生物动力系统模拟

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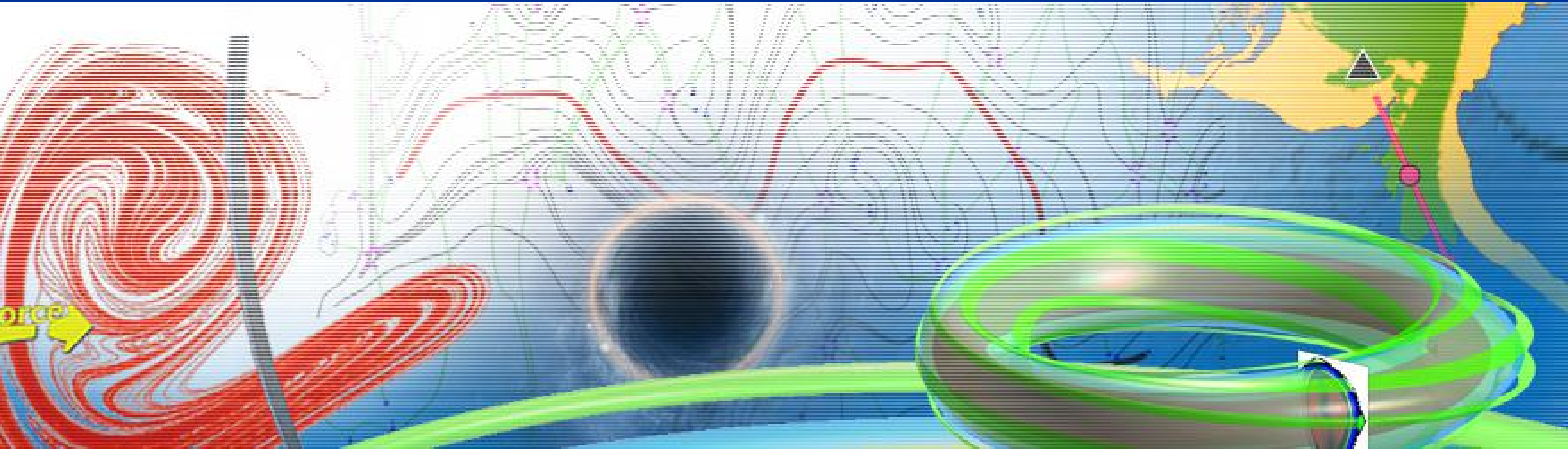


分子动力学模拟

系统层次动力学模拟

动力系统基本概念：状态空间、连续及离散系统、稳定性、系统终态的分类

线性系统理论： 线性系统的解析解，脉冲响应函数， 拉普拉斯变
换，控制理论初步

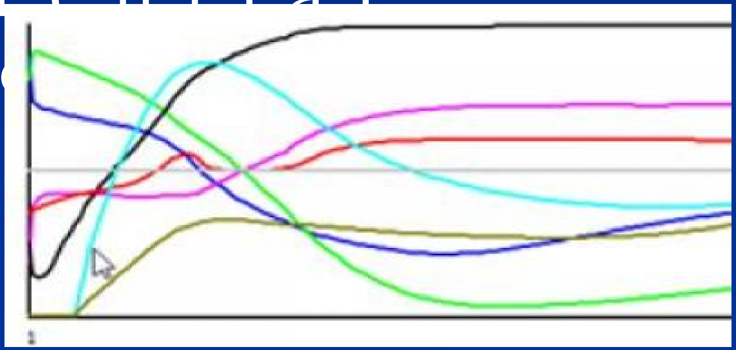
生物网络：对基因调控、信号传导、蛋白相互作用的网络建模实例分析

机体层次上的动力学模拟

Dynamical systems theory

An area of mathematics used to describe the behavior of complex dynamical systems, usually by employing differential equations or difference equati

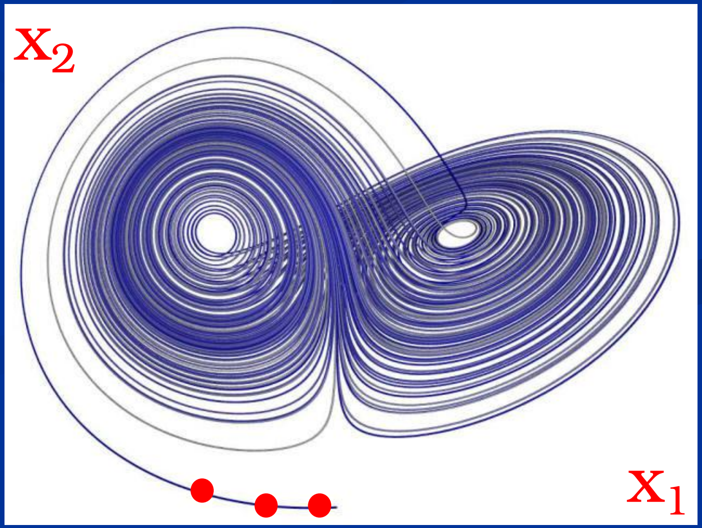
Continuous



$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p}, t)$$

$$\mathbf{x} = [\, x_1, x_2 \,, \ldots]$$

$$\mathbf{p} = [\, p_1, p_2 \,, \ldots]$$

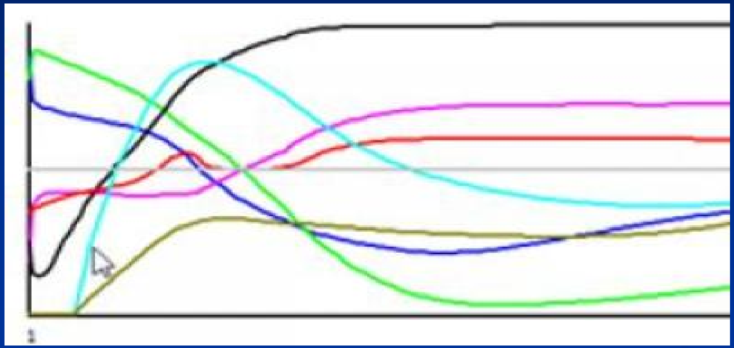


Discrete

$$\mathbf{x}(t+1) = f(\mathbf{x}(t), t)$$

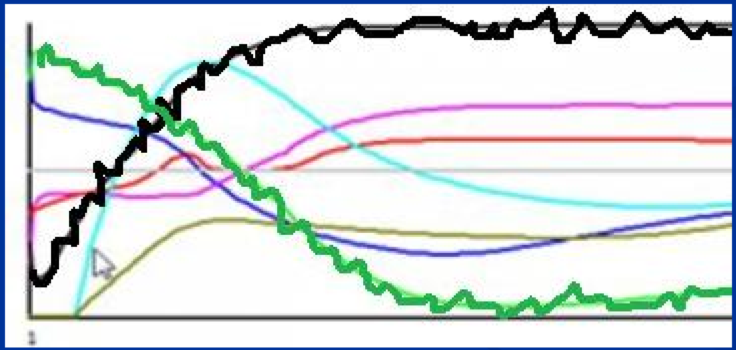
Deterministic vs stochastic systems

$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p}, t)$$



$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p}, t) + \xi(t)$$

noise term

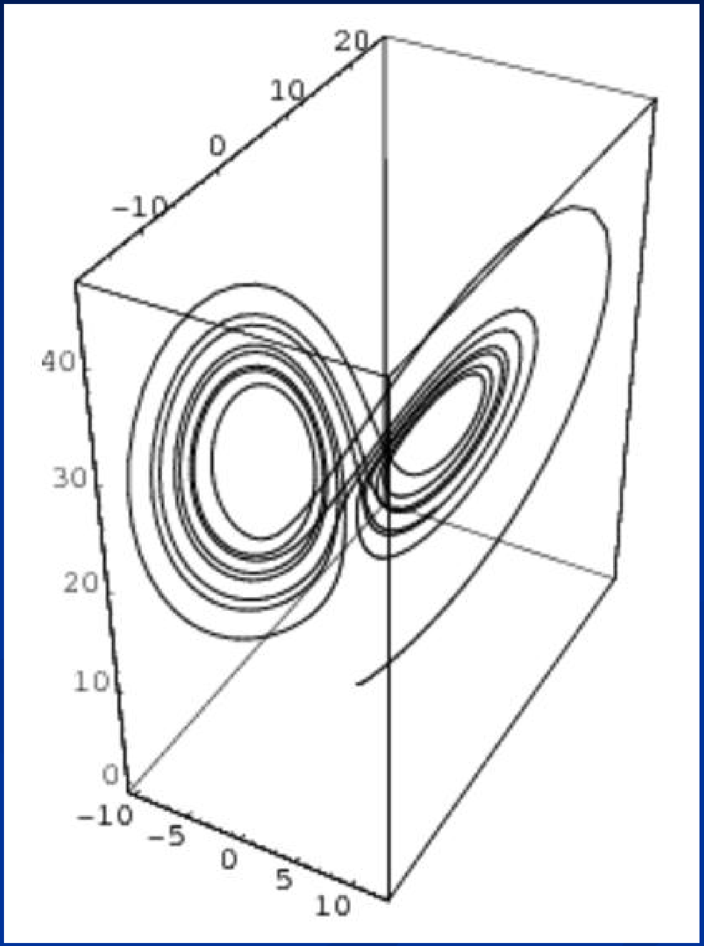


Random()
Rand()

Can a deterministic system manifests stochastic behav

Lorenz attractor

$$\dot{X} = \sigma (Y - X)$$
$$\dot{Y} = -X Z + r X - Y$$
$$\dot{Z} = X Y - b Z,$$



MIT professor
Mathematician
Meteorologist

During the 1950s, Lorenz became skeptical of the appropriateness of the linear statistical models in meteorology, as most atmospheric phenomena involved in weather forecasting are non-linear

Long-term weather forecasting is impossible

Butterfly effect

Small causes can have large effects

Sensitive dependence on initial conditions

A small change in one state of a deterministic nonlinear system can result in large differences in a later state

The butterfly effect is most familiar in terms of weather; it can easily be demonstrated in standard weather prediction models, for example. The climate scientists James Annan and William Connolley explain that chaos is important in the development of weather prediction methods; models are sensitive to initial conditions. They add the caveat: "Of course the existence of an unknown butterfly flapping its wings has no direct bearing on weather forecasts, since it will take far too long for such a small perturbation to grow to a significant size, and we have many more immediate uncertainties to worry about. So the direct impact of this phenomenon on weather prediction is often somewhat overstated

Sensitivity dependence on parameter values

$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p}, t)$$

$$\frac{d^2x}{dt^2} + \delta\frac{dx}{dt} - x + x^3 = \gamma\cos(t)$$

Example:
Duffing equation

Can anyone write it into the following form?

$$\dot{X} = \sigma(Y - X)$$
$$\dot{Y} = -XZ + rX - Y$$

$$\frac{dx_1}{dt} = x_2$$

$$\frac{dx_2}{dt} = -\delta x_2 + x_1 - {x_1}^3 + \gamma\cos(t)$$

Can anyone write it into the following form?

$$\dot{X} = \sigma\,(Y - X)$$
$$\dot{Y} = -X\,Z + r\,X - Y$$
$$\dot{Z} = X\,Y - b\,Z,$$

$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p})$$

$$\frac{dx_1}{dt} = x_2$$

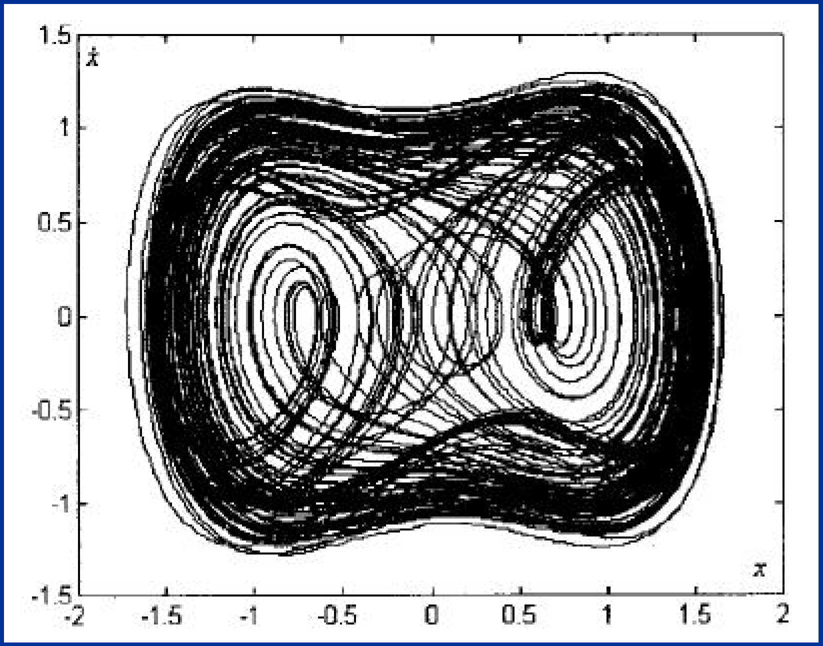
$$\frac{dx_2}{dt} = -\delta x_2 + x_1 - {x_1}^3 + \gamma\cos(x_3)$$

$$\frac{dx_3}{dt} = 1$$

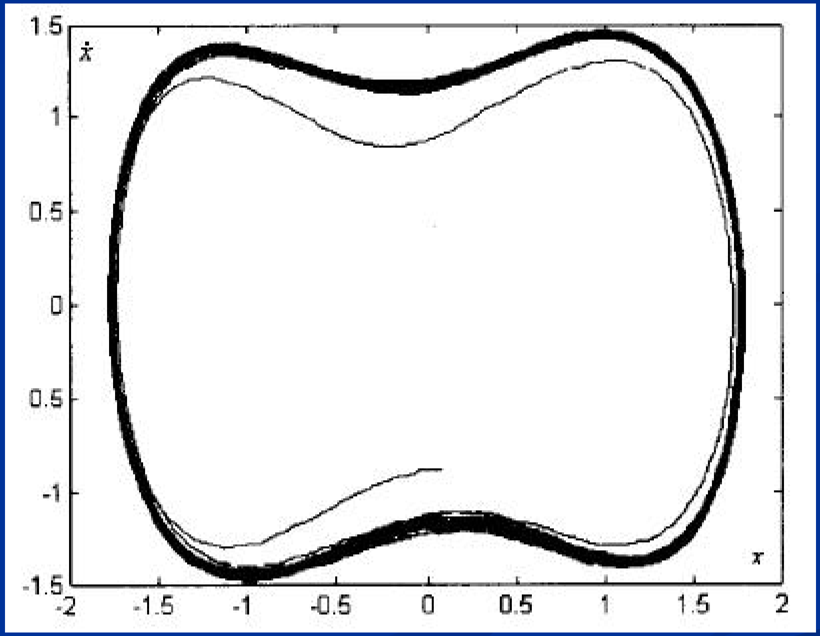
Phase diagram

$$\frac{dx_1}{dt} = x_2$$

$$\frac{dx_2}{dt} = -\delta x_2 + x_1 - {x_1}^3 + \gamma\cos(t)$$



$\gamma < \gamma_c$



$\gamma > \gamma_c$

This "sensitivity dependence on parameters" can be

Application to weak signal detection

$$\frac{dx_1}{dt} = x_2$$

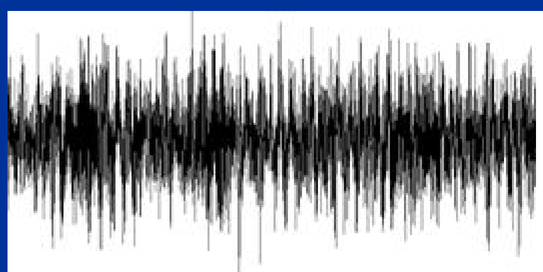
$$\frac{dx_2}{dt} = -\delta x_2 + x_1 - {x_1}^3 + \gamma_c \cos(t) + \text{signal}$$

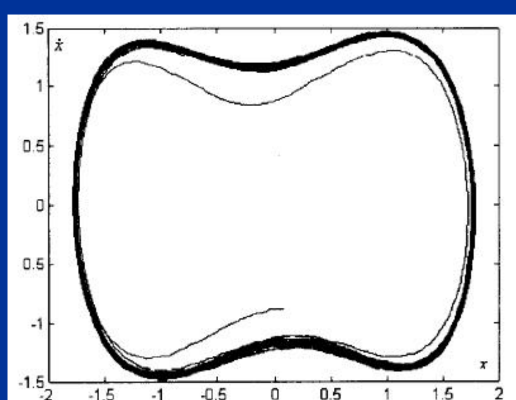
$\text{signal} = \varepsilon \cos(t) + \xi(t)$

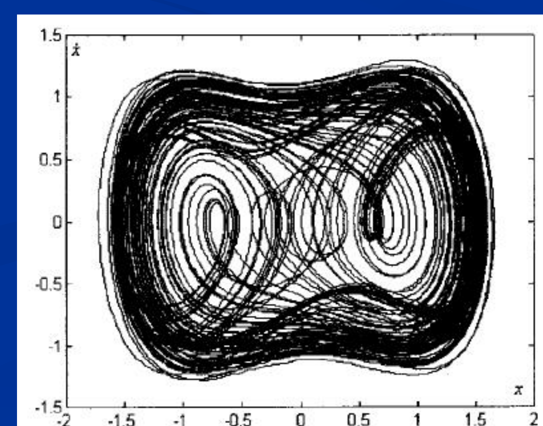
Contains useful signal

$\text{signal} = \xi(t)$

Sheer noise







The technique was developed in last century, by …

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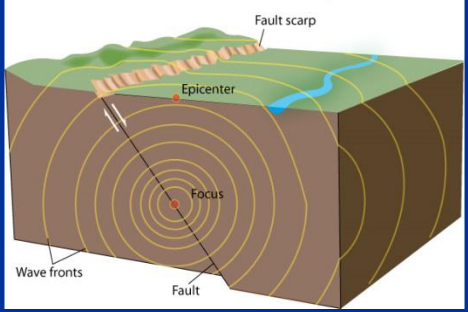
The Application of Chaotic Oscillators to Weak Signal Detection

Guanyu Wang, Dajun Chen, Jianya Lin, and Xing Chen

Successfully applied to

Seismic Waves Radiate from the Focus of an Earthquake



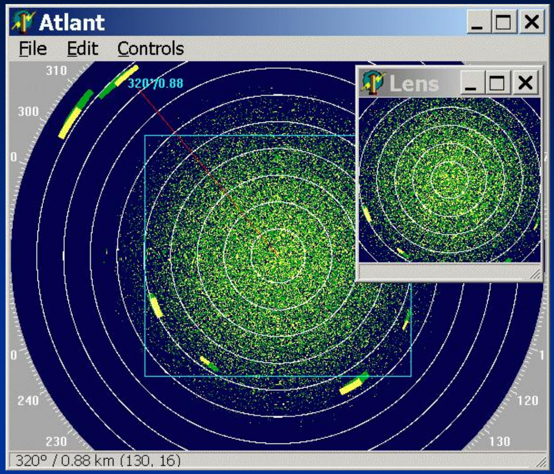
Geophys. J. Int. (2009) 178, 1493–1522 doi: 1

Chaotic system detection of weak seismic signals

Y. Li,[1] B. J. Yang,[2] J. Badal,[3] X. P. Zhao,[2] H. B. Lin[1,2] and R. L. Li[2]
[1] *Department of Information Engineering, Jilin University, Changchun 130026, China*
[2] *Department of Geophysics, Jilin University, Changchun 130026, China. E-mail: yangbaojun@jlu.edu.cn*
[3] *Physics of the Earth, Sciences B, University of Zaragoza, Pedro Cerbuna 12, Zaragoza 50009, Spain*

and many other fields …

Including radar signal detection



I was invited by … to help with radar detection design

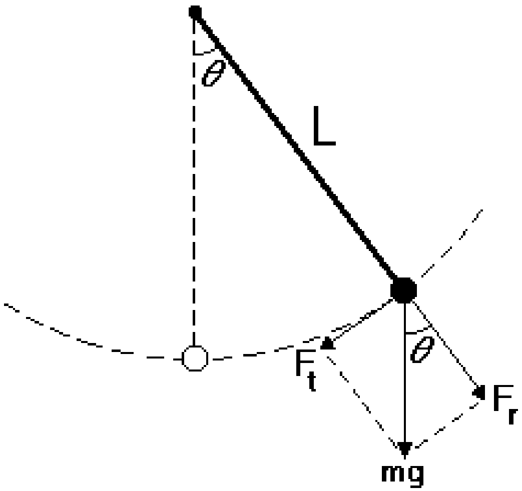
Dynamical systems theory are useful,

The application to biology would be fruitful.

Arrhythmia

Controlling chaos

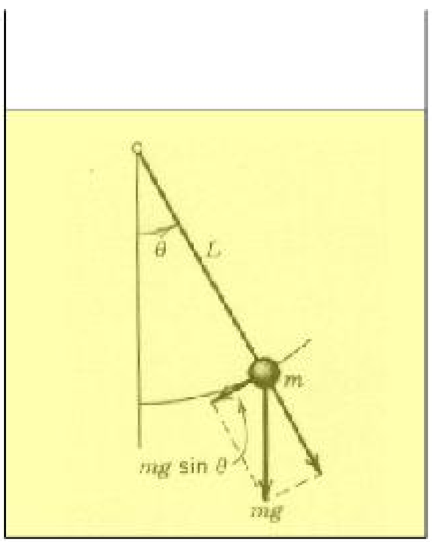
Duffing equation is related to pendulum



$$m\ell\ddot{\theta} = -mg\sin(\theta)$$

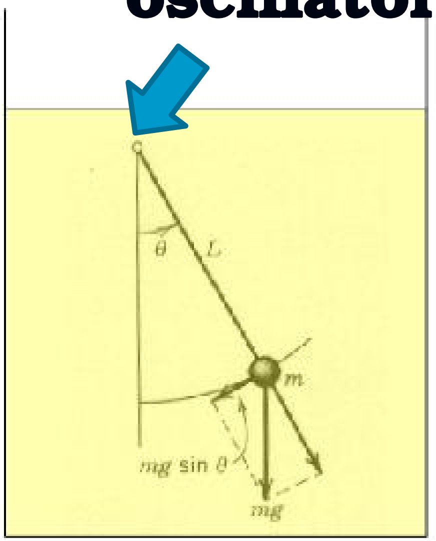
$$\ddot{\theta} + \frac{g}{\ell}\sin(\theta) = 0$$

$$\ddot{\theta} + \omega^2\sin(\theta) = 0 \qquad \omega = \sqrt{\frac{g}{\ell}}$$



$$\ddot{\theta} + \delta\dot{\theta} + \omega^2\sin(\theta) = 0$$

oscillator



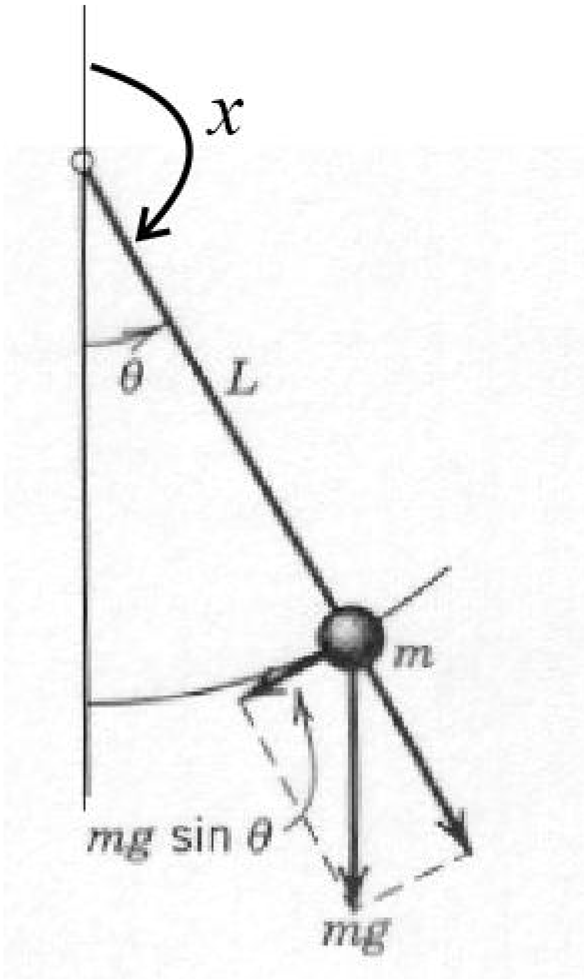
$$\ddot{\theta} + \delta\dot{\theta} + \omega^2 \sin(\theta) = \varepsilon \cos(\Omega t)$$

$$Sin(\theta) = \theta - \frac{\theta^3}{3!} + \cdots$$

$$\ddot{\theta} + \delta\dot{\theta} + \omega^2 \left(\theta - \frac{\theta^3}{6}\right) = \varepsilon \cos(\Omega t)$$

$$\frac{d^2x}{dt^2} + \delta\frac{dx}{dt} - x + x^3 = \gamma \cos(t)$$

Can we make them closer?

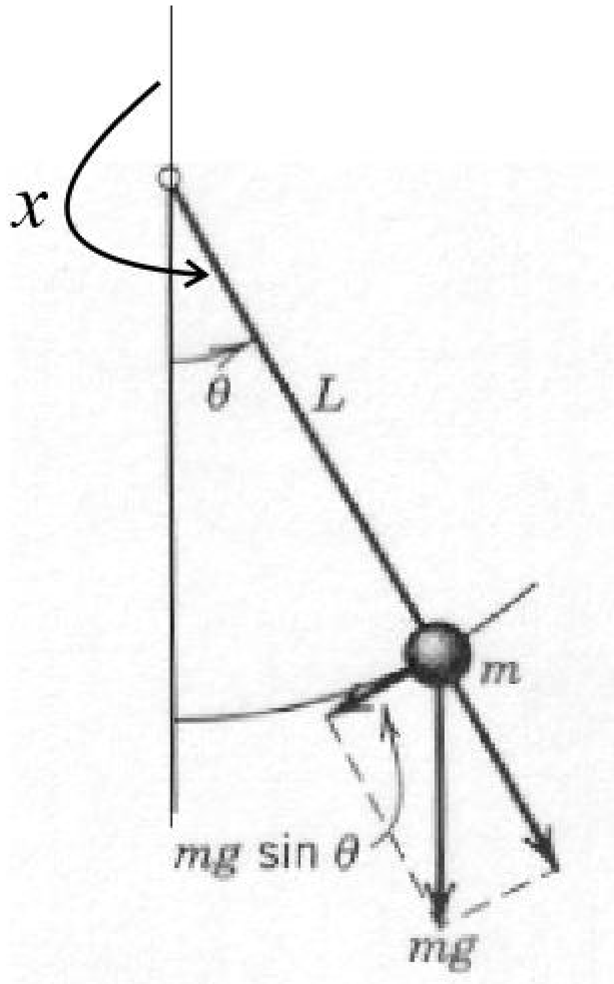


$$\theta = \pi - x$$

$$\ddot{\theta} + \delta\dot{\theta} + \omega^2 \sin(\theta) = 0$$
$$\ddot{x} + \delta\dot{x} - \omega^2 \sin(x) = 0$$

We succeed in converting it closer to the Duffing equation!

Let's try the following



$$\theta = x - \pi$$

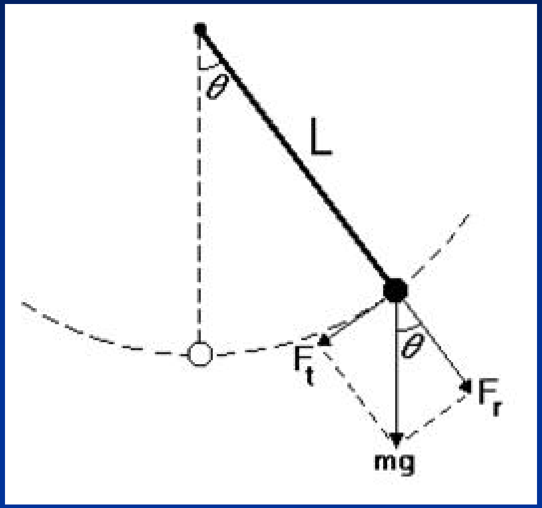
$$\ddot{\theta} + \delta\dot{\theta} + \omega^2 \sin(\theta) = 0$$

$$\ddot{x} + \delta\dot{x} - \omega^2 \sin(x) = 0$$

It is also OK!

Now let's convert

$$\frac{d^2\theta}{dt^2} + \sin(\theta) = 0$$



into

$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p})$$

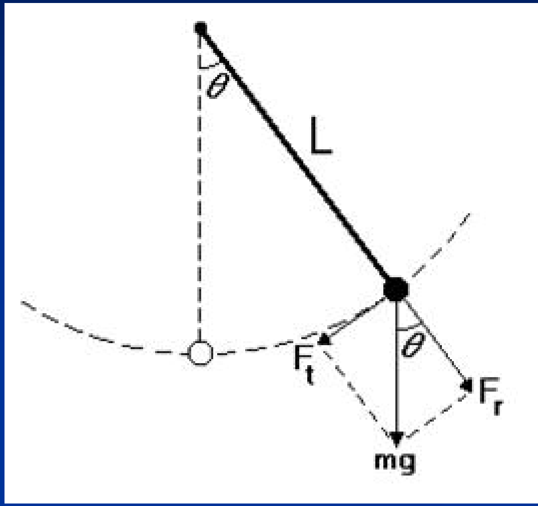
$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = -\sin(x)$$

Steady state $\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p}) = 0$

$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = -\sin(x)$$



$x = \pi$

$y = 0$

$x = 0$

$y = 0$

Stability of $\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p})$

Calculate the Jacobian matrix of $f(\mathbf{x}, \mathbf{p})$

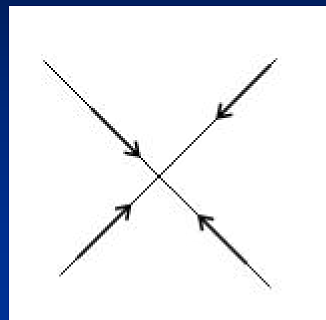
$$J_F(x, y) = \begin{bmatrix} \frac{\partial F_1}{\partial x} & \frac{\partial F_1}{\partial y} \\ \frac{\partial F_2}{\partial x} & \frac{\partial F_2}{\partial y} \end{bmatrix}$$

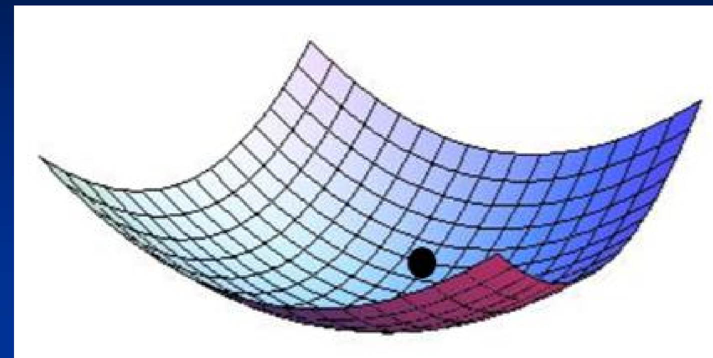
Then calculate the eigenvalues

$$\lambda = Re(\lambda) + Im(\lambda)i$$

When λ are real

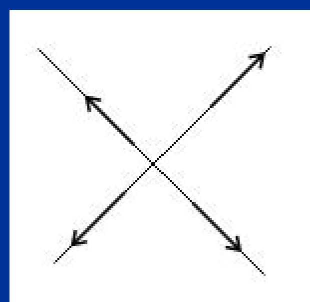
$\lambda_1 < 0$
$\lambda_2 < 0$





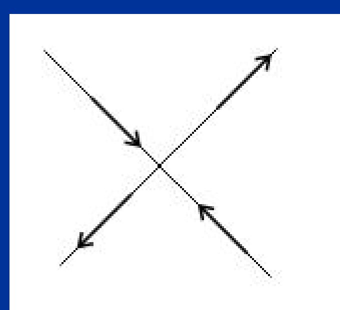
sink

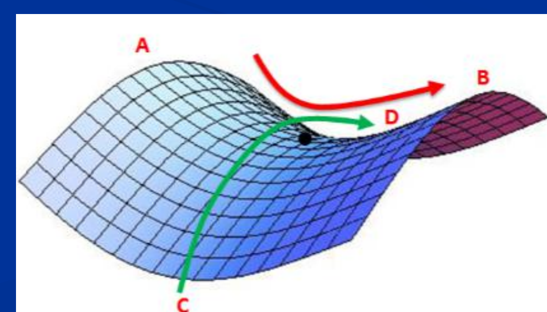
$\lambda_1 > 0$
$\lambda_2 > 0$



source

$\lambda_1 < 0$
$\lambda_2 > 0$

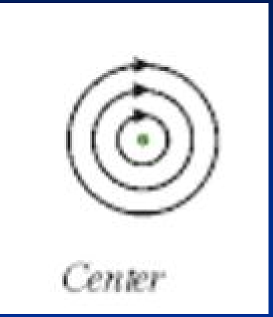




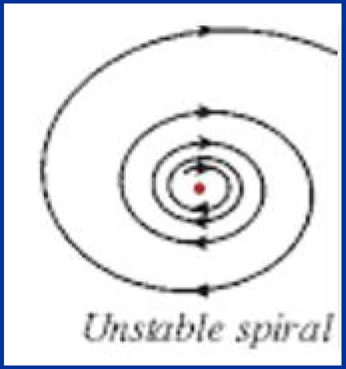
saddle

When λ have imaginary part

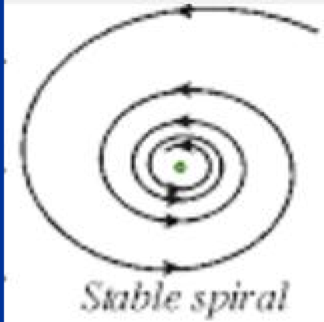
$Re(\lambda) = 0$



$Re(\lambda) > 0$



$Re(\lambda) < 0$



Stability

$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = -\sin(x)$$

Calculate the Jacobian ma

$$f(x,y) = \begin{pmatrix} y \\ -\sin(x) \end{pmatrix}$$

$$D_{(x,y)} \begin{pmatrix} y \\ -\sin(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\cos(x) & 0 \end{pmatrix}$$

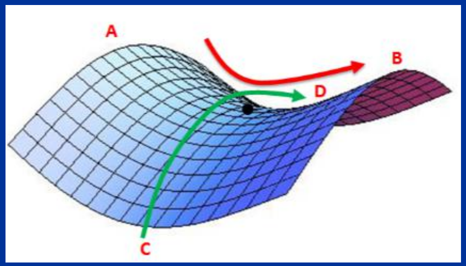
We first evaluate Jacobian at

$x = \pi$

$y = 0$

$$D_{(x,y)}f \begin{pmatrix} \pi \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Eigenvalues a $\lambda = \pm 1$.



As long as there is a positive eigenvalue, it is unstable.

This steady state is thus unstable

We then evaluate Jacobian at

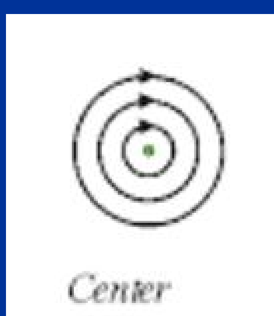
$x = 0$

$y = 0$

$$D_{(x,y)} f \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

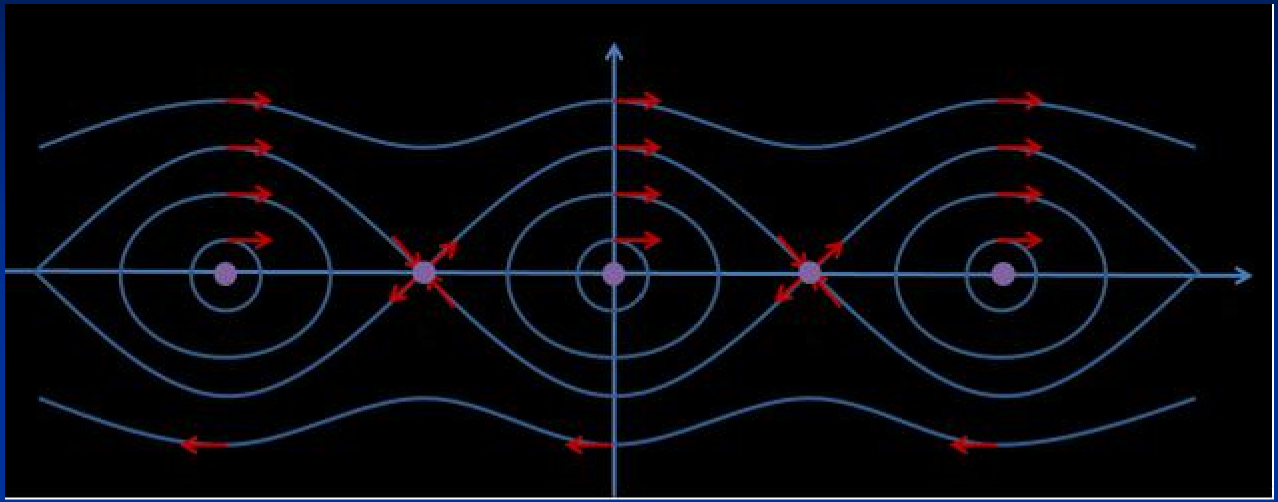
Eigenvalues ar $\lambda = \pm i$

The real part is 0,
not positive nor negative.



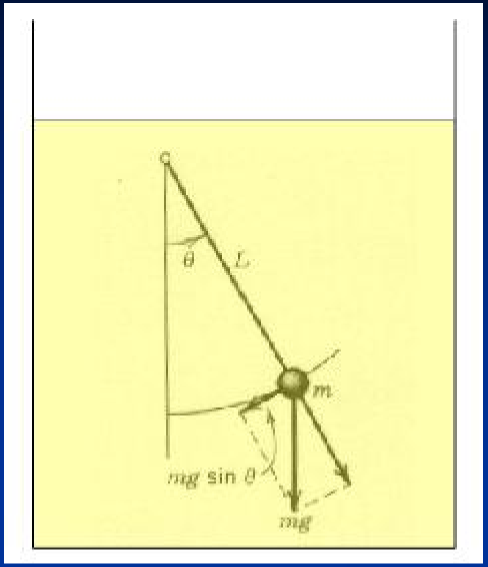
This steady state is marginally stable

Phase portrait



Now let's convert

$$\frac{d^2\theta}{dt^2} + \delta\frac{d\theta}{dt} + \sin(\theta) = 0$$



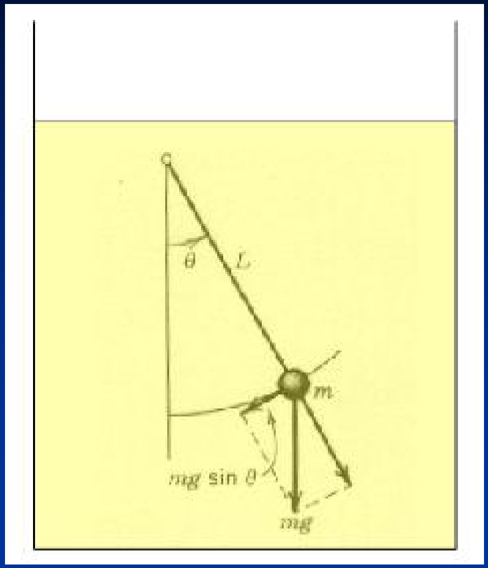
into

$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p})$$

$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = -\delta y - \sin(x)$$

Steady state



$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = -\delta y - \sin(x)$$

$x = 0$

$y = 0$

$x = \pi$

$y = 0$

Stability of $\frac{d\mathbf{x}}{dt} = f(\mathbf{x}, \mathbf{p})$

Calculate the Jacobian ma

$$f(x,y) = \begin{pmatrix} y \\ -\sin(x) - \delta y \end{pmatrix}$$

$$D_{(x,y)} \begin{pmatrix} y \\ -\sin(x) - \delta y \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\cos(x) & -\delta \end{pmatrix}$$

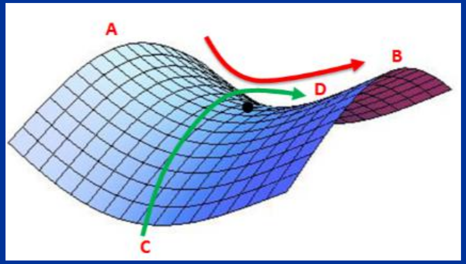
We first evaluate Jacobian at

$x = \pi$

$y = 0$

$$D_{(x,y)}f \begin{pmatrix} \pi \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & -\delta \end{pmatrix}$$

One can check that
one eigenvalue >0
the other < 0



This steady state is thus unstable

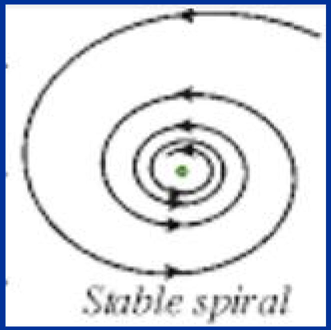
We then evaluate Jacobian at

$x = 0$

$y = 0$

$$D_{(x,y)}f\begin{pmatrix}0\\0\end{pmatrix} = \begin{pmatrix}0 & 1\\ -1 & -\delta\end{pmatrix}$$

One can check that
All the real part of eigenvalues are < 0



Stable spiral

This steady state is stable

Phase portrait