



# Modelling and simulation

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## I. Nonlinear maps and chaotic dynamics

### The (first) death of Laplace's Demon

LAPLACE (1749-1829):

assume an *intelligent, computing creature* exists, that – at a given time –

- has complete knowledge of the state of the world, i.e. knows the position and velocity of every particle in the universe
- knows the laws of nature which govern the motion of these particles
- can thus compute and predict the future of the world in every little detail

no room for: randomness, the free will, responsibility, guilt, merit ...

God(s) : spectator(s) who might have fixed initial conditions

apart from some *practical* problems (storage, computation),  
Laplace's demon has died several times ... (relativity, quantum mechanics)

POINCARÉ (1854-1912):

(even very simple) mechanical systems

- can exhibit very *complex* behavior
- may be extremely sensitive to small changes in the initial conditions
- might react in a highly non-linear manner to such changes  
(small causes → large consequences)
- therefore, cannot be predicted over *long* time intervals  
(not even with more and more accurate measurements of the present state)

such systems are nowadays called **chaotic**

Even in a classical, Newtonian world **Laplace's demon fails**

He/she cannot even predict a simple driven pendulum (sec. I.3)  
(not to mention the weather forecast... )

# I. Nonlinear maps and chaotic dynamics

## I.1. The logistic map

non-linear, one-dimensional discrete iteration which illustrates several features of chaotic systems  
(period doubling, Lyapunov exponent)

## I.2. Random number generators

application of non-linear maps for generating pseudo random numbers  
(basis of all Monte Carlo methods, see secs. 2,3)

## I.3. The chaotic pendulum

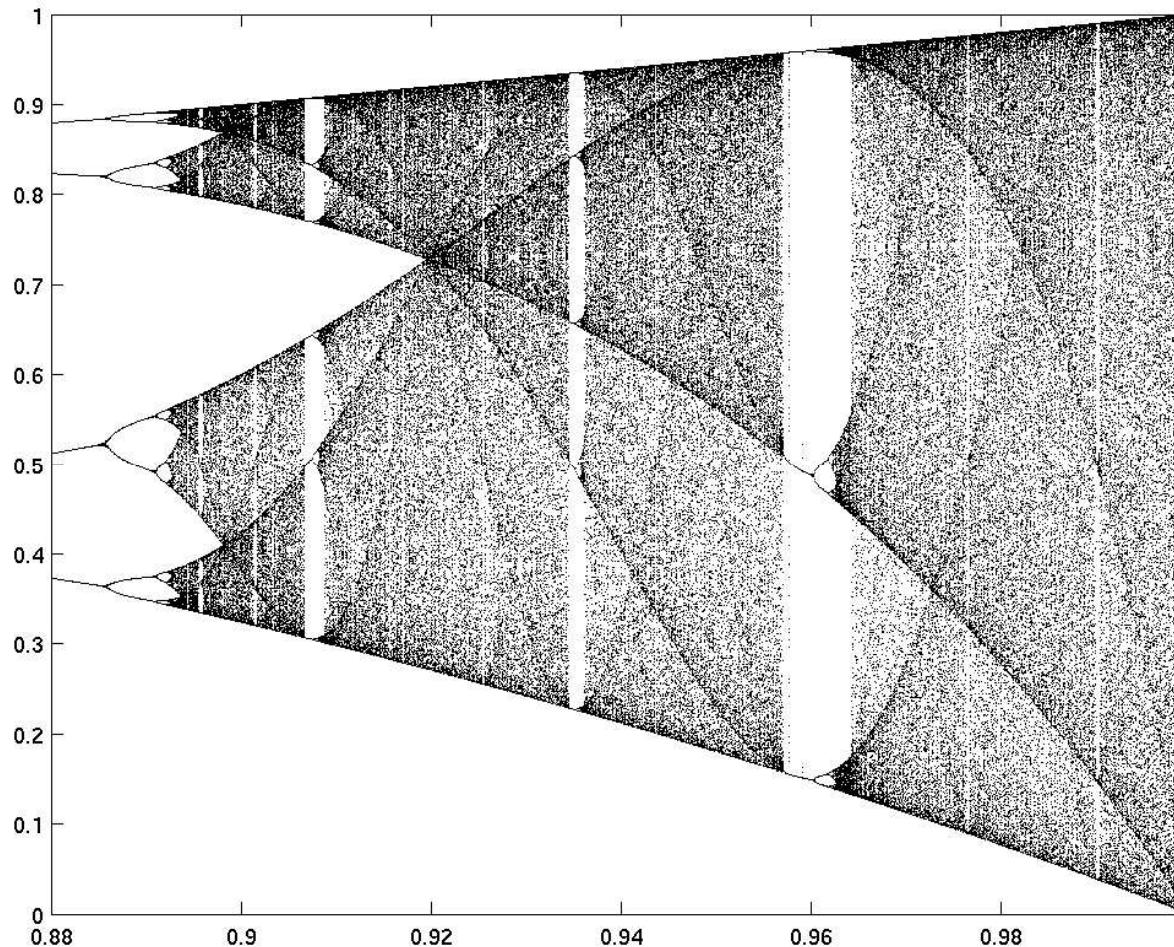
a simple pendulum, subject to an external periodic torque, displays highly complex, chaotic behavior  
(ordinary differential eqs., *Poincaré section*)



# Chapter I: Nonlinear Maps and Deterministic Chaos

## Modelling and Simulation, Michael Biehl

### 1. The logistic map



(portion of the bifurcation diagram, as explained below)

The discussion follows closely the chapter *Population Dynamics* in W. Kinzel and G. Reents, *Physics by Computer* (Springer, 1998).

# The logistic map

iteration of  $x \in [0, 1]$  with parameter  $r \in [0, 1]$ :  $x_{n+1} = f(x_n) = 4r x_n (1 - x_n)$

- P.F. Verhulst (1845)  
a (very) simple model of a single species population dynamics

$x \equiv$  population density, change from year to year:  $x_{n+1} - x_n = (4r - 1)x_n - 4r x_n^2$

**linear growth term** (reproduction  $\propto x$ ):  $(4r - 1)x = \begin{cases} < 0 & \text{for } r < 1/4 \text{ extinction} \\ > 0 & \text{for } r > 1/4 \text{ exp. growth} \end{cases}$

**non-linear restriction** (e.g. limited food supply):  $-4r x^2 < 0$   
hinders unlimited growth, prevents “population explosion”

- Prototype of a chaotic map, similar to those obtained from *Poincaré sections* of mechanical systems. Example: driven pendulum with friction, see sec. I.3.

## Fixed points and periodic attractors

one obvious fixed point:  $f(0) = 0, x = 0$  is reproduced in the iteration.

further observation:  $\lim_{n \rightarrow \infty} x_n = \begin{cases} x^* = 0 & \text{for } r < r_o = 1/4 \\ x^* > 0 & \text{for } r_o < r < r_1 \end{cases}$

when is a fixed point stable/unstable (attractive/repulsive)?

formally: consider small deviation from a candidate fixed point  $x^* = f(x^*)$

$$x_0 = x^* + \epsilon_o, \quad x_1 = f(x^* + \epsilon_o) \approx f(x^*) + \epsilon_o f'(x^*) = x^* + \underbrace{\epsilon_o f'(x^*)}_{\epsilon_1}, \quad f'(x) = 4r(1 - 2x)$$

after  $n$  iterations:  $\epsilon_n \approx f'(x^*) \epsilon_{n-1} \approx [f'(x^*)]^n \epsilon_o = \begin{cases} \rightarrow 0 & \text{for } |f'(x^*)| < 1 \\ \text{grows} & \text{for } |f'(x^*)| > 1 \end{cases}$

## Matlab routines

```
% logistic map
% the iteration x(i+1) = 4 r x(i) (1- x(i))
% is implemented and can be studied by the
% following scripts and functions:
%
```

---

```
function s = logstep(r,x,n)
```

```
% logstep.m defines the logistic map
% logstep(r,x,n) iterates 4*r*x*(1-x) n times
% beginning with initial value x
```

```
for i=1:n
    x = 4 * r * x * (1-x);
end
s=x;
```

---

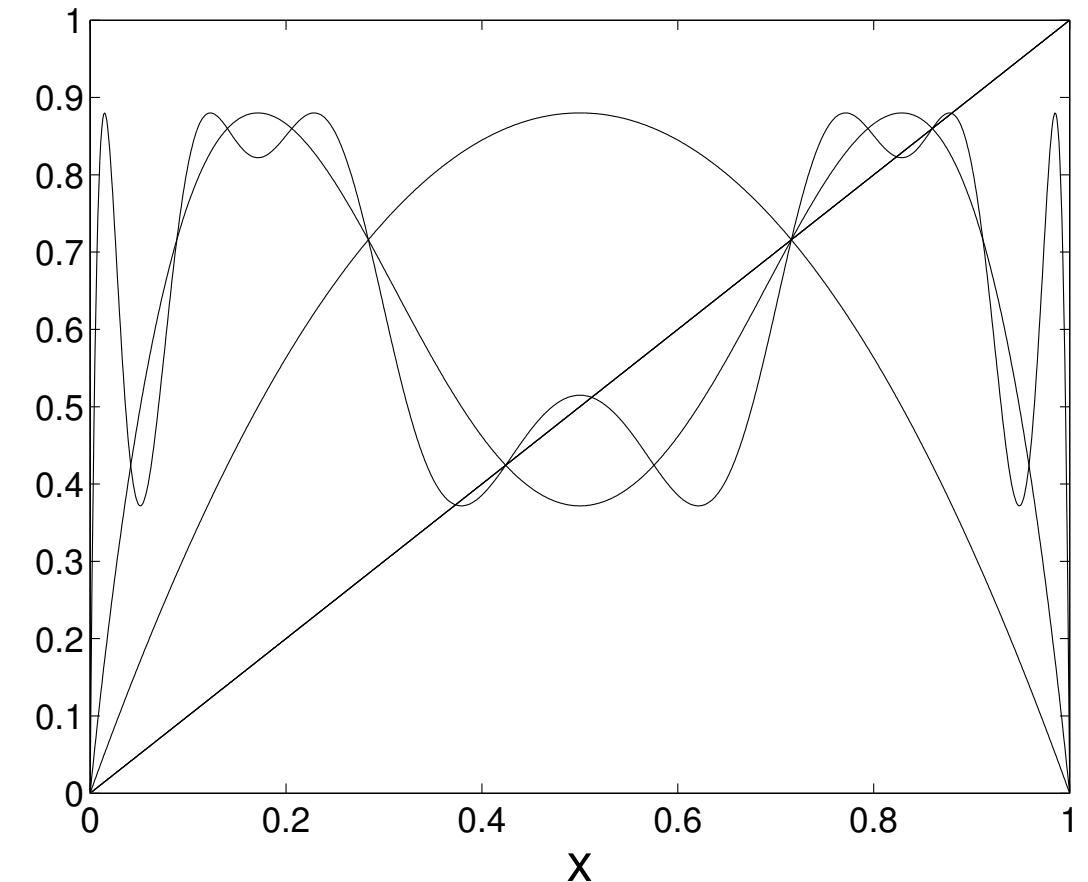
```
function fp = fplot(r,n)
```

```
% fplot(r,n) plots the n-fold iteration of the
% logistic map with parameter r (default: n=1)
% as x(i+1) vs. x(i)
% (includes f(x)=x for n=0)
```

```
if nargin==1
    n=1;
end
```

```
x = 0:0.001:1;
y = x;
for i =1:n
    y = logstep(r,y,1) ;
end
plot(x,y,'k-'); hold on;
plot(x,x,'k-'); hold off;
```

---



**Fig. 2:** The logistic map  $f(x) = 4rx(1 - x)$ , the two-fold iterated  $f^{(2)}(x) = f(f(x))$  and  $f^{(4)}(x)$  for  $r = 0.88$ . Intersections with  $y = x$  correspond to stable or unstable fixed points.

```

function s = iterplot(r,xinit,nsteps)

% function iterplot(r,xinit,nsteps)
% performs nsteps iterations of the logistic map
% with parameter r and plots
% a) the x-values vs. "time"
% b) the sequence of x-values as x(i) vs x(i-1)

x= xinit * ones(1,nsteps);
xprev = x;
time = 1 : nsteps;

for i=2:nsteps
    x(i) = logstep(r,x(i-1),1);
    xprev(i) = x(i-1);
end

figure(1);
plot(time,x,'k-*')
title([' r = ' num2str(r,'%0.4f')], 'FontSize',18);
axis([ 0 nsteps+1 -0.01 1.01 ] );
axis square;

figure(2);
x1= ones(1,2*nsteps-2); x2= ones(1,2*nsteps-2);

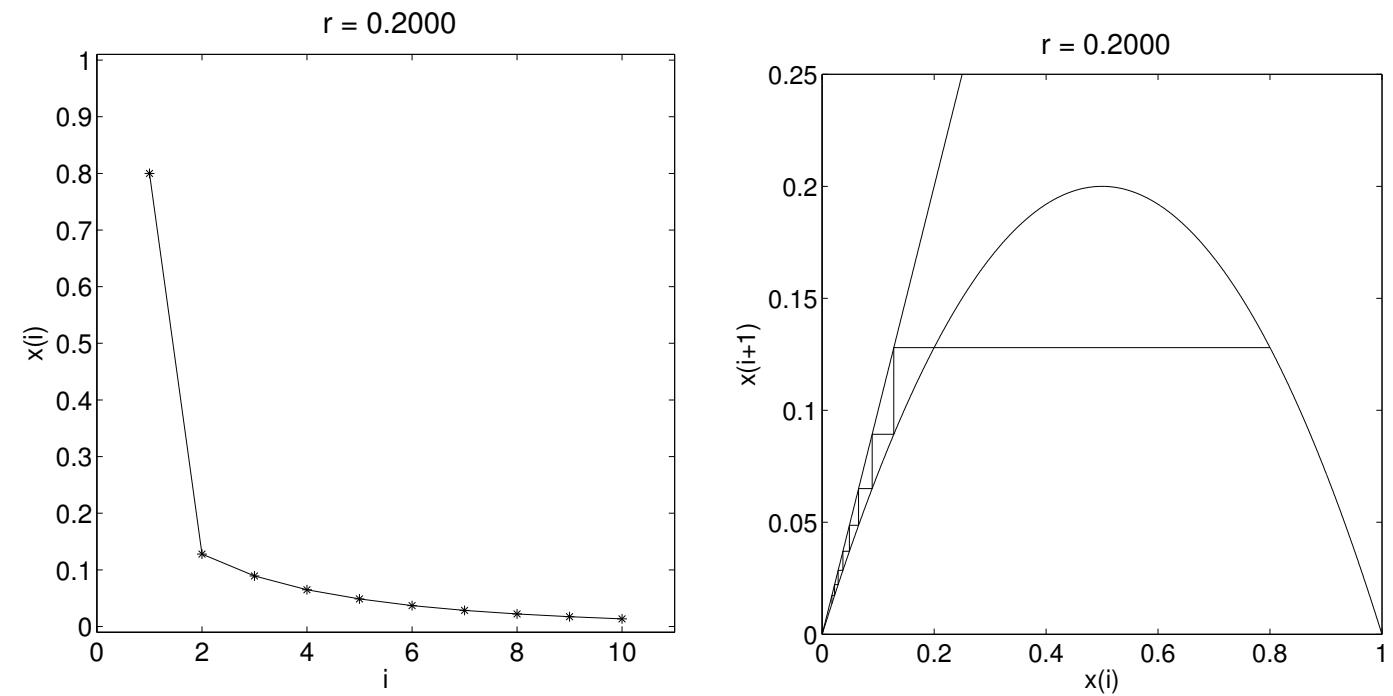
for i=1:nsteps-1
    x1(2*i-1) = x(i); x2(2*i-1) = x(i);
    x1(2*i)   = x(i); x2(2*i)   = x(i+1);
end

```

```

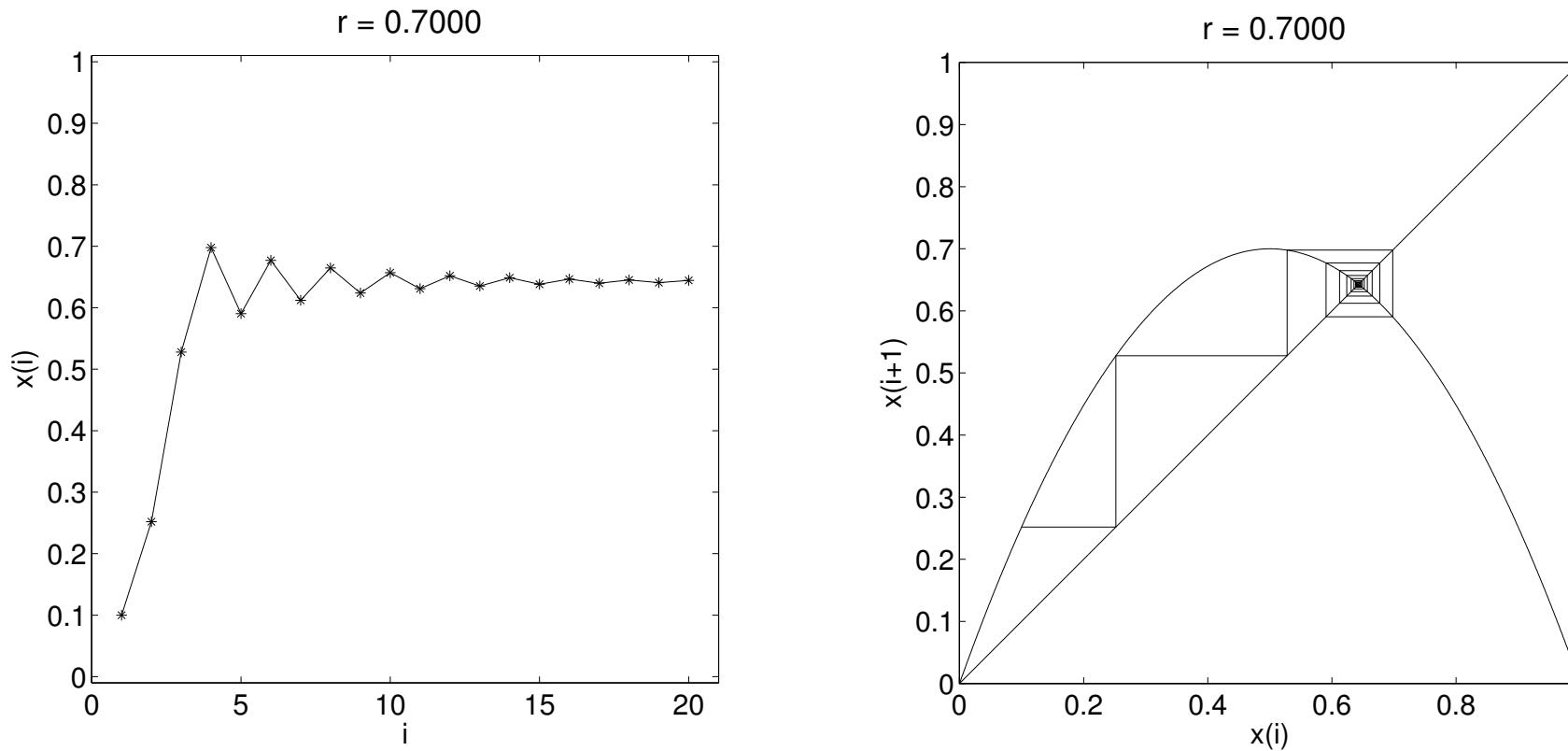
plot(x1(2:2*nsteps-2),x2(2:2*nsteps-2));
hold on;
fplot(r,1);
title([' r = ' num2str(r,'%0.4f')], 'FontSize',18);
axis square; hold off;

```



**Fig. 3:** The iteration for  $r = 0.2$  converges to  $x = 0$

## Convergence to a single, non-zero fixed point



**Fig. 4:** Iteration with  $r = 0.7$ : the f.p.  $x = 0$  is unstable and  $x_n$  tends to  $x^* \approx 0.64$  even from small initial values. Note that  $|f'(0)| > 1$  whereas  $|f'(x^*)| < 1$ ; as  $f'(x^*) < 0$ , the sign of the deviation from  $x^*$  alternates.

single non-zero f.p.:

$$x^* = 1 - \frac{1}{4r}$$

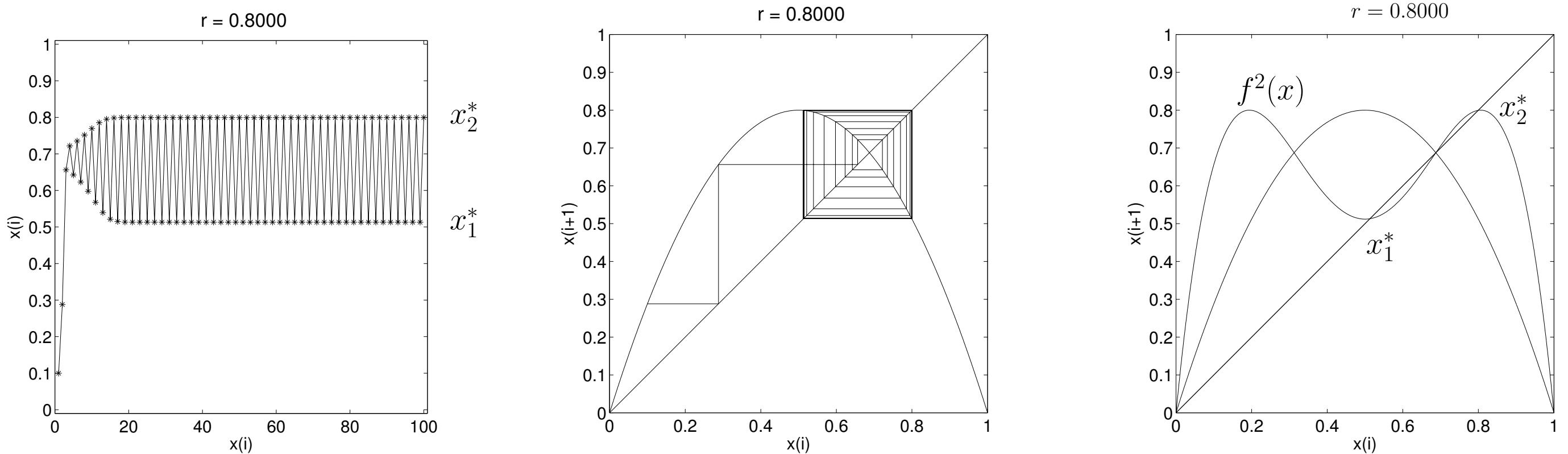
corresponding derivative:  $|f'(x^*)| = |2 - 4r| = \begin{cases} < 1 & \text{for } r < r_1 = 3/4 \\ > 1 & \text{for } r > r_1 \end{cases}$

**for  $r > r_1 = 3/4$  all single f.p. are unstable!**

## The route to chaos: period doubling

for  $r \gtrsim 3/4$  the simple fixed point is replaced

- by an attractor with period two:  $x_1^*, x_2^*$ , with  $f(x_1^*) = x_2^*$  and  $f(x_2^*) = x_1^*$   
or, equivalently
- by 2 fixed points of the two-fold iterate:  $f^{(2)}(x_j^*) = f(f(x_j^*)) = x_j^* (j = 1, 2)$

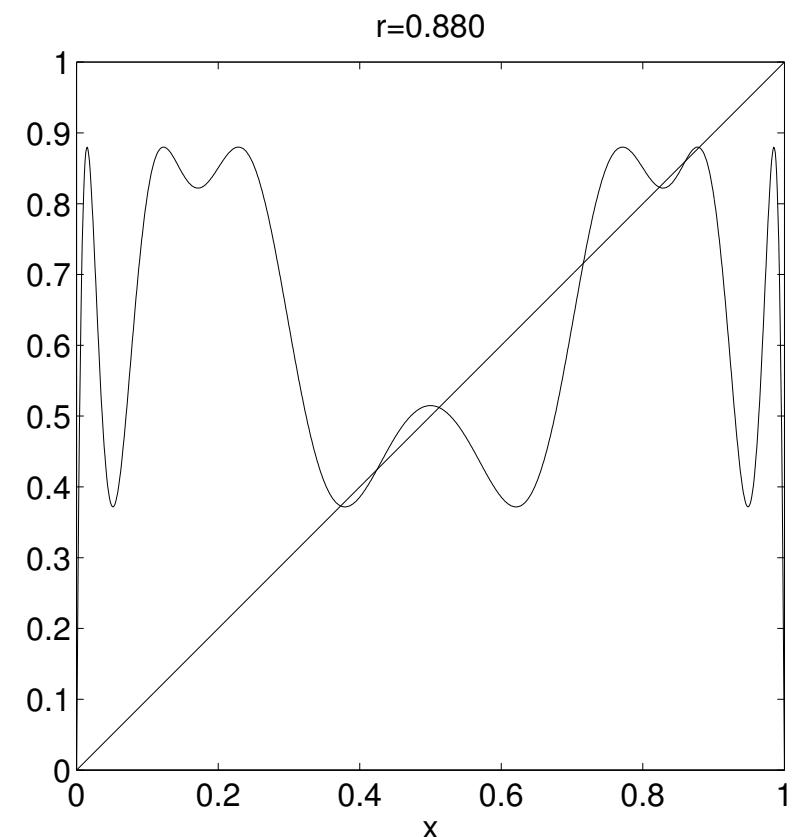
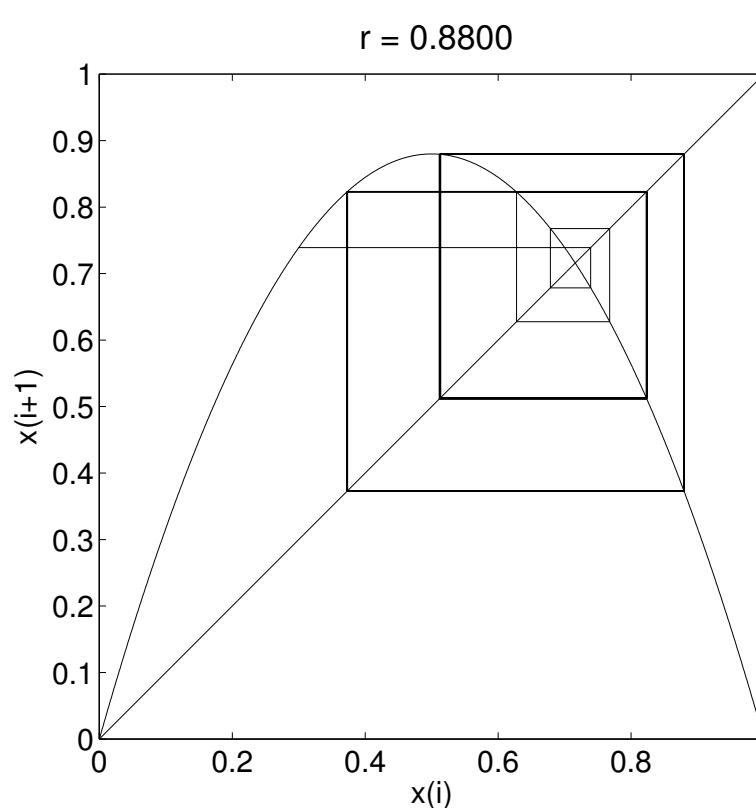
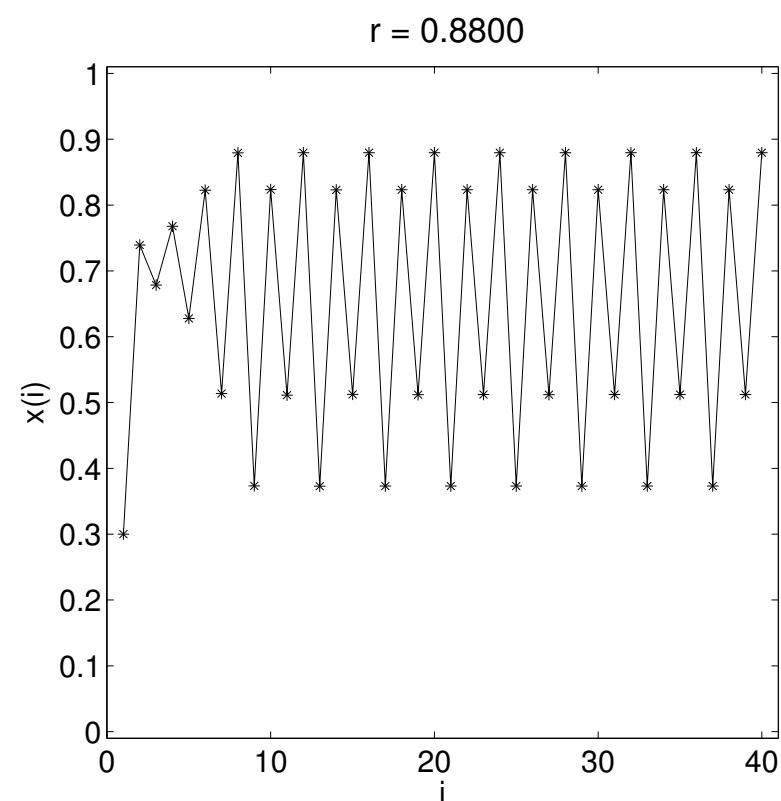


**Fig. 5:** Attractor of period 2 for  $r = 0.80$ , the 2-fold iterate has 2 attractive f.p.

stability condition is analogous to the previous study for single f.p. of  $f(x)$ :

$$|f^{(2)'}(x_{1,2}^*)| > 1 \text{ for } r > r_2 = (1 + \sqrt{6})/4 \approx 0.8624$$

for  $r \gtrsim r_2$  the 2-cycle is replaced by a stable 4-cycle



**Fig. 6:** Attractor of period 4 for  $r = 0.88$ ,  $f^{(4)}$  has 4 attractive and 4 repulsive f.p.

### period doubling scenario:

- at every **bifurcation point**  $r_k$ , a  $2^{k-1}$ -cycle becomes unstable and is replaced by a stable  $2^k$ -cycle
- the sequence of  $r_k$  approaches for  $k \rightarrow \infty$  a limiting value  $r_\infty \approx 0.8925$

## Matlab routine

```
function rp = rplot(rmin,rmax,rinc,iter,iwaste)

% rplot(rmin,rmax,rinc,iter,iwaste)
% performs iwaste {800} initial iterations of the
% logistic map, the following iter {200} steps are
% plotted versus r in the range (rmin,rmax) with
% increment rinc {0.0001}

if nargin < 5
    iwaste = 800;
end
if nargin < 4
    iter=200;
end
if nargin < 3
    rinc=0.0001;
end

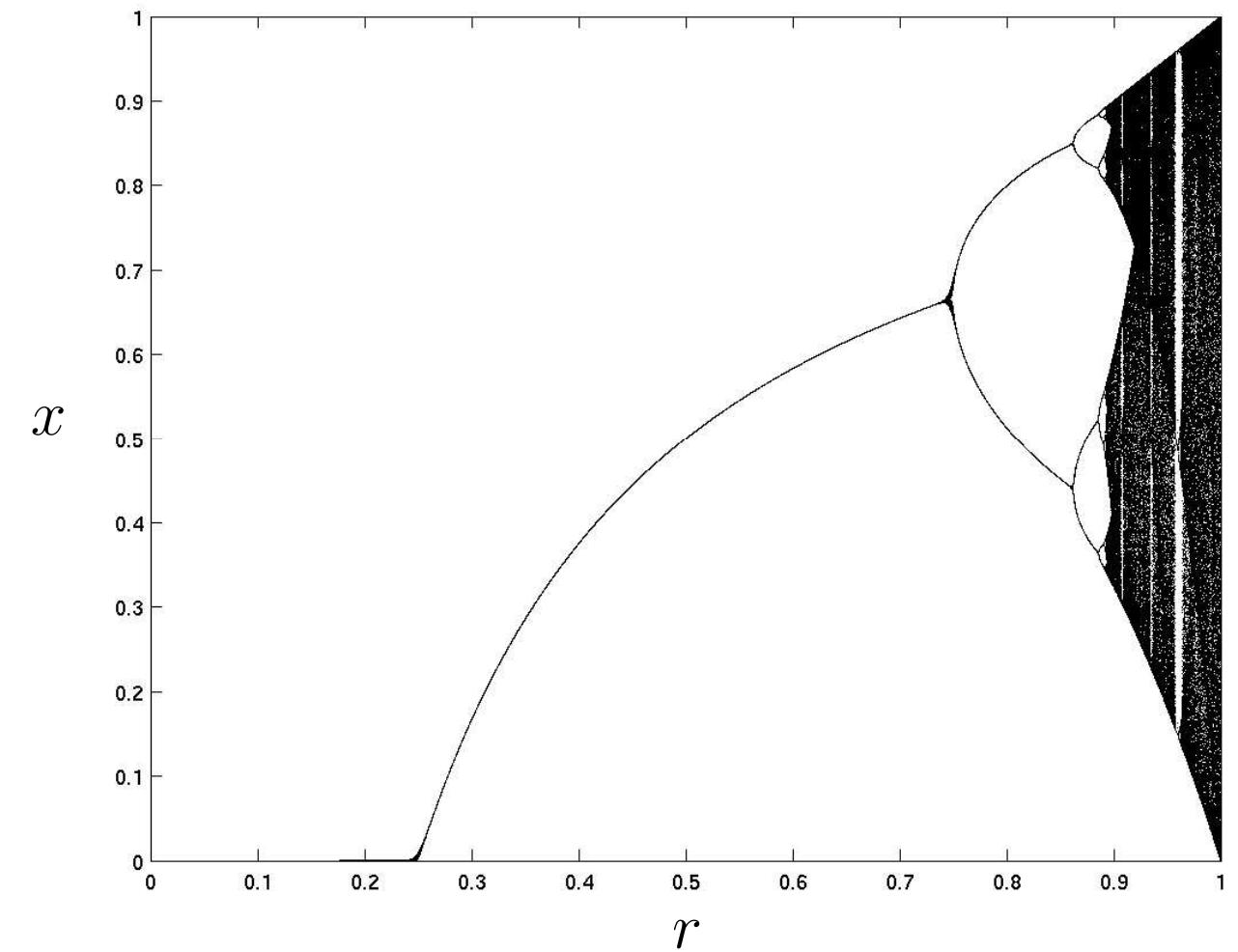
% number of r values
nofr = floor( (rmax-rmin)/rinc);

rr=rmin*ones(1,nofr);
x = ones(nofr,iter);

for j=1:nofr
```

```
    rr(j)= rmin + j* rinc;
    x(j,1)=logstep(rr(j),0.2,100);
    for i=2:iter
        x(j,i) = logstep(rr(j),x(j,i-1),1);
    end
end

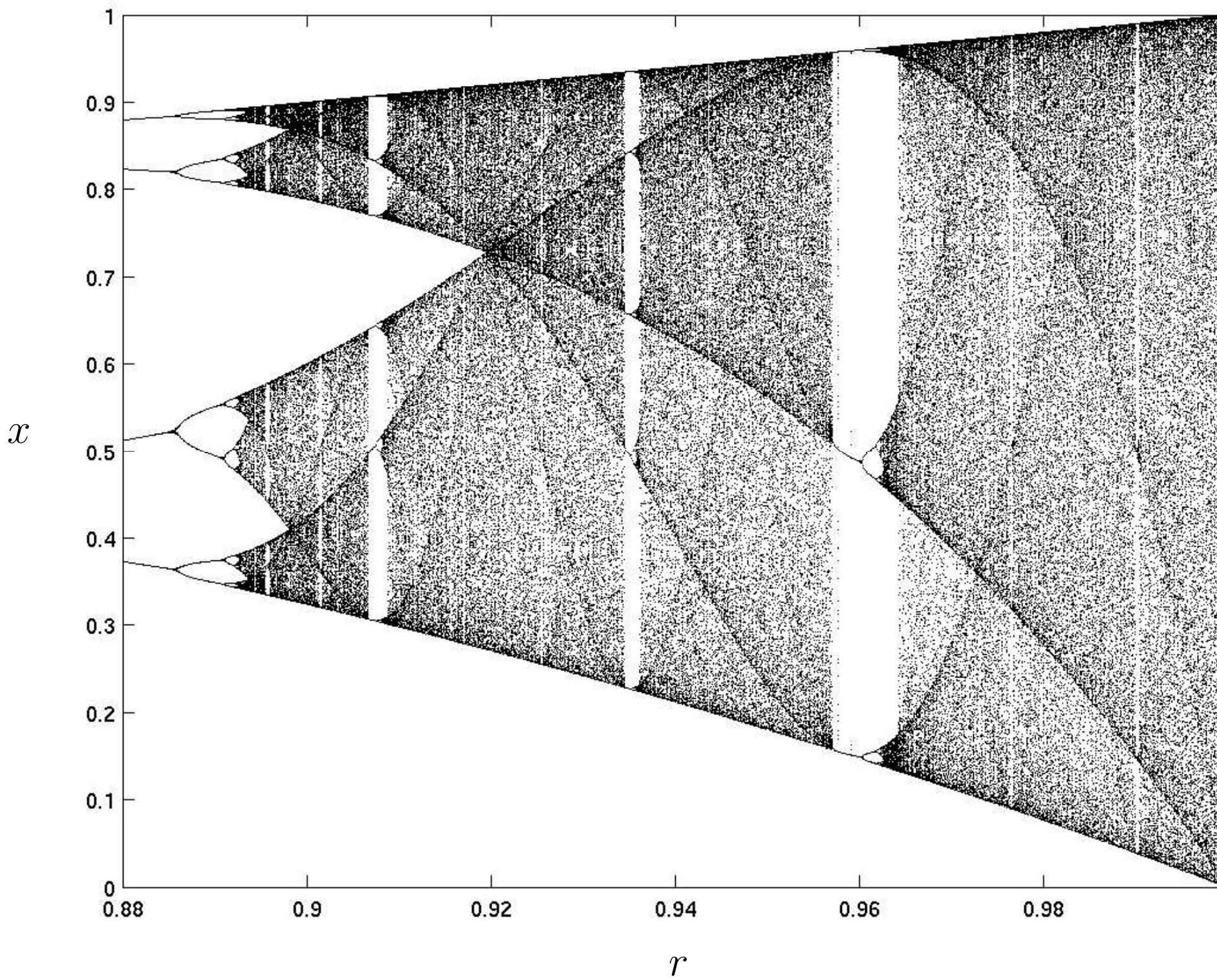
plot(rr, x(1:nofr,2:iter),'k.', 'MarkerSize',0.1)
axis([rmin rmax 0.0 1.0]);
```



**Fig. 7:** The bifurcation diagram,  $x$ -values vs.  $r$

## The bifurcation diagram

plot of the  $x$ -values (vs.  $r$ ) that occur in the iteration after an initial phase  
(here: 800 initial iterations, then 200 values recorded)



**Fig. 8:** The bifurcation diagram in the region of  $r \geq 0.88$

## The Feigenbaum constant

Bifurcation points can be identified by searching for fixed points  $f^{(\ell)}(x^*) - x^*$  and the  $r$ -value where  $|f^{(\ell)'}(x^*)| = 1$ . Note: this becomes very involved for large  $\ell$ .

An important observation:

the sequence of bifurcation points approaches  $r_\infty$  as

$$r_k \approx r_\infty - \frac{c}{\delta^k} \quad \text{for large } k$$

with the so called **Feigenbaum constant**

$$\delta = \lim_{k \rightarrow \infty} \frac{r_k - r_{k-1}}{r_{k+1} - r_k} \approx 4.669202$$

The importance of the Feigenbaum constant is due to its **universality**.

It occurs in all one-dim. iterations with a *smooth*  $f(x)$  *with a single hump* and even in many experimental systems that show **period doubling**.

## Matlab routines

```
function r = channelplot(rr,bins,iter,iwaste,top)
% channelplot(r,bins,iter,iwaste) performs iwaste
% {1000} initial iterations of the log. map with
% parameter r, then generates a histogram for the
% occurrence of x-val. in the subsequent iter {10000}
% steps, bins {1000} controls the number of bins,
% top {iter/100} is the maximal occurrence displayed

if nargin < 2
    bins=1000;
end
if nargin < 3
    iter=10000;
end
if nargin < 4
    iwaste=1000;
end
if nargin < 5
    top = iter/100 ;
end

x= 0.1 * ones(1,iter);
x(1) = logstep(rr,0.2,iwaste+1);
for i=2:iter
    x(i)= logstep(rr,x(i-1),1);
end
plot(0,0); axis ([0 1 0 top]); hold on;
title(['r =' num2str(rr,'%.5f')], 'FontSize',18);
```

```
hist(x,bins); hold off;



---



```
function c = channelmovie(rmin,rmax,rinc,dt)
% channelmovie(rmin,rmax,rinc,dt)
% generates a sequence of channel plots for
% r-values between rmin and rmax {1}. r is
% incremented by rinc {0.0001} after dt {1/50} sec.

if nargin < 4
    dt=1/50;
end
if nargin < 3
    rinc = 0.0001;
end
if nargin < 2
    rmax = 1;
end

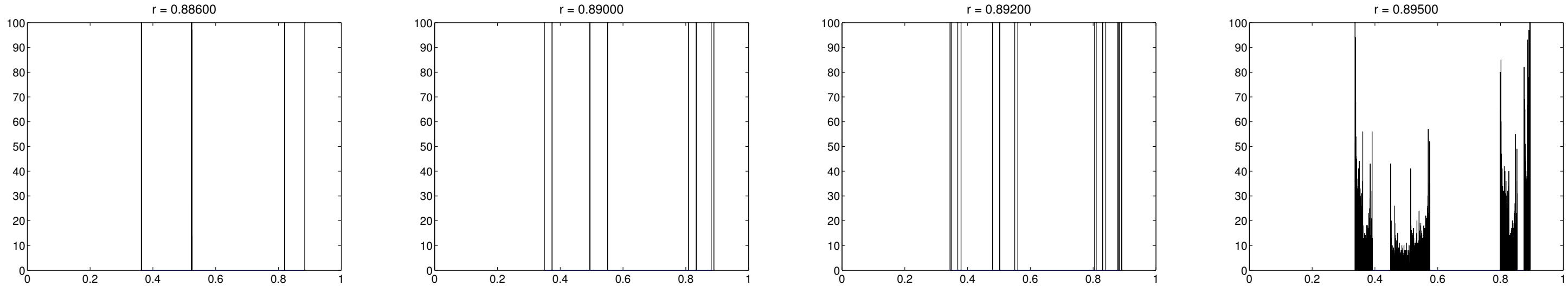
number = floor( (rmax-rmin)/rinc )

for i=1: floor( (rmax-rmin)/rinc )
    r = rmin + i * rinc;
    channelplot(r)
    pause(dt)
end
```


```

# Period doubling

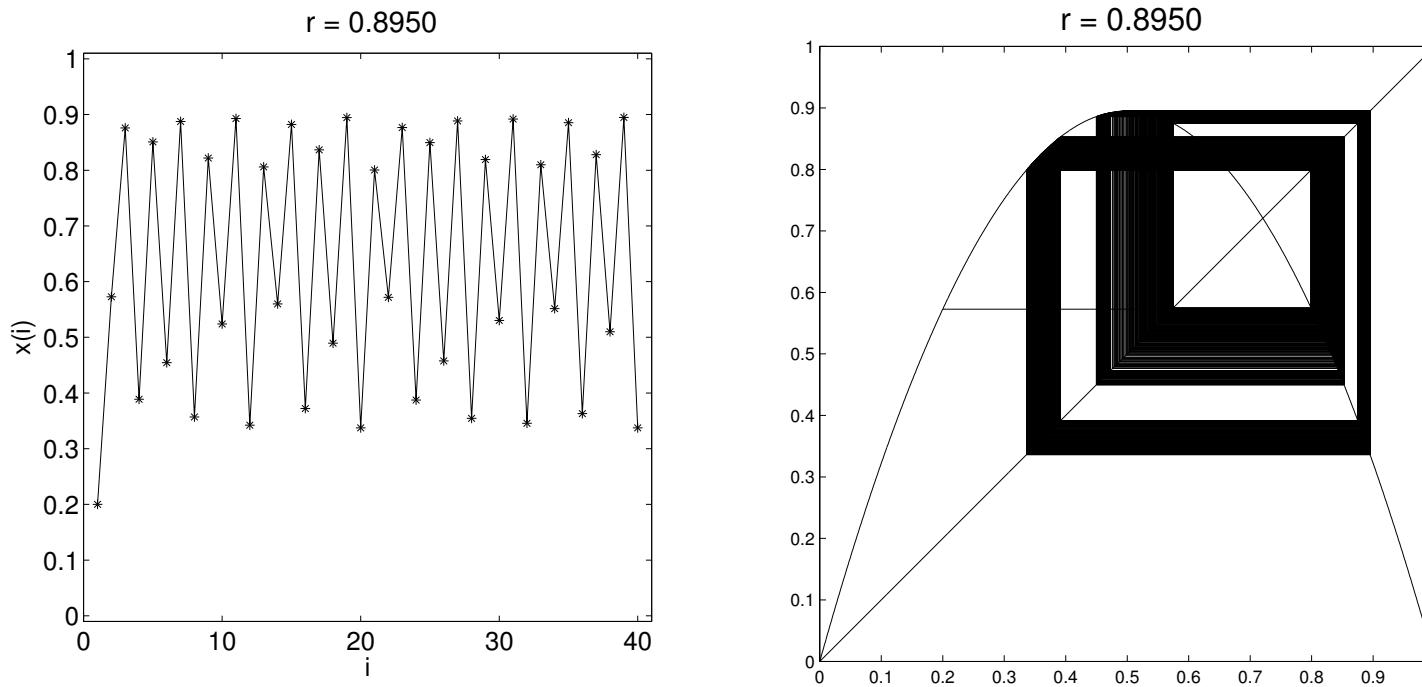
histograms for the occurrence of  $x$ -values for increasing  $r$ :



**Fig. 9: Stable attractors with periods 4,8,16 and a chaotic orbit with 4 bands**

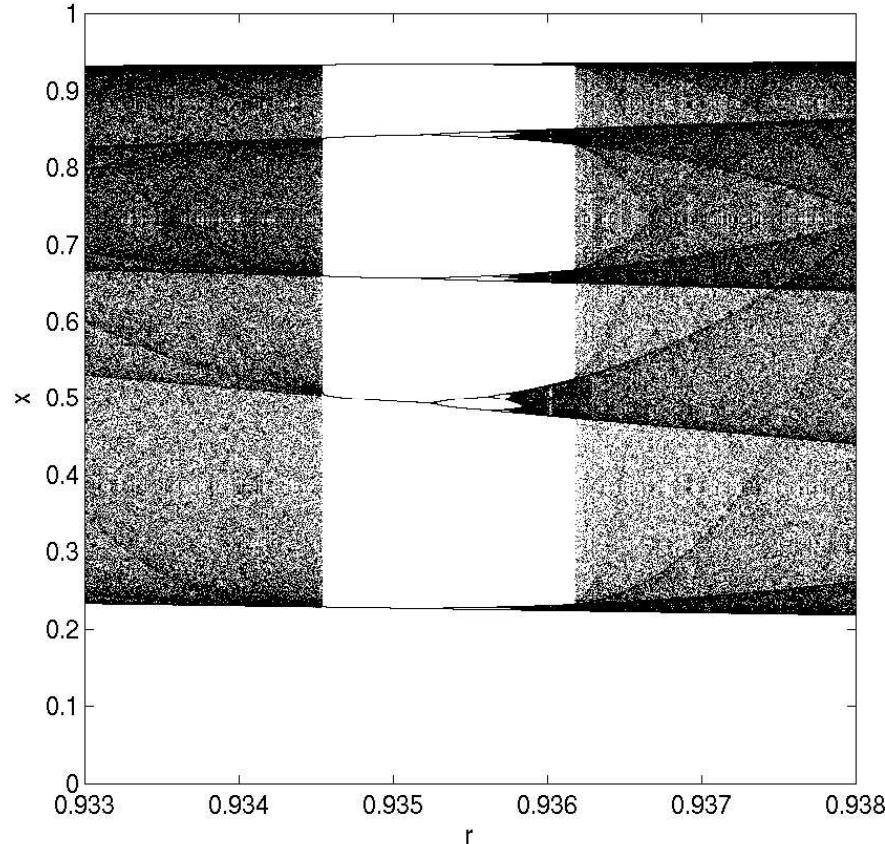
## The chaotic region

for  $r \gtrsim r_\infty$  periodic attractors are replaced by *chaotic orbits* which **fill** (one or several) intervals of  $x$ -values by means of a *quasiperiodic sequence* :



## Windows of periodic behavior

within the chaotic region one finds *windows* with periodic orbits:



**Fig. 11:** A window of period 5 in the vicinity of  $r = 0.935$ . Suggestion: run channelmovie(0.933,0.938,0.00001) to observe how period doubling leads to chaotic behavior again.

One can show: the bifurcation diagram contains every integer period, i.e. there are infinitely many windows!

In each of these windows  $w$ , period doubling leads to chaotic behavior at a limiting value  $r_\infty^w$ . Again, the sequence of bifurcation points  $r_k^w$  converges to  $r_\infty^w$  according to the Feigenbaum scenario:

$$r_k^w \approx r_\infty^w - \frac{c^w}{\delta^k}$$

Here,  $c^w$  may depend on the actual window, but  $\delta$  is the Feigenbaum constant.

## Deterministic chaos

What precisely is chaotic in the *chaotic region*?

Iterate, say, 100 times from initial values  $x_0$  and  $x_0 + \epsilon$  with, e.g.,  $\epsilon = 10^{-12}$

– for a **periodic attractor**, e.g.  $r = 0.935$ :

`logstep(0.935,0.2 ,100)` yields 0.49617646948447...

`logstep(0.935,0.2+epsilon,100)` yields 0.49617646948447...

**small initial deviations remain small and vanish!**

– for a **chaotic orbit**, e.g.  $r = 0.97$ :

`logstep(0.97,0.2 ,100)` yields 0.92484...

`logstep(0.97,0.2+epsilon,100)` yields 0.2782...

**small initial deviations become very large!**

The logistic map

- defines a simple **deterministic** iteration  
(it is not, e.g., a stochastic process)
- becomes **unpredictable** in the chaotic regime  
because of the sensitivity to initial conditions

Note: this is not “just a problem of numerical precision”, but, of course, accuracy becomes a problem. In a computer, the  $x_i$  are only evaluated to machine precision  $\delta$ , in general. So, the above results for the chaotic regime are certainly completely “wrong”, as already  $x_1$  differs from the true value by  $\mathcal{O}(\delta)$ .

**The Lyapunov exponent** quantifies the sensitivity to initial conditions.

Consider the iterations from two slightly different initial values:

$$\begin{array}{ccccccc} x_0 & \rightarrow x_1 & \rightarrow x_2 & \dots & & & \\ x_0 + \epsilon_o & \rightarrow x_1 + \epsilon_1 & \rightarrow x_2 + \epsilon_2 & \dots & \text{with the sequence of} & \epsilon_i, & i = 0, 2, \dots \end{array}$$

After  $n$  iterations:  $|\epsilon_n| = |f^{(n)}(x_o + \epsilon_o) - f^{(n)}(x_o)| \equiv \epsilon_o e^{\lambda n}$

In the limit  $\epsilon_o \rightarrow 0$  and  $n \rightarrow \infty$ , the r.h.s. defines the **Lyapunov exponent**  $\lambda$ .

Noting that  $\lim_{\epsilon_o \rightarrow 0} \frac{f^{(n)}(x_o + \epsilon_o) - f^{(n)}(x_o)}{\epsilon_o} \equiv \left. \frac{d f^{(n)}(x)}{dx} \right|_{x=x_o}$

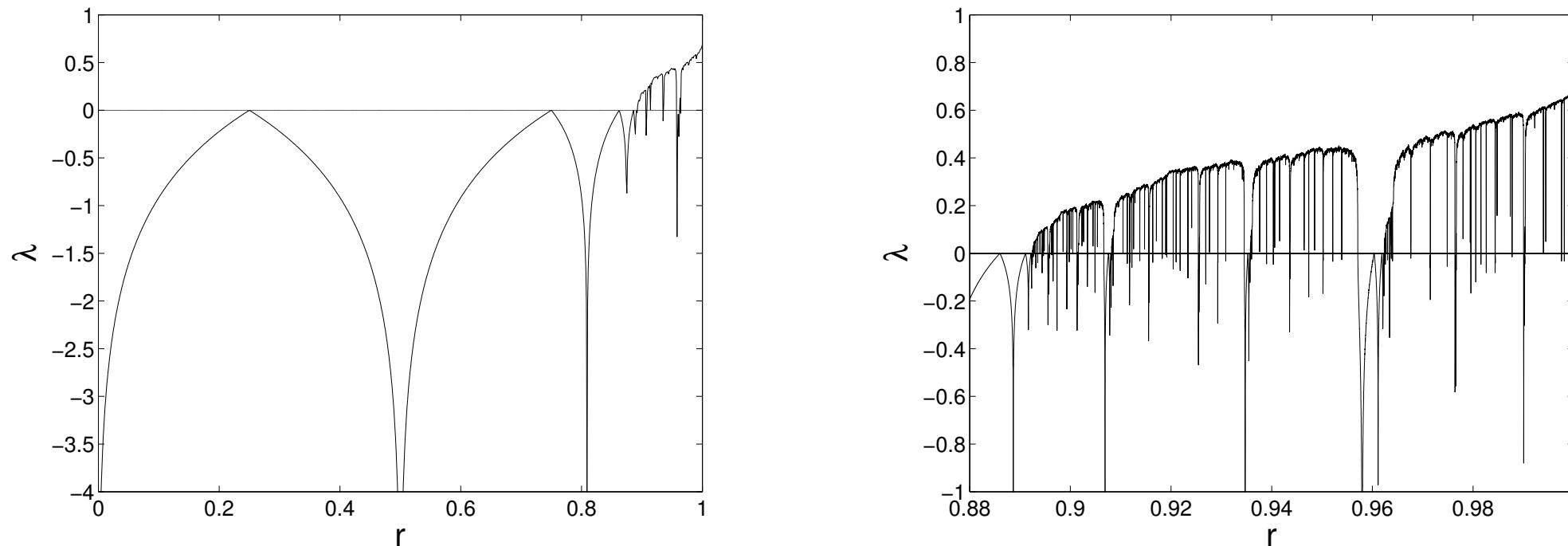
and using the chain-rule  $\frac{d[f(g(x))]}{dx}|_{x=x_o} = f'(g(x_o)) g'(x_o)$

we can write

$$\lambda = \lim_{n \rightarrow \infty} \frac{1}{n} \ln \left| \left. \frac{df(f(f \dots f(f(x)) \dots))}{dx} \right|_{x=x_o} \right| = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \ln |f'(x_i)|.$$

We can determine  $\lambda$  from a single sequence of  $x_n$ !

Lyapunov exp. obtained from scanning  $r$  and performing 1000 iter. for each value:



**Fig. 12:** Exponent  $\lambda$  vs.  $r$  for the entire range (left) and close-up (right) for  $r \geq 0.88$ . The resolution of the plot is limited by the increment in  $r$  (left: 0.001, right: 0.0001).

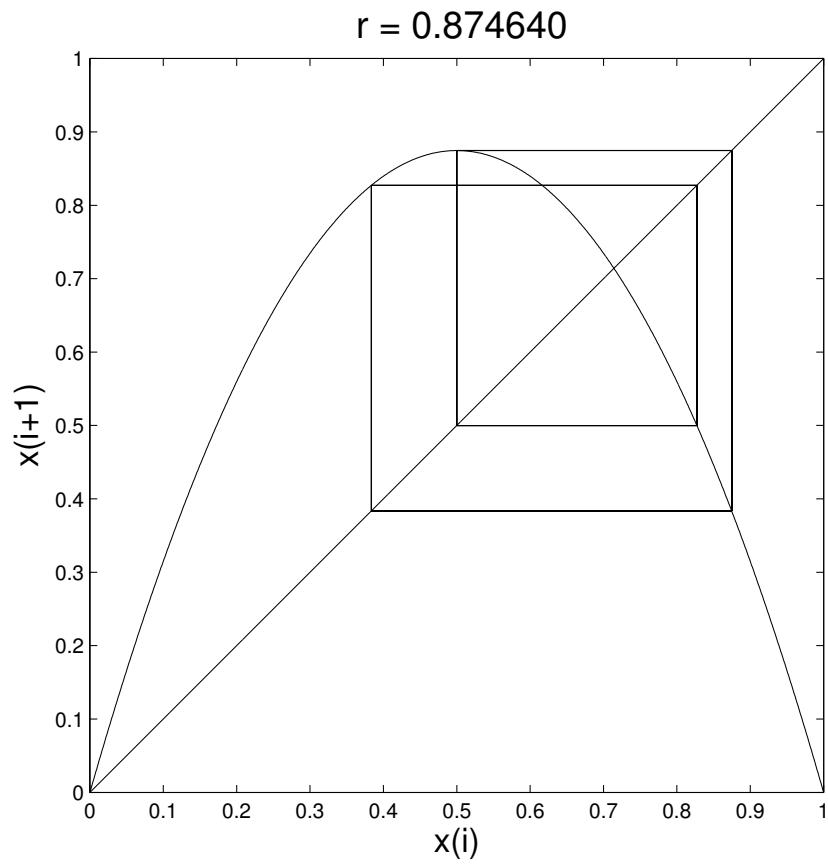
- $\lambda < 0$ : negative exponents indicate **convergent behavior** towards a stable attractor or single fixed point.  
Small initial deviations vanish as  $n \rightarrow \infty$ .
- $\lambda > 0$ : positive exponents indicate **chaotic behavior**.  
Initial deviations grow exponentially with  $n$  and the system is very sensitive to initial deviations.

special cases:

- $\lambda = 0$ : zero exponents indicate **marginal stability**.

Values of  $r$  with  $\lambda \rightarrow 0^-$  mark bifurcation points where an attractor becomes unstable and is replaced by one with double period. In principle we could determine the  $r_k$  from the Lyapunov plot in order to estimate the Feigenbaum constant, for instance.

- $\lambda \rightarrow -\infty$ : diverging exponents mark **superstable orbits** in which deviations (close to the attractor) vanish extremely fast. One finds  $\lambda \rightarrow -\infty$  for all periodic cycles that contain the value  $x = 1/2$ , because  $f'(1/2) = 0$  and  $\ln f'(1/2) \rightarrow -\infty$ .



**Fig. 13: Superstable attractor with period four.**

In each interval  $[r_k, r_{k+1}]$  of  $r$ -values with periodic orbits, there is exactly one value  $r = R_k$  which yields a superstable cycle.

Furthermore, the  $R_k$  approach  $r_\infty$  according to the Feigenbaum scenario. Corresponding statements hold true for all windows of periodic behavior in the chaotic regime.