2. Complex Dynamics:

a. The Logistic Map

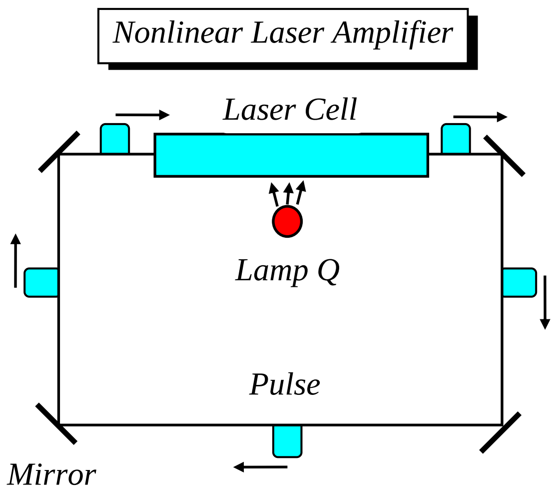


Figure 5: Experimental setup of laser racetrack.

A simple laser amplification system that shows both orderly and chaotic behavior is illustrated in Fig. 5. This somewhat schematic situation represents many actual systems in chemistry, physics, and other branches of science. For example, it can stand for the excitation of vibrational modes in molecular collisions or describe population dynamics.

The gas atoms in the laser cell are excited initially by a flashlight (Lamp ***Q***) to a maximum population inversion (normalized to) ***I = 1***. Then, at some time, an initial laser pulse of intensity $I_0 < 1$ is emitted from the cell and deflected by mirrors back into the cell. Here, it will partially be absorbed by exciting gas atoms, but will also stimulate emission of light with the same frequency. Consequently, another pulse will emerge from the cell with intensity I_1 which must be proportional to the incoming intensity I_0. It is also proportional to the maximum intensity possible, i.e., proportional to the content $(1 - I_0)$ of the cell remaining after the previous pulse has been emitted.

This is a repetitive process, where the intensity I_{n+1} of the outgoing pulse depends on the intensity I_n of the previous, incoming, pulse. Keeping track only of the last pulse and neglecting the small change in the population inversion, for simplicity, one arrives at the **iterative map**

$$I_{n+1} = \mu \cdot I_n \cdot (1 - I_n) \quad \text{or} \quad f(I) = \mu \cdot I(1 - I) \quad (I>0) \qquad (4)$$

Graphic Iteration

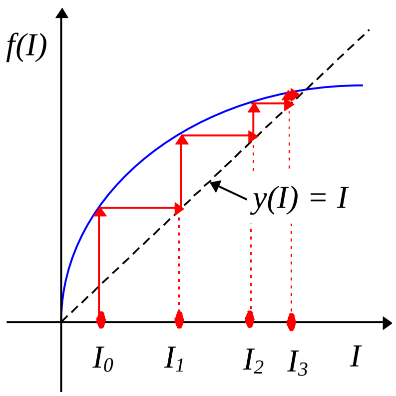


Figure 6: Iterating a map by reflexion at diagonal.

Here, the quantity μ is the overall **gain or amplification** factor of the setup. Such functions *f(I)* determining the behavior of a dynamical system by iteration

I, f(I), f(f(I)), f(f(f(I))), f(f(f(f(I)))), ...

are called **mapping**s or **map**s. The above map (Equ. 4) is known as quadratic or "**logistic map**", because one of the situations it describes is the development of a population *I* for a constant overall food supply. In this latter case, *I = 1* is the maximum sustainable population, and the food supply remaining, once a population of the size *I* has been satisfied, is proportional to (*1 - I*). Then, the population is expected to grow, generation by generation, like $I_{n+1} \propto I_n \exists (1 - I_n)$, which is equivalent to Equ. (4).

To get an idea of the sequence of steps given by a map, one can apply the simple **graphic procedure** illustrated in the sketch. The forward trajectory of the system following the map *f* is given by the sequence $I, f(I), f^{2}(I), \ldots, f^{n}(I), \ldots$, the backward trajectory is given by $I, f^{-1}(I), f^{-2}(I), \ldots, f^{-n}(I), \ldots$. The sequence can be viewed as a "staircase" defined by the curve *f(I)* and *y(I) = I.*

The point I_0 is a **"periodic" point**, if $f^{n}(I_0) = I_0$. A **fixpoint** is defined by the condition $f(I_0) = I_0$ and represents, graphically, an intersection between the curves *f(I)* and *y(I) = I.* Fixpoints can be **"attractors"** or **"repellors"**, depending on whether or not trajectories starting in the neighborhood of I_0 will converge. The separation of two trajectories starting at I_0 and $I_0+\Delta I$ *is given by*

$$|\Delta f| = |f(I_0+\Delta I) - f(I_0)| = |\Delta I| \cdot |(df/dI)| \qquad (5)$$

Hence, their initial separation grows or shrinks, depending on whether the derivative is larger or smaller than unity. Therefore,

$$\left|\left(\frac{df}{dI}\right)_{I_0}\right| < 1 \qquad (I_0 = Attractor) \qquad \left|\left(\frac{df}{dI}\right)_{I_0}\right| > 1 \qquad (I_0 = Repellor) \qquad (6)$$

In the case of the logistic map defined in Equ. 2, one calculates the fixpoint from the condition

$$\mu I - \mu I^2 = I$$

leading to

$$\mu I^2 = I(\mu - 1)$$

and

$$I_{Fixpoint} = \frac{\mu - 1}{\mu} \tag{7}$$

In addition, $I = 0$ is a trivial fixpoint, since $f(0)=0$. In the present application to a laser system, where I represents an intensity, the range of acceptable I values is the positive real axis. For example, **for $\mu = 2.5$, the fixpoint is located at $I = 0.6$**. The derivative of the function representing the logistic map,

$$df/dI = \mu \cdot (1-2I) \tag{8}$$

and

$$\left| \left(\frac{df}{dI} \right)_{I=(\mu-1)/\mu} \right| = |2 - \mu| \tag{9}$$

is =0.5 and, hence, smaller than unity. Therefore, the above fixpoint is an attractor, i.e., all trajectories will converge to it.

In the following, some calculations of the behavior of the laser amplifier are made with the mathematical software package ***MATHCAD*** {mathcad\Logistic_MAPi.MCD}, to demonstrate numerically the different orderly or chaotic conditions for this system.

The figure shows the ***logistic map*** (see Equ. 4) and some *related maps* (for k≠1) of the kind

$$f(x) := \mu x^k \left(1 - x^k\right)^{1/k} \tag{10}$$

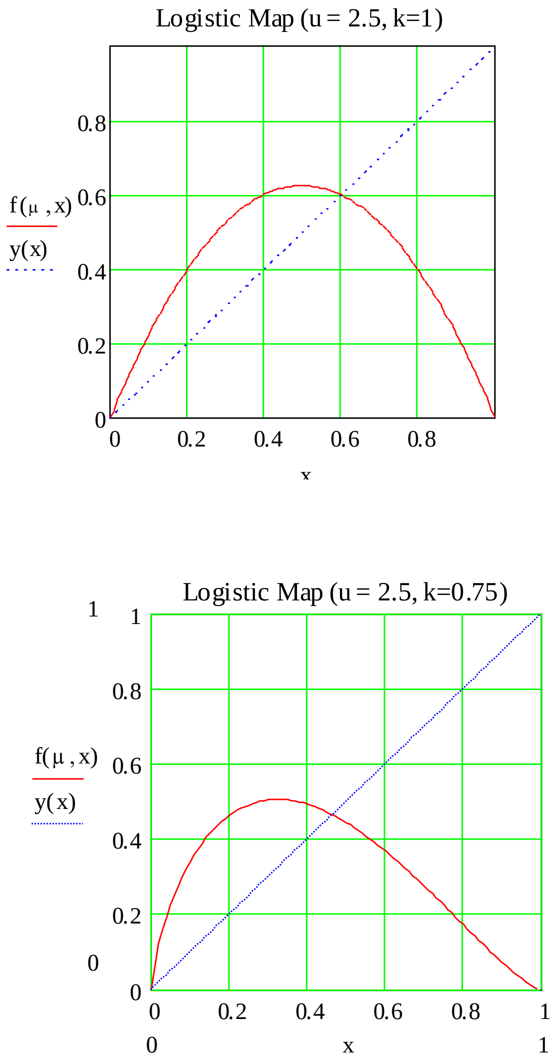


Figure 7: Two homologues of the logistic map, for different k values.

where μ is the gain or amplification factor already introduced. The parameter ***k is a real "tuning" parameter*** deforming the symmetric logistic bell-shaped curve and shifting the maximum left or right of the symmetry point *x = 0.5*. This latter family of maps has properties similar to those of the logistic map. However, the numbers and values of the fixpoints can obviously be different and, therefore, also the iterative trajectories. Also shown in each graph is the "diagonal" *y(x)* = x. Intersections between the map and the function *y* indicate ***fixpoints of the map***.

The plots in Fig. 8 have been calculated with the *MATHCAD* software package {mathcad\Logistic_MAPi.MCD}. It illustrates the iterative ***trajectories***, i.e., the set of points

$$\psi_i = \begin{pmatrix} f(\mu, x_{i-1}) \\ x_{i-1} \end{pmatrix} \qquad (11)$$

for the two maps plotted in Fig.8, and an initial value of $x_0 = 0.75$. In both cases, the trajectory is attracted to the respective fixpoint, the intersection of the map $f(\mu, x)$ and $y(x) = x$. Taking a different initial value x_0' will lead to trajectories that are slightly modified, in particular for the early iterates. However, these latter trajectories will also be attracted to the respective fixpoint of each map. The following discussion and numerical calculations pertain to the

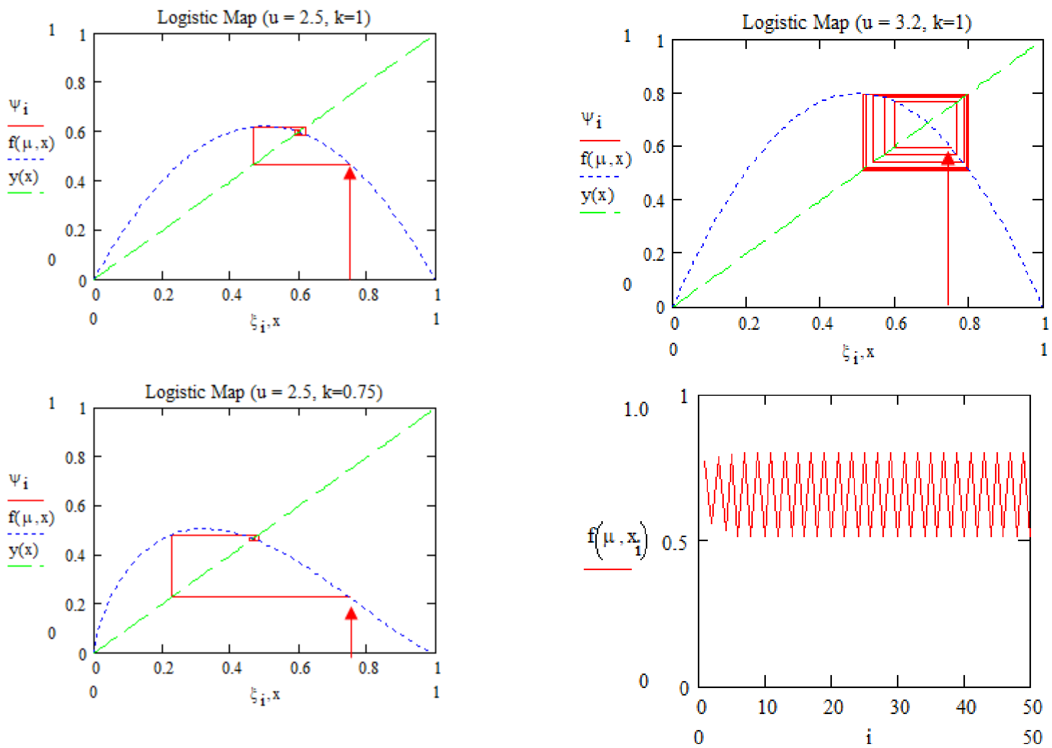


Figure 8:Behavior of maps for different *k* and μ.

original logistic map with $k=1$, unless explicitly specified otherwise.

The above examples illustrate a stable behavior of the laser system. It will settle down to a steady-state operation, once it has passed the initial oscillatory phase. By changing the gain factor μ, which can be accomplished by extracting more or less intensity out of the beam, the steady-state operating point (the fixpoint of the logistic map) will change. For small enough gains, there will be no fixpoint, except for the trivial fixpoint of $x = 0$. According to Equ. 7, this is the case for $\mu \leq 1$. Then, the stable operation point is the one with no output intensity: The laser extinguishes.

For $\mu \geq$ *3.0* the maps looks qualitatively the same as before for smaller values of μ. However, as seen in top panel of the figure, the trajectory ***changes in character***. It does so, regardless of initial value x_0. The trajectories are still attracted to the fixpoint but do no longer converge to it for $n \rightarrow \infty$. Instead, the system oscillates back and forth between two values x_1 and x_2, it has become ***bistable***. The lower panel of the figure illustrates this oscillation. The process of developing such an instability is termed ***"bifurcation"*** or ***"frequency doubling"***.

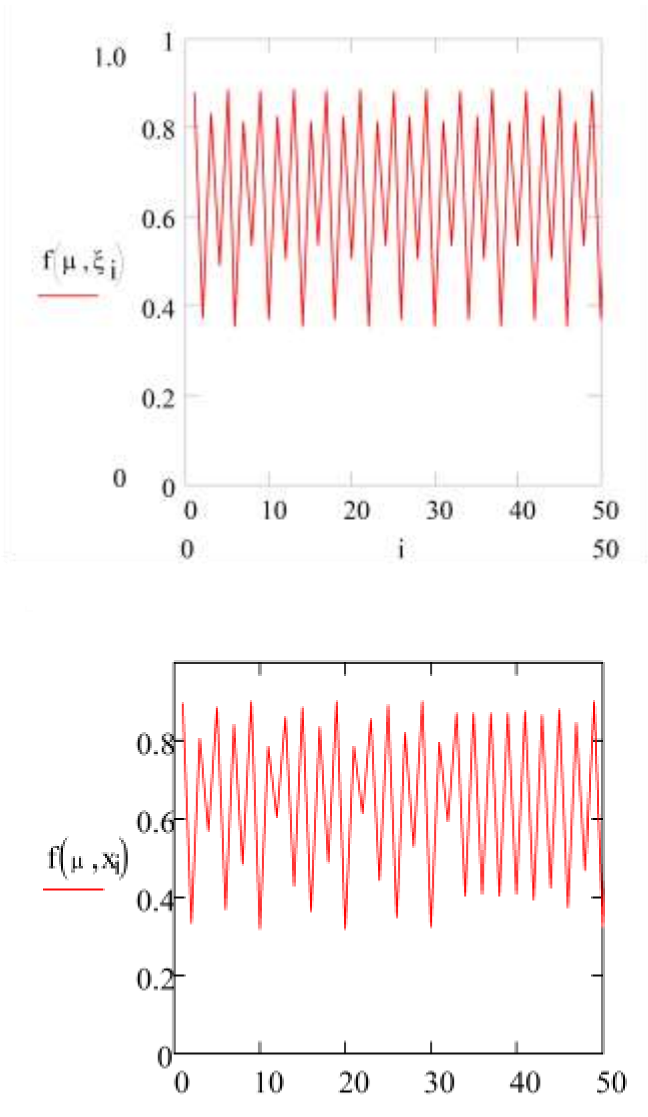


Figure 9: Iterations for different values of the gain (amplification) factor μ.

The first bifurcation for the logistic map occurs at $\mu = 3.0$. But this is not the only one. At $\mu = 1.1 + \sqrt{6} = 3.549$, a ***second bifurcation*** occurs. For slightly larger values of μ, the system oscillates between ***four*** points x_1 ,…, x_4. This behavior of the system is illustrated in Fig. 9. After an oscillation with larger amplitude (*0.887→ 0.355*), there is always one with a slightly smaller amplitude (*0.813 →0.540*).

Already for slightly larger gain factors, $\mu \geq 3.6$, the period-doubling domain ends. The system shows an ***intermittent behavior***, where time intervals of periodic behavior are interspersed with multi-stable or chaotic oscillations. Such behavior is illustrated in Fig. 9 for μ = *3.61*. Here, an initial chaotic behavior is followed by quasi-orderly periodic behavior for later iterations (approximately between *i= 35* and *i =45*).

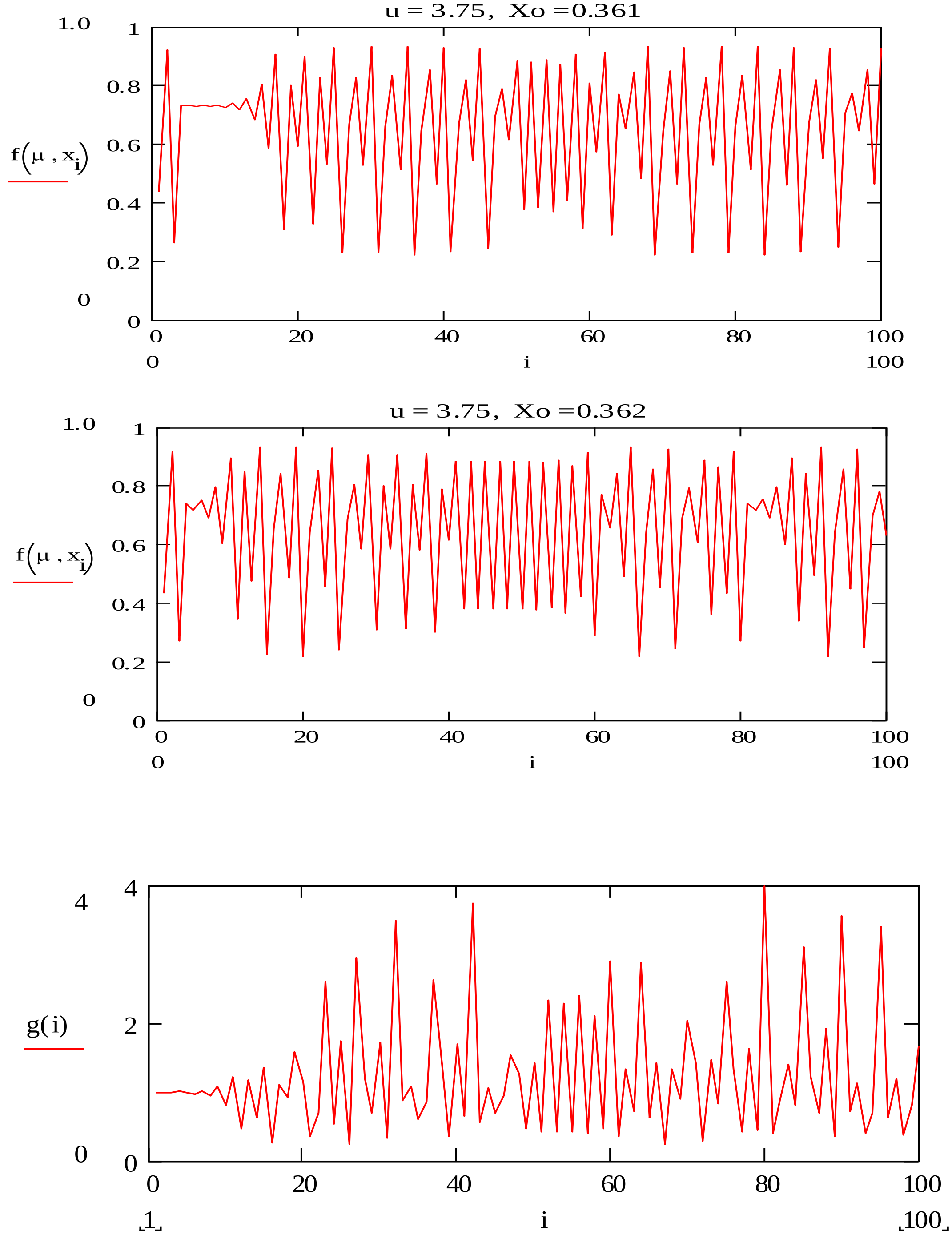


Figure 10: Sensitivity to initial conditions x_0, for μ=3.75 (compare top 2 panels) and ratio of the two trajectory coordinates (bottom).

Increasing the gain factor even further, for $\mu > 3.6$, the system described by the logistic map behaves mostly chaotically, although there are some "windows" on the μ axis where the laser exhibits regular or at least quasi-orderly behavior. Chaotic behavior is illustrated on Fig. 10. Here, for $\mu = 3.75$, the iterations are shown for two slightly different initial conditions, $x_0 = 0.361$ (top panel) and $x_0' = 0.362$ (middle panel). The ratio of both, $g(i) = x_i/x_i'$ is plotted in the bottom panel of Fig. 10. The irregular, chaotic character of both iterative trajectories is obvious from the two upper panels. Furthermore, the bottom panel demonstrates the ***sensitivity to initial conditions*** of the system dynamics.

It is also of interest to be able to make an analytical prediction how a system will behave, without numerical trials and errors. Specifically, one is interested in finding out how one can evaluate whether a system will behave orderly or chaotically, when there are periodic orbits on which the system settles after some finite time. To develop a stability criterion, one may examine simple one-dimensional classical mechanics, where the motion is driven by a potential V. Stationary states emerge in force equilibrium, i.e. where the potential gradient is zero.

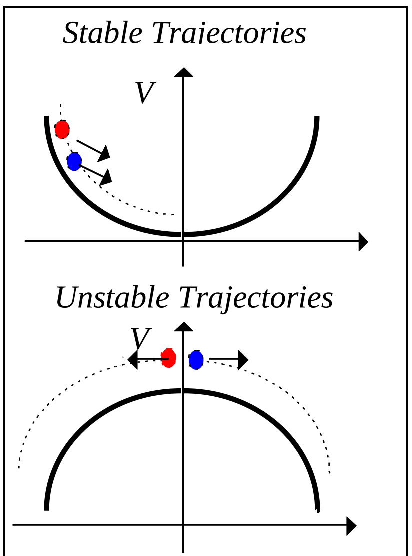


Figure 11: Stable and unstable equilibrium (stationary) states.

The upper case in the sketch of Fig.11 depicts a stable situation, where two particles are driven toward the same (***stable***) equilibrium point (minimum of V), despite the fact that they started at slightly different initial positions. The trajectories are attracted to the equilibrium point and even come to rest there, if there is some action equivalent to friction. Quite different is the behavior of the same particles, if they are placed on the top of a potential, which is also a point of (here, however, ***unstable***) equilibrium. In this latter case, slightly different initial placement can lead to dramatically different, diverging trajectories. Now, the particles tend to move away from the equilibrium point of V. An unstable equilibrium point represents a repellor.

b. Liapunov stability theory

A generalization of the above illustration to iterative maps, based on the ***Liapunov exponent*** (or function) leads to an identification of chaotic domains. Assume again a one-dimensional map $x_{n+1} = f(x_n)$ and 2 neighboring initial starting points, x and $(x+\varepsilon)$, with a small $\varepsilon > 0$. After n iterations, the trajectories will be at points $f^{\,n}(x)$ and $f^{\,n}((x+\varepsilon))$. One can then define the function

$$\delta(\varepsilon,n) := | f^{\,n}(x) - f^{\,n}((x+\varepsilon))| =: |\varepsilon| \cdot e^{\lambda n} \qquad (12)$$

This equation really defines the parameter λ, which is called the ***Liapunov exponent***. It is obvious that for $\lambda > 0$, the trajectories diverge exponentially with increasing number of iterations, while they converge for $\lambda < 0$.

The *Liapunov exponent* can be calculated realizing that

$$\ln|\{ f^{\,n}(x) - f^{\,n}((x+\varepsilon))\}/ \varepsilon | = \lambda\, n \qquad (13)$$

and

$$\lambda \approx (1/n) \cdot \ln|(df^{\,n}/dx)| \qquad (14)$$

Furthermore, by definition of the iteration $f^{\,n}$,

$$f^{\,n}(x) = f(x_{n-1}) = f(f(x_{n-2})) = f(f(f(x_{n-3}))) = f(f(f(x_{n-4}))) = \ldots\ldots,$$

with $x_0 = x$. Then, the ***chain rule*** for differentiation yields

$$\frac{df^{\,n}}{dx} = \frac{df(x_{n-1})}{dx_{n-1}} \cdot \frac{dx_{n-1}}{dx} = \frac{df(x_{n-1})}{dx_{n-1}} \cdot \frac{dx_{n-1}}{dx_{n-2}} \cdot \frac{dx_{n-2}}{dx} = \ldots\ldots\ldots =$$

$$df^{n}/dx = f'(x_{n-1}) \cdot f'(x_{n-2}) \cdot f'(x_{n-3}) \cdot f'(x_{n-4}) \cdots \qquad (15)$$

Here the derivatives are to be taken at the different points x_n along the trajectory. With

$$\ln\left|\frac{df^n}{dx}\right| = \ln\prod_{i=0}^{n-1}|\,f'(x_i)\,| = \sum_{i=0}^{n-1}\ln|\,f'(x_i)\,|, \qquad (16)$$

one has finally for the ***Liapunov exponent :***

$$\lambda = \frac{1}{n}\cdot\sum_{i=0}^{n-1}\ln|\,f'(x_i)\,| \qquad (17)$$

connecting the divergence or convergence of iterations with the derivatives of the function *f* at the individual iterations x_i. A term *i* in the sum is positive, if there is divergence of the trajectories at point x_i, while it is negative, when trajectories converge at this point.

According to the above discussion, one expects that ***whenever a Liapunov exponent becomes positive, the motion is chaotic***. Equ. 8 explains why in the *MATHCAD* illustrations of the logistic map, different behavior resulted simply when the gain factor μ was changed. This gain factor μ also controls the derivative of the function *f* in the neighborhood of an intersection of the map *f(x)* with the function *y(x) = x,* making such an intersection a ***fixpoint***, an ***attractor***, or a ***repellor***.

Figure 12 shows on top the iterates (*fix or periodic*

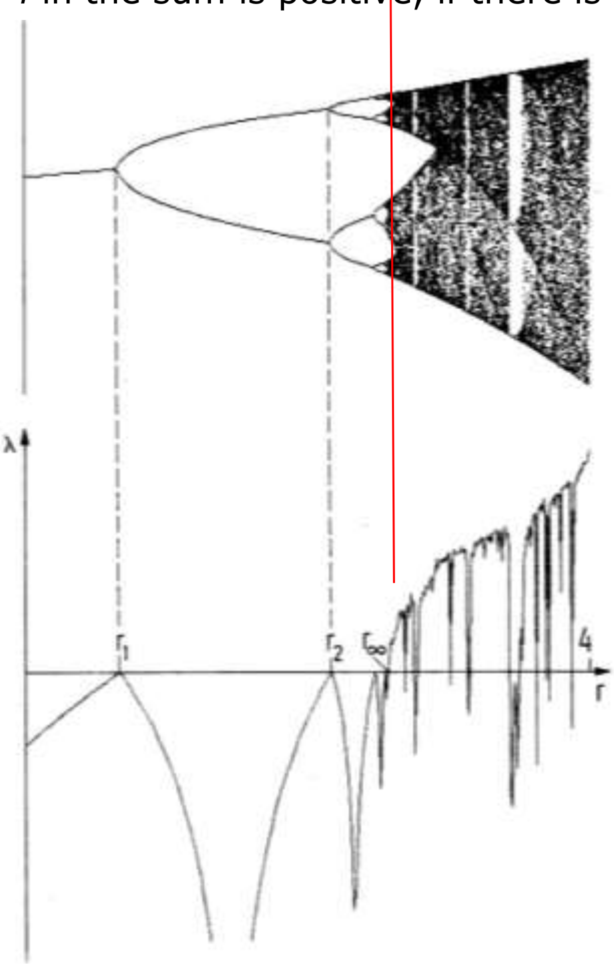


Figure 12: Asymptotic iterates and Liapunov exponent for the logistic map (r:=μ).

points x_n, for large *n*) for the ***logistic map*** and some of the ***related maps*** of the kind

$$f(x) := \mu x^k \left(1 - x^k\right)^{1/k} \qquad (10)$$

defined earlier in this section. At the bottom of the figure, the Liapunov exponent is plotted for the logistic map ($k = 1.0$), both quantities plotted versus the gain factor μ. One observes a correlation between the gain factors μ_i, for which $\lambda(\mu_i) = 0$, and successive period doubling (bifurcation). ***Successive period doubling is a possible route to chaos in dynamical systems.*** The distance between successive bifurcations becomes increasingly smaller. Their scaling is given by the ***Feigenbaum numbers***.

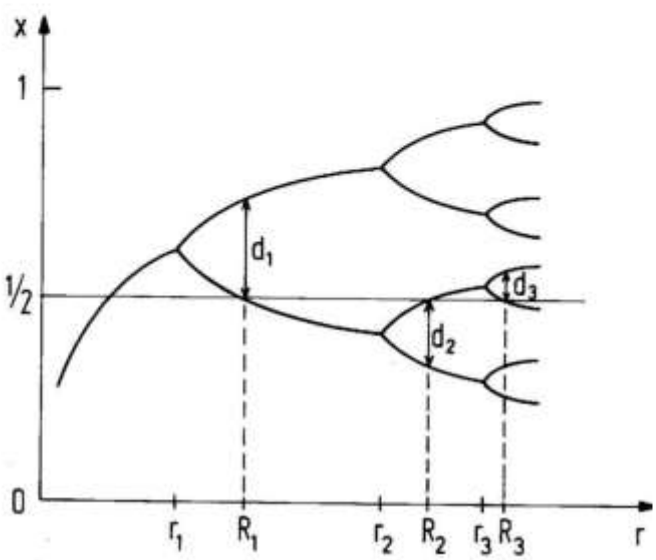


Figure 13: Bifurcation "tree" for the logistic map.

Feigenbaum Scaling

$$r_n = r_\infty - const \cdot \delta^{-n}, n \gg 1$$
$$r_\infty = 3.5699456$$
$$\delta = 4.66920160 \qquad (18)$$
$$\frac{d_n}{d_{n+1}} = -\alpha, \quad n \gg 1$$
$$\alpha = 2.502907875$$

Beyond $\mu = \mu_\infty$, the Liapunov exponent becomes generally positive, and the system behaves in general chaotically. For larger gains, chaoticity dominates. However, one observes that there are intermittent regions, where $\lambda < 0$ and, therefore, ordered motion exists (***order within chaos***). For a system described by an *m*-dimensional map, there is an *m*-dimensional surface of associated Liapunov exponents.

Briefly some remarks concerning methods of analysis of maps, in particular the search for periodic orbits. Periodic points of period n of a map *f* can be deduced from the stable (attractor) fixpoints of $f^{\,n}(x)$. Fixpoints are defined by $f^n(x)=x$. They are attractors, when $|df^{\,n}/dx|\leq 1$. Figure 14 illustrates the method for triple periodic points for $\mu := 1.0 + \sqrt{8}$. Here one plots $f^{\,3}(x)$ and checks whether there are tangent points of the curve with the diagonal $y(x)=x$. For tangent points, $f^{\,3}(x)=x$ (fixpoint) and $|df^{\,3}/dx|=1$ (attractor). In the case shown, intensities of approximately $x=0.17$, 0.52, and 0.98 are visited by the system in sequence.

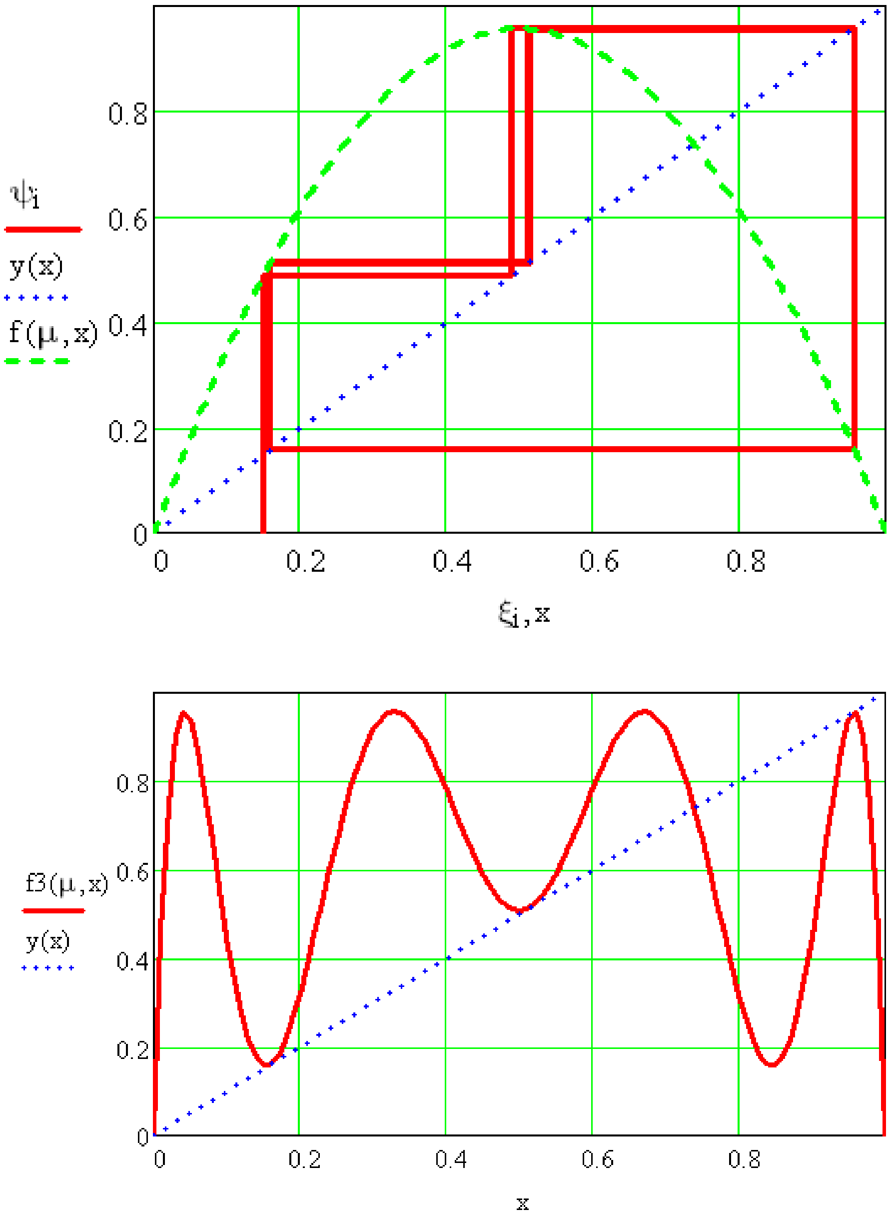


Figure 14: Search for period tripling in logistic map *f* with μ=3.828. Function *f* and iterative trajectory (top). Finding fixpoints of function *f*³(x) as intersections and touching tangents (bottom).

The task of analyzing the behavior of systems described by maps reduces essentially to one of finding the special points of the map transformation, such as fixpoints and periodic points. Following this, one is interested in the stability of the orbits in the neighborhood of these points, i.e., whether the points represent attractors or repellors. The analysis is applicable to many classes of physical, chemical, and biological systems. Therefore, one needs criteria similar to what is offered by the Liapunov coefficient discussed above. This is achieved by casting the earlier observed relations between Liapunov coefficient (or function) into a more general mathematic formulation that can be adapted to individual cases. The following is adapted from Kondepudi & Prigogine.

The concept of a stationary state of a system can be visualized with Fig. 11 illustrating stationary points on a potential. These points are defined by a perfect balance of forces, which add up to exactly zero at the equilibrium points of the potentials. The top panel of Fig. 11 shows a stable situation. If slightly displaced from the equilibrium point, the conservative forces will drive the system back to that point, which is obviously an attractor. The situation for the stationary point of the inverted potential shown at the bottom of Fig. 11 is the reverse of that. That point is an unstable equilibrium point, a repellor of trajectories.

The following discussion will assume a generic, multi-dimensional system with k=1,2,…,r degrees of freedom (independent coordinates). An example for such a system is a chemical reactor with several materials {A, B, C, D,…} present in different concentrations. Any intrinsic state *X* of that system will have values along all *r* degrees of freedom. In the example, the set of all concentrations {[A], [B], [C], [D], …} defines the state. To define a system trajectory through an ensemble of states, one also needs the time rate of change of all coordinates.

In the mathematical formalism, state *X* and its rate of change (Z) are each represented by a corresponding *r*-dimensional state vector,

$$\vec{X} = \left(X_1, X_2, \ldots., X_r\right) \qquad \text{and} \qquad \dot{\vec{X}} = \frac{d}{dt}\vec{X} = \vec{Z}\left(X_1, X_2, \ldots., X_r; \lambda\right) \quad (19)$$

Rigorously, Z is a vector field, and λ in Equ. 19 stands for additional parameters required to complete the equations of motion (19). Obviously, a stable (stationary) state X_s is time independent, which implies for each of its components X_{sk} that

$$\frac{d}{dt}X_{sk} = Z_k\left(X_{s1}, X_{s2}, \ldots., X_{sr}; \lambda\right) = 0 \qquad (k = 1, 2, \ldots., r) \qquad (20)$$

For any two different states X' and $X'' = X' + \delta X$, a distance

$$L(X', X'') = |X' - X''| = L(|\delta[X|) > 0 \qquad (21)$$

can be defined, which has to be a positive function to make sense. It should not depend on the signs of individual variations δx_k. In a one-dimensional system such as represented by the Logistic Map, this distance is simply the numerical difference of the n^{th} iterate of two trajectories starting at different initial values. For two state vectors, one could use the quadratic difference between them,

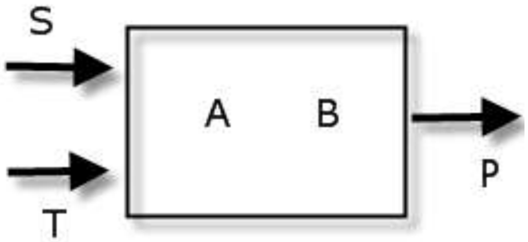
$$L\left(\vec{X}', \vec{X}''\right) = L\left(\left|\delta X\right|\right) := \left|\sum_k \left(\delta X_k\right)^2\right| \qquad (22)$$

In general, one has to require of a stable state that the distance between it and a nearby state will decrease in time, hence,

$$\frac{d}{dt}L(\left|\delta X\right|) < 0 \qquad (23)$$

Actually, Equs. 22 and 23 define a "Liapunov Function" or, in a more general case, a Liapunov functional.

As an illustrative example (Kondepudi & Prigogine), one may examine the kinetic equations describing a set of coupled chemical reactions taking place simultaneously in a chemical reactor:



$$\begin{aligned} S+T &\xrightarrow{k_1} A \\ S+A &\xrightarrow{k_2} B \\ A+B &\xrightarrow{k_3} P \end{aligned} \tag{24}$$

Figure 15: Chemical reaction system with intrinsic states defined by {[A].[B]}.

Here, the quantities k_i are the reaction constants. One is interested under what conditions a steady-state would result, producing a set of constant concentrations [A] and [B], which would then result in a constant stream of reaction products *P*.

Interpreting the two interesting concentrations as the two coordinates, $X_1 = [A]$ and $X_2 = [B]$, one derives the equations of motion for the concentrations,

$$\begin{aligned} \frac{d}{dt}X_1 &= k_1 \cdot [S] \cdot [T] - k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2 = Z_1\left(\vec{X},[S],[T]\right) \\ \frac{d}{dt}X_2 &= k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2 = Z_2\left(\vec{X},[S],[T]\right) \end{aligned} \tag{25}$$

In the above expression for dX_1/dt the dependence on [S] and [T] is an example of what the parameter λ in Equ. 19 represents.

The conditions for stability are that the rates dX_i/dt = 0, and therefore, starting with the second of the above two rates, one has

$$\begin{aligned} \frac{d}{dt}X_2 = 0 \;&\rightarrow k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2 = 0 \\ &\rightarrow k_2 \cdot [S] \cdot X_1 = k_3 \cdot X_1 \cdot X_2 \end{aligned} \tag{26}$$

and

$$\frac{d}{dt}X_1 = 0 \;\rightarrow\; k_1 \cdot [S] \cdot [T] - k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2 = 0$$
$$\rightarrow\; k_1 \cdot [S] \cdot [T] = 2k_2 \cdot [S] \cdot X_1 \qquad (27)$$

Therefore, any stationary state has to satisfy

$$\boxed{X_{s1} = [A]_s = \frac{k_1[T]}{2k_2}} \text{ and } \boxed{X_{s2} = [B]_s = \frac{k_2[S]}{k_3}} \qquad (28)$$

If it does, the state will either be in stable or unstable equilibrium (see Fig. 11). A stable state has to satisfy condition (23), namely that small variations δX_1 and δX_2 about the stable vector $\{X_{s1}, X_{s2}\}$ should disappear in time. Hence, for a stable state,

$$\frac{d}{dt}L(|\delta X_1|, |\delta X_2|) < 0 \qquad (29)$$

using the definition adopted for the distance function L, for example that of Equ. 22. However, other equivalent definitions are acceptable. To test the validity of condition (29) for a given state, one can follow a simple procedure of inserting into Equ. (25) the expressions

$$X_k(\text{t}) = (X_{sk} + X_k(\text{t})) \quad (k=1, 2) \qquad (30)$$

Of course, the specific coordinates of the stationary state X_s are not time dependent. In linear approximation, one may neglect terms of higher order such as $(X_k \cdot X)_\ell$. One then gets expressions for $d(\delta X_k)/dt$ needed to test the condition of Equ. (29).