} = \text{Re}(a \begin{bmatrix} A_+ \\ B_+ \end{bmatrix} e^{-i\omega_+ t} + b \begin{bmatrix} A_- \\ B_- \end{bmatrix} e^{-i\omega_- t}) \quad (22)$$

The constants  $a$  and  $b$  are determined by the initial conditions. Now:

- Discuss pure periodic solutions ( $b=0$  or  $a=0$ ). Ellipses



- Superpose to get solutions with  $x = y = 0$  at  $t = 0$ .  $a = B_-$ ,  $b = -B_+$ .

$$\begin{bmatrix} A_{\pm} \\ B_{\pm} \end{bmatrix} = f \begin{bmatrix} i \\ \pm 1 \end{bmatrix} \quad (23)$$

Now we:

- Factor out sum and difference frequencies
- Write solution as a product of a rapidly oscillating part and a slowly rotating vector
- Voila!

The lecture will finish with a few plots of the orbits in the  $xy$  plane, for various values of  $f$ .

We hope to organize an informal field trip to *Musée des Arts et Metiers* to see Foucault's original pendulum.

### 1.1.8 Lectures 11 and 12: Numerical solutions

Introduction to concept of numerical approximation; reduction from infinite dimensional operator to finite dimensional operator; "Consistency" (convergence; accuracy of approximation; Approximation of first and second derivatives by finite difference (second order). Taylor polynomials for functions that don't have a convergent Taylor series, or even infinitely many derivatives. Methods for numerical solution of ODE. Use of Automization. Euler method. Mid-point method (RK2); derivation of fourth-order Runge-Kutta; implementation of Runge-Kutta in Python; error estimates; (Adaptive step-size implementation deferred). Examples of performance; What happens if the rhs is has fewer than four derivatives?

Approach to RK derivation: Derive coefficients for one-step (Euler) and two-step (midpoint) methods. Then turn to 4th order case, which is done by the same idea, but with more algebra. A lot more algebra. To spare students the pain, we will only summarize the algebra enough to make it clear that the general attack on the second order case carries over to fourth order. It is a little miracle.

Numerical stability. Illustration for Euler method applied to exponentially damped 1D system.