Dimension Reduction: Analysis and Algorithms

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(based on a review with A. Stuart)

Instructions for Audience

I've nagged speakers for 2.5 days.
Now you have the opportunity to take revenge.
Please do!

Modeling

Confining complex real-world situations into succinct systems of equations (e.g., Newton's laws of mechanics). The central theme of the exact sciences.

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A "second level" of modeling is required to obtain useful models. This second step is often called **dimension reduction**, **coarse-graining**, **homogenization**, or simply, **modeling**.

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- Too **complex** to be solved.
- Dynamics of interest take place in a (low-dimensional) **subspace** $\mathcal{X}$ of $\mathcal{Z}$.
- Objective: find a self-contained description of the dynamics in $\mathcal{X}$ without resolving the dynamics in $\mathcal{Y}=\mathcal{Z}/\mathcal{X}$.

Using coordinates $x \in \mathcal{X}$ and $y \in \mathcal{Y}$:

$$\frac{dx}{dt} = f(x,y) + \alpha(x,y)\frac{dU}{dt}$$

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microscopic

The goal is to obtain a **reduced**, **macroscopic, closure** equation in $\mathcal{X}$:

$$\frac{dX}{dt} = F(X) + A(X)\frac{dU}{dt}$$

macroscopic

such that $X(t)$ approximates well the component $x(t)$ of the full dynamics.

Running Themes

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- **Controlled versus uncontrolled approximation**
  Dimension reduction is sometimes backed by analysis, along with error estimates (e.g., systems with **scale separation**). In other cases, it is based on heuristic reasoning, and scope of validity is unknown (e.g., K-ε models of turbulence).

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- **Deterministic versus stochastic**
  Dynamics in $\mathcal{Z}$ and $\mathcal{X}$ may be either deterministic or stochastic. We classify systems accordingly as **DD**, **DS**, **SD**, and **SS**.

Running Themes (cont.)

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- **Reduction principle**
  Two steps: identification of the subspace $\mathcal{X}$ (often not known) and derivation of dynamics in $\mathcal{X}$.

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- **Path-wise versus distributions**
  Often the dynamical system is "lifted" to an evolution of probability distribution. Higher dimensional but linear (hence, functional analytical techniques).

Mori-Zwanzig Formalism

A general technique to (formally) reduce the dimensionality of systems of **ODEs**. Developed in the context of irreversible stat. mech. In essence, a rewriting of the equations in a suggestive form.

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The basic idea: (1) treat $x(t)$ as a given function and integrate (formally) the y-equation. The solution $y(t)$ depends on the entire history of $x(t)$ ("**variation of constants**"). (2) Substitute $y(t)$ in the x-equation, resulting in a closed reduced system.

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$$\frac{dx(t)}{dt} = \tilde{f}(x(t)) + \int_0^t K(x(t-s),s)\,ds + \mathcal{N}(x(0),y(0),t)$$

"Markovian" "memory" "noise"

Generalized Langevin Equation

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(Spatial) **Homegenization**: dynamics depend on small scale features, but phenomena of interest are on large scales (e.g., porous media, climate prediction).

(Temporal) **Averaging**: dynamics include short timescale features, but phenomena of interest over long time scales (e.g., molecular conformations, climate prediction).

Scale Separation (cont.)

In our context, *x(t)* are the "**slow**" variables, whereas *y(t)* are the "**fast**" variables:

$$\frac{dx}{dt} = f(x,y) + \alpha(x,y)\frac{dU}{dt}$$

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Several scenarios, depending on the functions f,g,α,β.

Attracting Manifolds

Goes back to Tikhonov (East) and Levinson (West).

Starting point: ODEs with scale separations:

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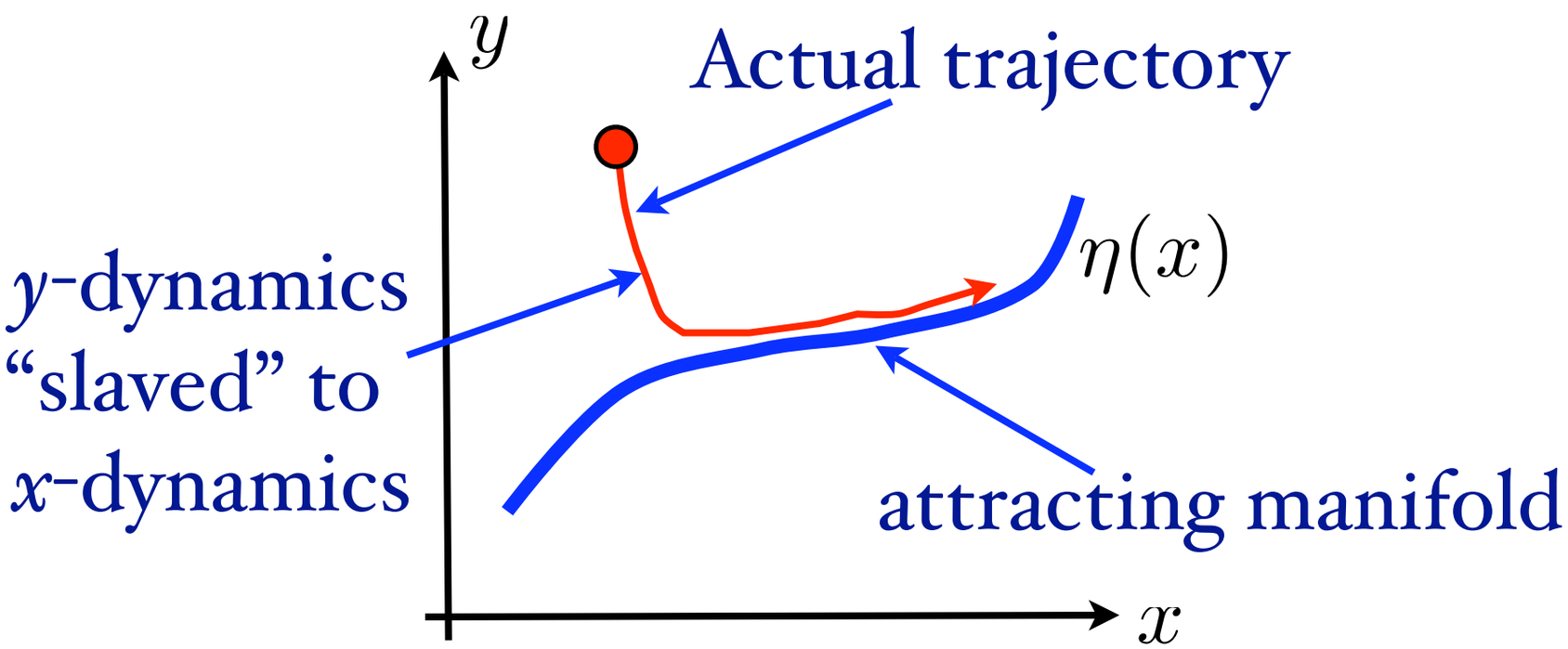
Systems of **class DD**


y
Actual trajectory
y-dynamics
"slaved" to
x-dynamics
$\eta(x)$
attracting manifold
x

Example:

$$\frac{dx_1}{dt} = -x_2 - x_3$$
$$\frac{dx_2}{dt} = x_1 + \frac{1}{5}x_2$$
$$\frac{dx_3}{dt} = \frac{1}{5} + y - 5x_3$$
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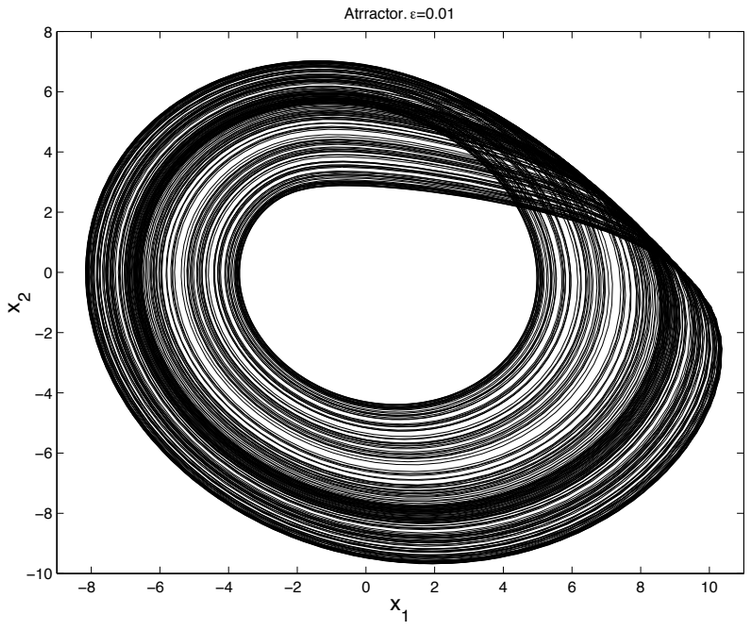

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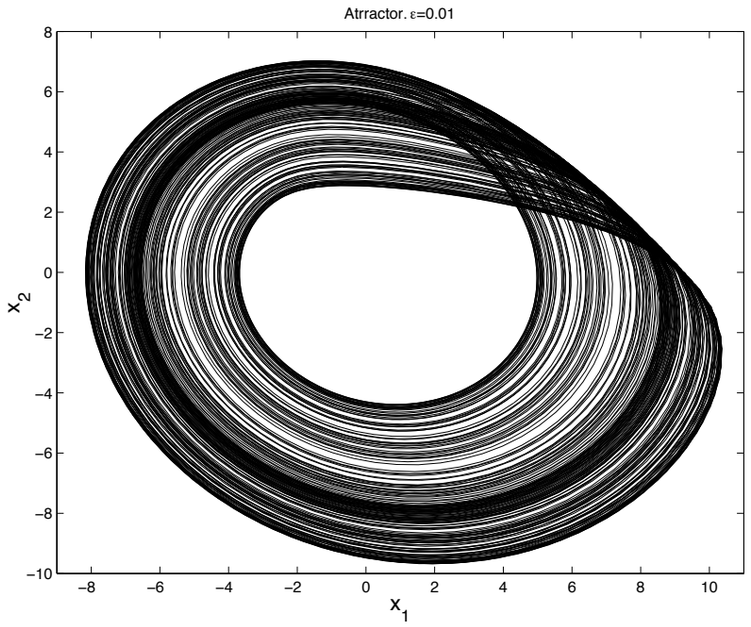

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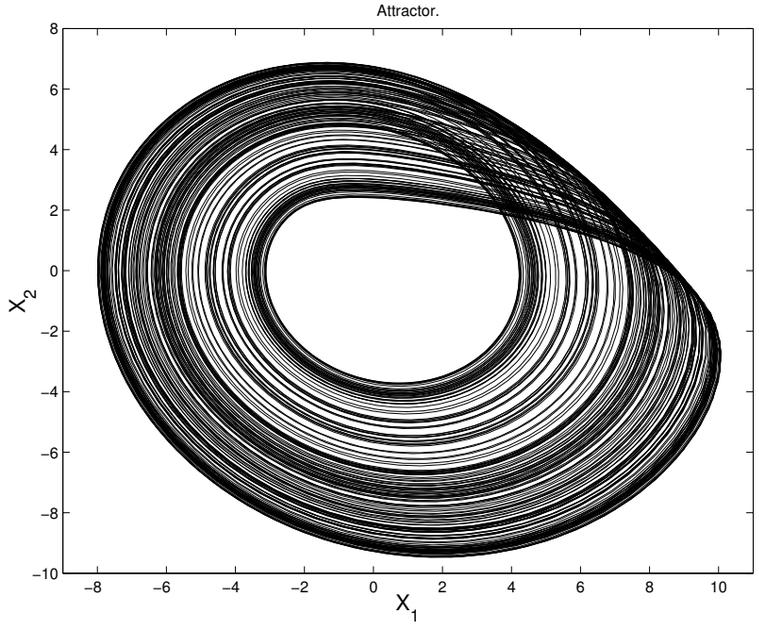

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Assumption: for fixed x, the y-dynamics are **ergodic**.

Let $\varphi_x^t(y)$ denote the solution operator of the y-dynamics:

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Ergodic dynamics induce a **Young measure** on Y:

$$\mu_x(A) = \lim_{T\to\infty} \int_0^T I_A(\varphi_x^t(y))\, dt$$

measure depends on x

indicator function

independent of y

Averaging (cont.)

Anosov's theorem states that *x(t)* converges uniformly on any bounded time interval to the solution *X(t)* of the **averaged equation**:

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- Extension to non-unique invariant measure (differential inclusions, Artstein).
- Invariant measure may depend on *y(0)*.

Application: Stiff Hamiltonian Systems

Ubiquitous in molecular systems: Hamiltonian systems with strong potential forces resuling in **fast oscillatory motion** around a sub-manifold, along with weaker forces responsible for **conformational changes** over longer timescales (Rubin and Ungar, 1957, Neistadt 1984, Bornemann and Schuette 1997).

$$H(z,p) = \frac{1}{2}\sum_i \frac{p_i^2}{2m_i} + V(z) + \frac{1}{\epsilon^2}U(z)$$

"soft" potential **"stiff" potential**

The stiff potential is minimal on a smooth submanifold $\mathcal{M}$.

Goal: approximate solution by a flow on $\mathcal{M}$.

Example: a two-particle system

constraining manifold y=0

$$H(x,p,y,v) = \frac{1}{2}(p^2+v^2) + V(x) + \frac{\omega^2(x)}{2\epsilon^2}y^2$$

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Naive solution: set $y=0$.
Wrong!

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Assumption: energy E does not depend on ε, hence $y \to o$ as $\varepsilon \to o$.

Naive solution: set $y=o$.
Wrong!

This system is still not in the desired form of scale separation because the "slow" (x,p) equations depend on ε.

Change variables:
$\eta = y/\varepsilon$.

Transformed system of equations:

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

$$\frac{dp}{dt} = -V'(x) - \frac{\omega'(x)}{2}\eta^2 \quad \textbf{slow}$$

$$\frac{d\eta}{dt} = \frac{1}{\epsilon}v \quad \textbf{fast}$$

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Applying the **averaging principle** (here, a variation of Anosov's theorem)

$$\frac{dX}{dt} = P$$
$$\frac{dP}{dt} = -V'(X) - J\,(\omega^{1/2}(X))'$$

constant depending on initial data

effective (Fixman) potential (non-trivial)

Stochastic Averaging

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If for fixed x the y-dynamics is ergodic with invariant measure $\mu_x(dy)$, then as $\varepsilon \to o$, $x(t)$ converges uniformly to $X(t)$:

$$\frac{dX}{dt} = \int_y f(X,y) \mu_X(dy)$$

class SD

Sketch of proof (asymptotic analysis can be backed up by a limit theorem):

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$$\frac{dx}{dt} = f(x,y)$$
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Step 2: power series expansion:

$$\phi(x,y,t) = \phi_0(x,y,t) + \epsilon\,\phi_1(x,y,t) + \ldots$$

Step 3: equate terms of same order:

***O(1/ε)* terms**: $\mathcal{L}_0\phi_0 = 0$

$$\mathcal{L}_0\phi = -\frac{\partial}{\partial y}(g\,\phi) + \frac{1}{2}\frac{\partial^2}{\partial y^2}(\beta^2\,\phi)$$ **the generator of the *y*-dynamics**

solution: $\phi_0(x,y,t) = \pi(x,t)\phi^x_{eq}(y)$ ← **invariant distribution of *y*-dynamics**

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Solvability condition: right-hand side orthogonal to the kernel of $\mathcal{L}_\circ{}^*$ (constant functions). Integrate over y:

$$\frac{\partial\pi}{\partial t} = -\frac{\partial}{\partial x}\left[\pi(x,t)\left(\int f(x,y)\phi^x_{eq}(y)\,dy\right)\right]$$

$$\frac{\partial \pi}{\partial t} = -\frac{\partial}{\partial x}\left[\pi(x,t)\left(\int f(x,y)\phi_{eq}^{x}(y)\,dy\right)\right]$$

Step 4: We identify this equation as the **Liouville equation** of the **deterministic** system

$$\frac{dX}{dt} = \int f(X,y)\phi_{eq}^{X}(y)\,dy \equiv F(X)$$

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This asymptotic expansion can be made into a rigorous convergence proof (e.g., through limit theorem for semi-groups).

Stochastic Limits

A more subtle case of scale-separated system occurs for the following scaling:

x-equation contains a "fast" term

$$\frac{dx}{dt} = \frac{1}{\sqrt{\epsilon}} f_0(x,y) + f_1(x,y)$$

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The setting is such that $f_o(x,y)$ **averages to zero** under the invariant measure of the y-dynamics. A large term that averages to zero becomes, as $\varepsilon \to o$, **white noise**.

Asymptotic expansion

Step 1: Switch to the Kolmogorov equation:

$$\frac{\partial \phi}{\partial t} = \frac{1}{\epsilon}\mathcal{L}_0\phi + \frac{1}{\sqrt{\epsilon}}\mathcal{L}_1\phi + \mathcal{L}_2\phi$$

$$\mathcal{L}_0\phi = -\frac{\partial}{\partial y}(g\,\phi) + \frac{1}{2}\frac{\partial^2}{\partial y^2}(\beta^2\,\phi) \qquad \mathcal{L}_1\phi = -\frac{\partial}{\partial x}(f_0\,\phi) \qquad \mathcal{L}_2\phi = -\frac{\partial}{\partial x}(f_1\,\phi)$$

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Step 2: Asymptotic series expansion:

$$\phi(x,y,t) = \phi_0(x,y,t) + \sqrt{\epsilon}\phi_1(x,y,t) + \epsilon\phi_2(x,y,t) + \ldots$$

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solution: $\phi_0(x,y,t) = \pi(x,t)\phi_{eq}(y)$

$O(1/\sqrt{\varepsilon})$ terms: $\mathcal{L}_0\phi_1 = -\mathcal{L}_1\phi_0$

Solvability condition requires that integral of RHS be zero.

$$\text{RHS} = \frac{\partial}{\partial x}\left[f_0(x,y)\phi_{eq}(y)\pi(x,t)\right]$$

This follows from the properties of f_o.

Solution: $\phi_1 = -\mathcal{L}_0^{-1}\mathcal{L}_1\phi_0$

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Again, apply same solvability condition, and obtain an equation for the (leading order) marginal $\pi(x,t)$:

$$\frac{\partial\pi}{\partial t} = -\int \mathcal{L}_1\mathcal{L}_0^{-1}\mathcal{L}_1\phi_{eq}(y)\pi(x,t)\,dy + \int \mathcal{L}_2\phi_{eq}(y)\pi(x,t)\,dy$$

Step 4: identification of reduced problem:

$$\frac{\partial \pi}{\partial t} = \underbrace{-\int \mathcal{L}_1 \mathcal{L}_0^{-1} \mathcal{L}_1 \phi_{eq}(y)\pi(x,t)\,dy}_{\textbf{diffusion}} + \underbrace{\int \mathcal{L}_2 \phi_{eq}(y)\pi(x,t)\,dy}_{\textbf{drift}}$$

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We identify the equation for the marginal $\pi(x,t)$ as a Kolmogorov equation of a **diffusion process** $X(t)$.

The drift and diffusion may be difficult to evaluate analytically due to the need to invert $\mathcal{L}_0$.

Example:

$$\frac{dx}{dt} = \frac{1}{\sqrt{\epsilon}} yx - \lambda x$$

$$\frac{dy}{dt} = -\frac{1}{\epsilon} y + \frac{1}{\sqrt{\epsilon}} \frac{dV}{dt}$$

$f_0(x,y)$

$f_1(x,y)$

Ornstein-Uhlenbeck process

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$$\mathcal{L}_0 \phi = \frac{\partial}{\partial y}(y\,\phi) + \frac{1}{2}\frac{\partial^2 \phi}{\partial y^2} \quad \Rightarrow \quad \phi_{eq}(y) = \frac{1}{\sqrt{\pi}} e^{-y^2}$$

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$$\frac{\partial \pi}{\partial t} = -\frac{\partial}{\partial x}\left[\left(\frac{1}{2} - \lambda\right) x\pi\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left(x^2\,\pi\right)$$

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$$\frac{dX}{dt} = \left(\frac{1}{2} - \lambda\right) X + X \frac{dU}{dt}$$

Reduced SDE

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$$X(t) = X(0) \exp\left[-\lambda t + U(t)\right]$$

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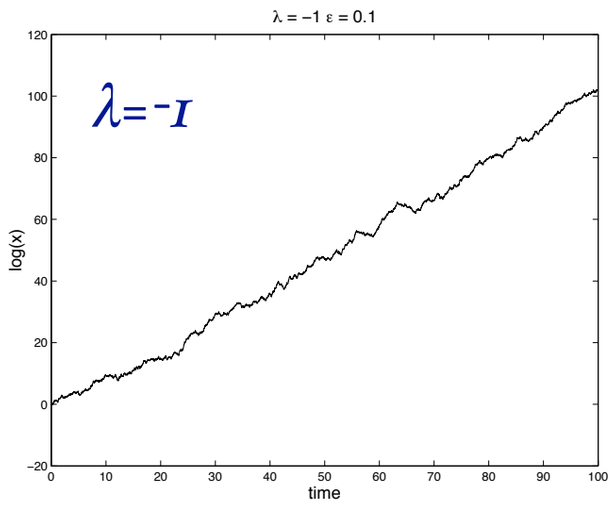
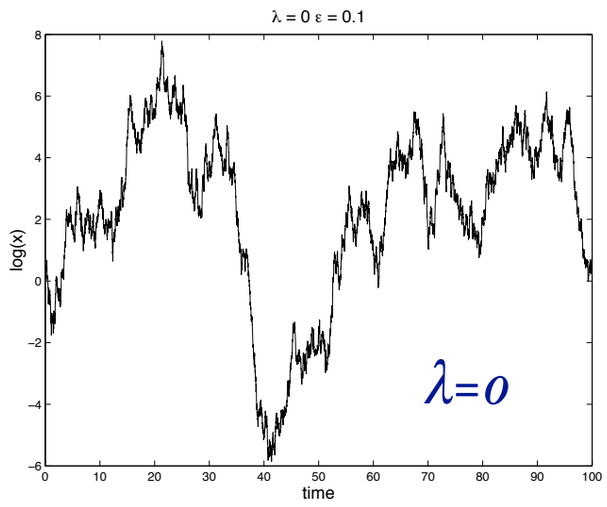
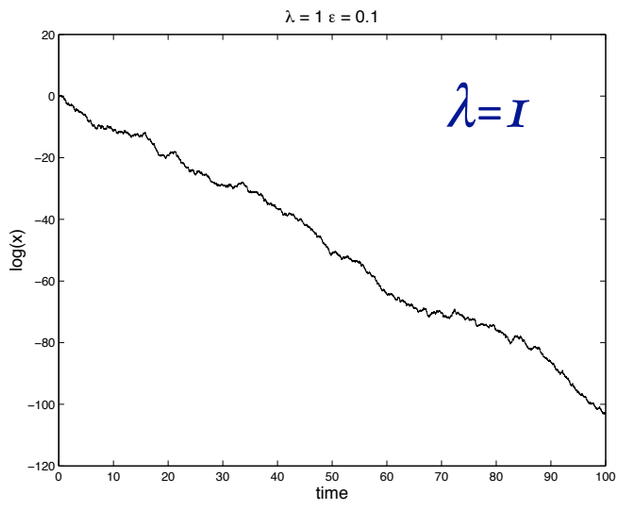
Numerical solution of $\log x(t)$ for $\varepsilon = 0.1$.







Example of Class DS

We dealt with systems of the following form that yields dimension reduction of **class SS**.

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y-equation independent of x (skew-symmetric, not essential)

The same type of arguments remain valid if the y-dynamics are deterministic, but sufficiently-well **mixing**.

Example:

$$\frac{dx}{dt} = x - x^3 + \frac{4}{90\sqrt{\epsilon}} y_2$$

$$\frac{dy_1}{dt} = \frac{10}{\epsilon}(y_2 - y_1)$$

$$\frac{dy_2}{dt} = \frac{1}{\epsilon}(28y_1 - y_2 - y_1 y_3)$$

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$(\sigma = 0.126)$ **class DS.**

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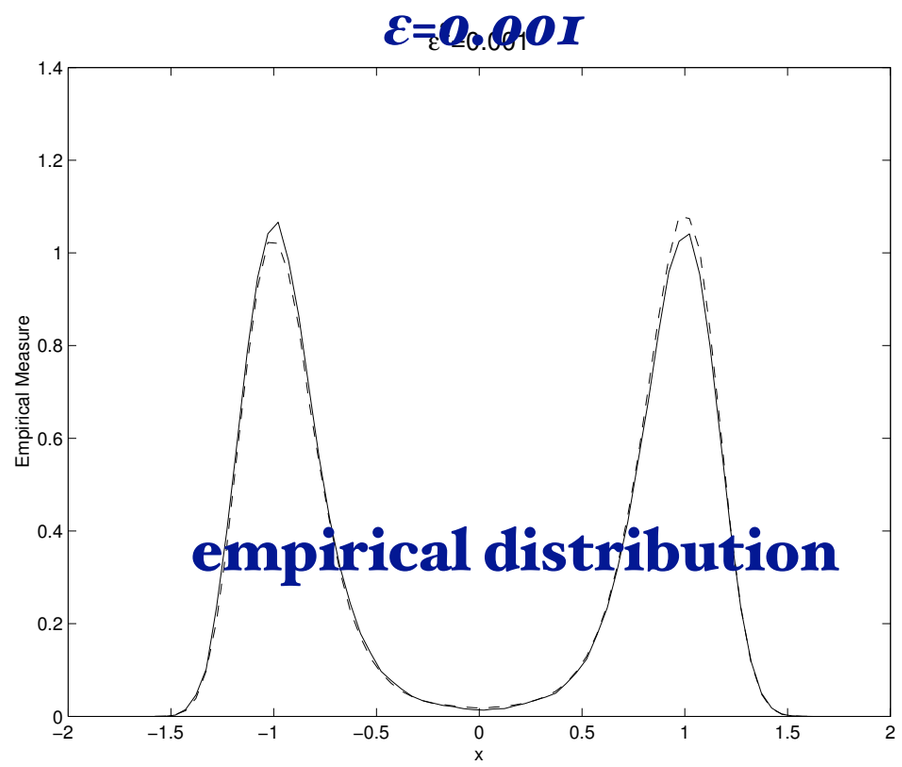
Reduced equation describes noisy particle in quartic potential. Equlibrium distribution is **bi-modal**.



Large Systems

Large Systems

Another class of systems for which the reduced system can be derived rigorously as a limit of the full dynamics, is systems which many DOFs. The reduced system is obtained in the limit where the number of DOFs tends to infinity (the "**thermodynamics limit**").

An instance of such systems are mechanical systems of **heat baths**. (Will be addressed in detail in tomorrow's lecture).

Also systems of **class DS**.

Birth-Death Systems

Chemical reactions are commonly modeled by stochastic birth-death systems.

The model:

There are m **species** with populations $x=(x_1,x_2,\ldots,x_m)$.

There are n **reactions** with rates $h_i(x)$ and stoichiometry numbers v_{ij}.

Can easily be simulated by the **Gillespie algorithm** (generative simulation of cont.-time Markov chains)

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- **Update** $x(t)$ accordingly and return to step 2.

The Gillespie algorithm provides a "pathwise" description. Alternatively, one can consider the **master equation** (the discrete analog of the Fokker-Planck equation).

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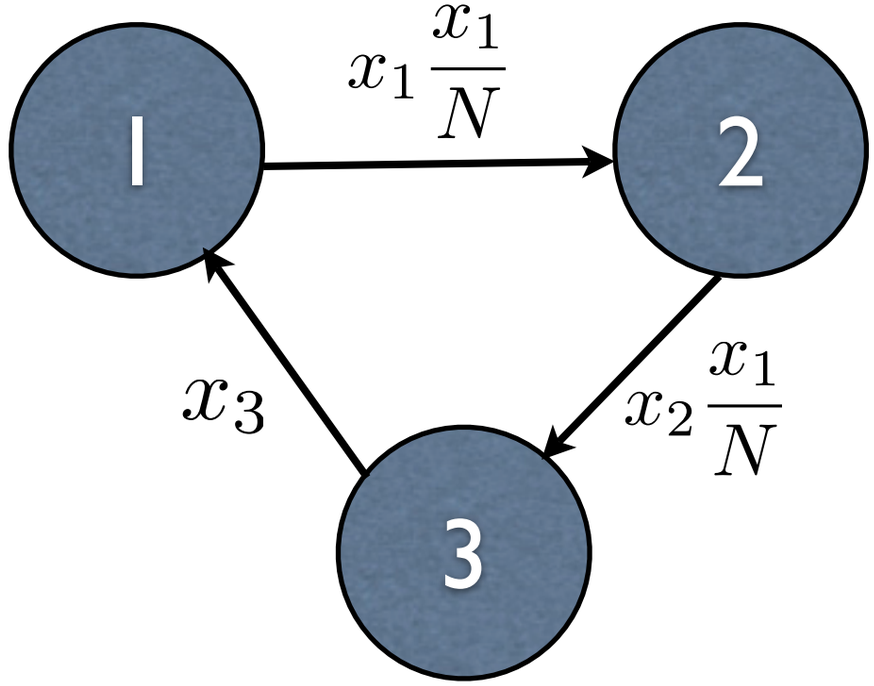
Example: a 3-species system

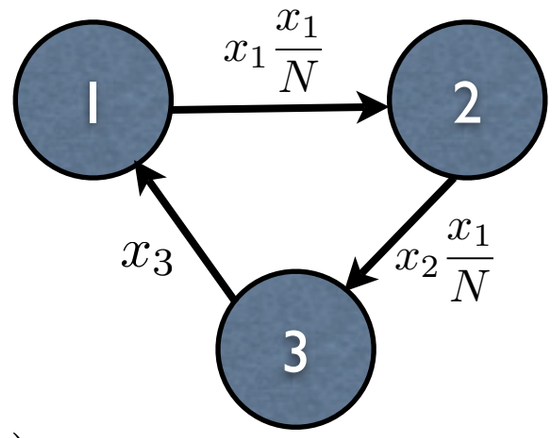


At time t=0:

$x_1 = 0 \quad x_2 = 0 \quad x_3 = N$

***N* is the total number of particles**

The **master equation**: for $p(x_1,x_2,x_3,t)$



$$\begin{aligned}\frac{dp}{dt} &= \frac{(x_1+1)^2}{N}p(x_1+1,x_2-1,x_3) - \frac{x_1^2}{N}p(x_1,x_2,x_3) \\ &+ \frac{x_1(x_2+1)}{N}p(x_1,x_2+1,x_3-1) - \frac{x_1x_2}{N}p(x_1,x_2,x_3) \\ &+ (x_3+1)p(x_1-1,x_2,x_3+1) - x_3p(x_1,x_2,x_3)\end{aligned}$$

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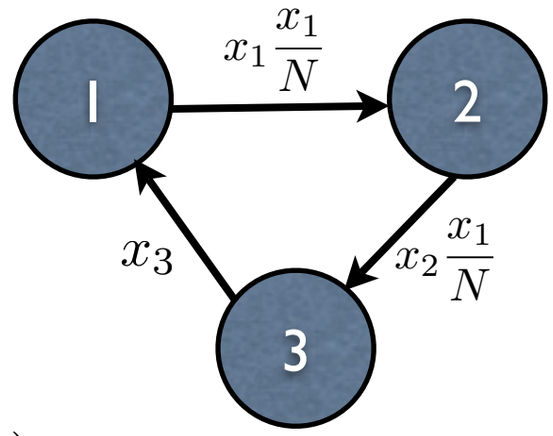

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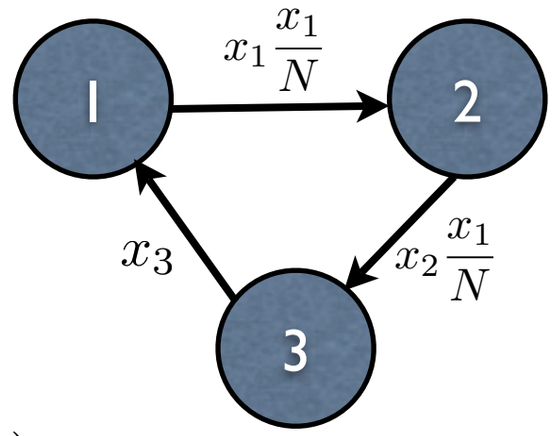
Because occupancies are $O(N)$, each reaction changes by little the "**density**" $X_i=x_i/N$.

The **master equation**: for $p(x_1,x_2,x_3,t)$



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Van-Kampen's Ω-expansion:
A change of variables. Treat the X_i as continuous variables.

$$\rho(X_1,X_2,X_3) = p(NX_1,NX_2,NX_3)$$

The master equation in terms of $\rho(X_1,X_2,X_3)$:

$$\begin{aligned}\epsilon\frac{d\rho}{dt} &= (X_1+\epsilon)^2\rho(X_1+\epsilon,X_2-\epsilon,X_3) - X_1^2\rho(X_1,X_2,X_3)\\ &+ X_1(X_2+\epsilon)p(X_1,X_2+\epsilon,X_3-\epsilon) - X_1X_2\rho(X_1,X_2,X_3)\\ &+ (X_3+\epsilon)\rho(X_1-\epsilon,X_2,X_3+\epsilon) - X_3\rho(X_1,X_2,X_3)\end{aligned}$$

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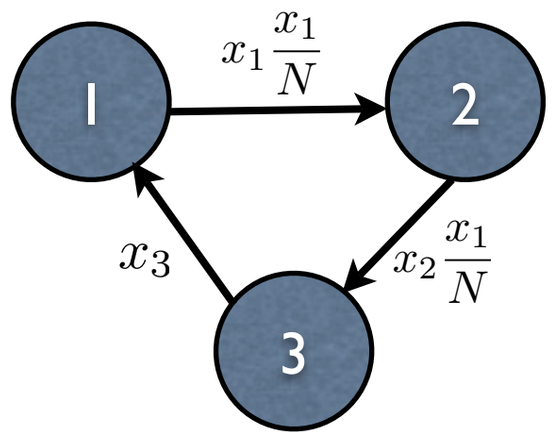
This is the **Liouville equation** of the (deterministic) system (the **rate equations**):

$$\begin{aligned}\frac{dX_1}{dt} &= -X_1^2 + X_3\\ \frac{dX_2}{dt} &= -X_1X_2 + X_1^2\\ \frac{dX_3}{dt} &= -X_3 + X_1X_2\end{aligned}$$



class SD

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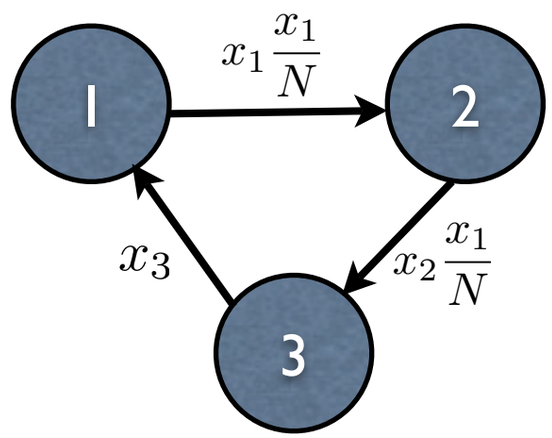
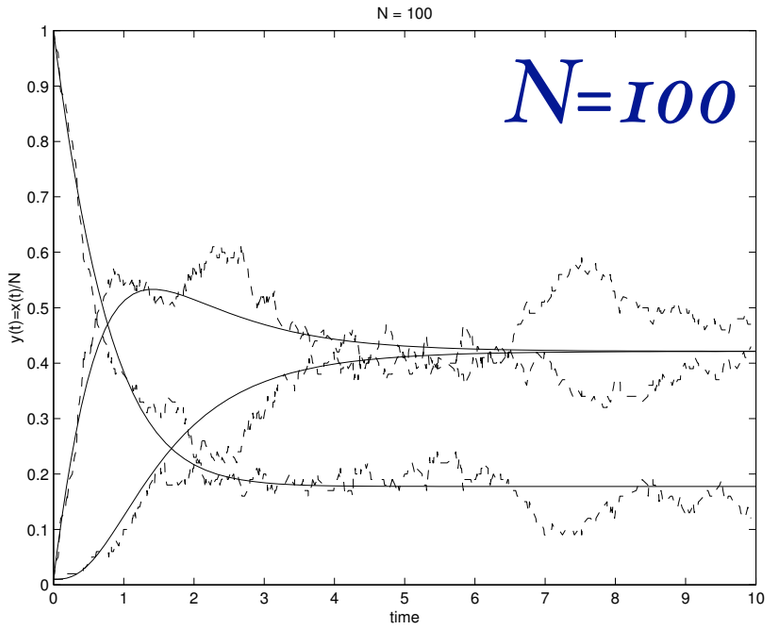


if $O(\varepsilon)$ terms are retained one gets a second-order Fokker-Planck equation of a stochastic system.

class SS

Numerical simulation:
Comparison between a single realization of the Gillespie algorithm with the solution of the deterministic reduced system.



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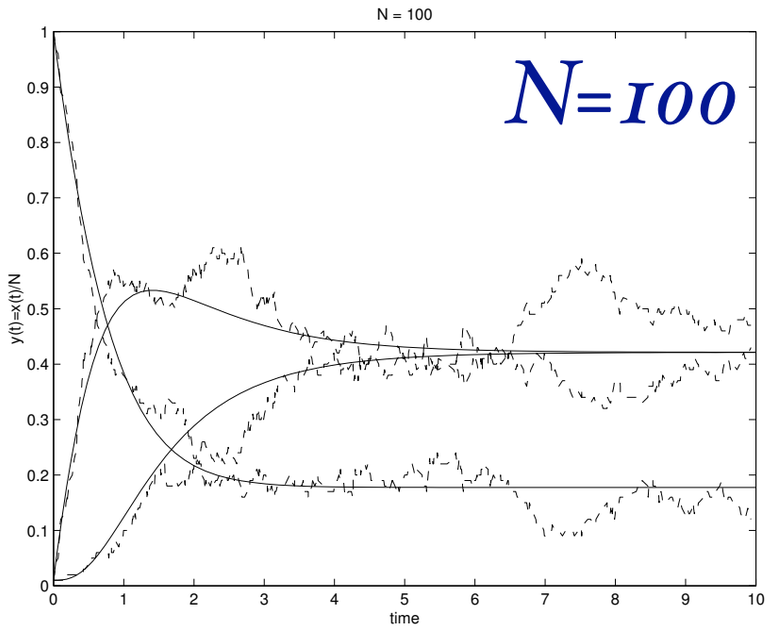

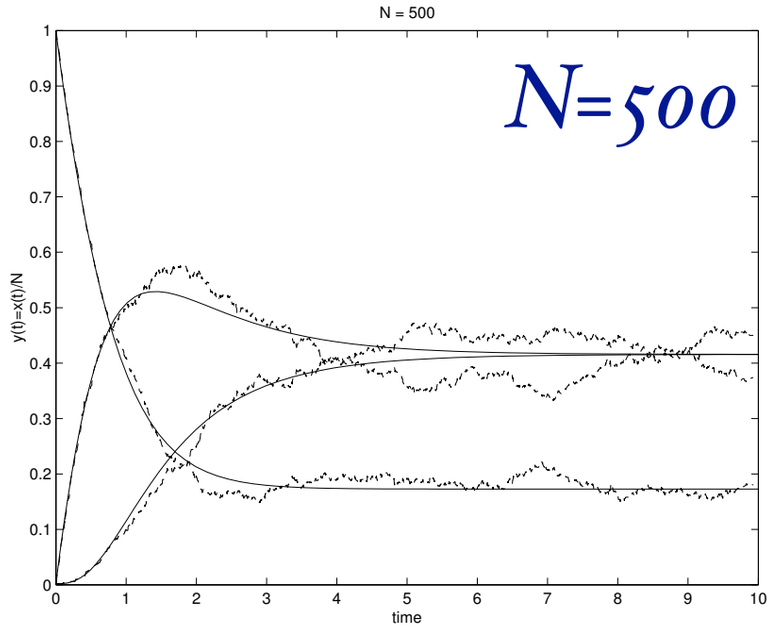

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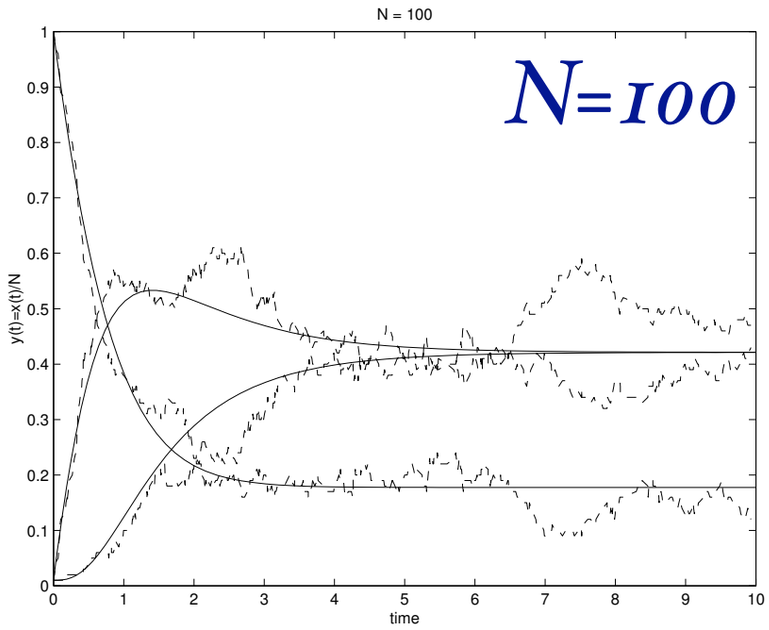

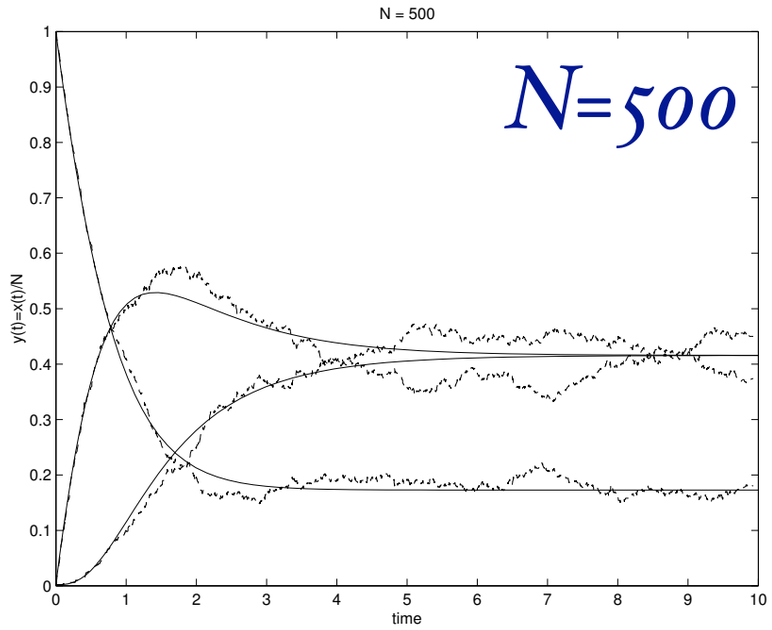

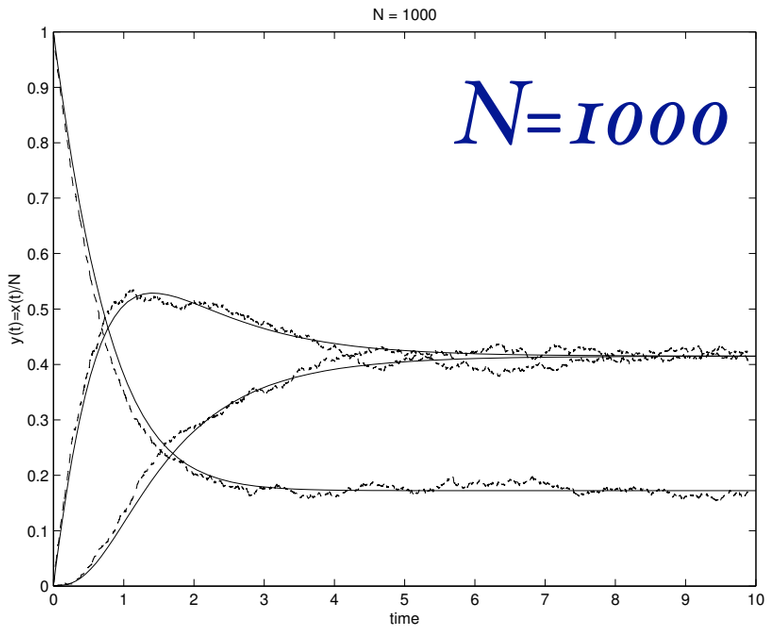

Algorithms

We have seen two classes of systems in which dimension reduction can be **rigorously** obtained as a limit (scale separation and large systems).

Most case of (real) interest do not belong to any of these classes (at least not in a strict sense), yet, “something needs to be done”.

In the remaning of this lecture we will review **uncontrolled approximations**, as well as **computational algorithms** of dimension reduction.

[I apologize in advance: I will only refer to a small part of the recent developments.]

Projective Integration

Kevrekidis and co-workers 2003 and later

Suppose we have a deterministic system with **scale separation**, but we are unable to derive the reduced model. **Goal**: approximate *x(t)*.

$$\frac{dx}{dt} = f(x,y)$$
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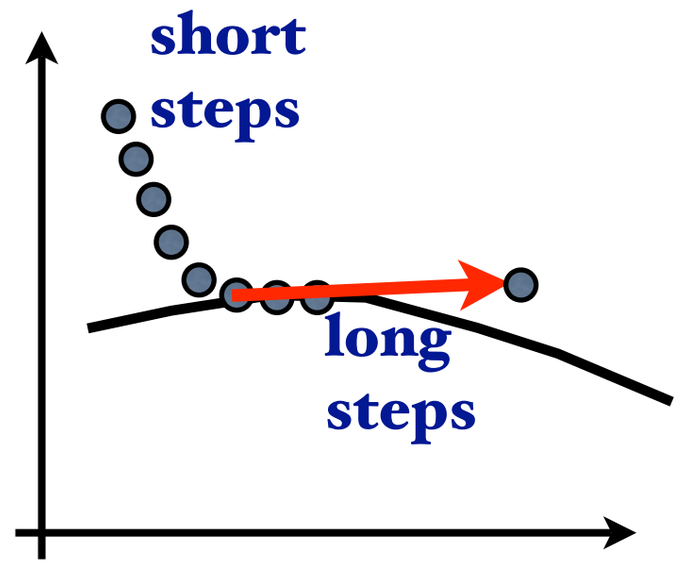
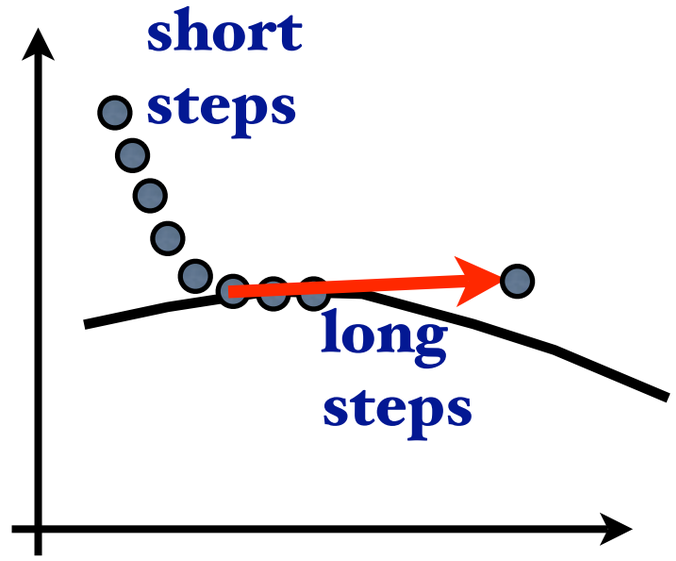
Case I: for fixed x the y-dynamics are attracted to an invariant manifold.

Algorithm: perform a number of short time steps to let y reach the invariant manifold. Evalulate the time-derivative of x, and then advance x by a "large" step.



Projective integration scheme:

given $\quad (x_n, y_n)$



Integrate the y-equation with "**small**" time steps $\delta t < \varepsilon$, for a time long enough to reach the manifold:

$$y_{n,m+1} = y_{n,m} + \frac{\delta t}{\epsilon}\, g(x_n, y_{n,m}) \qquad i = 0, \ldots, M-1$$

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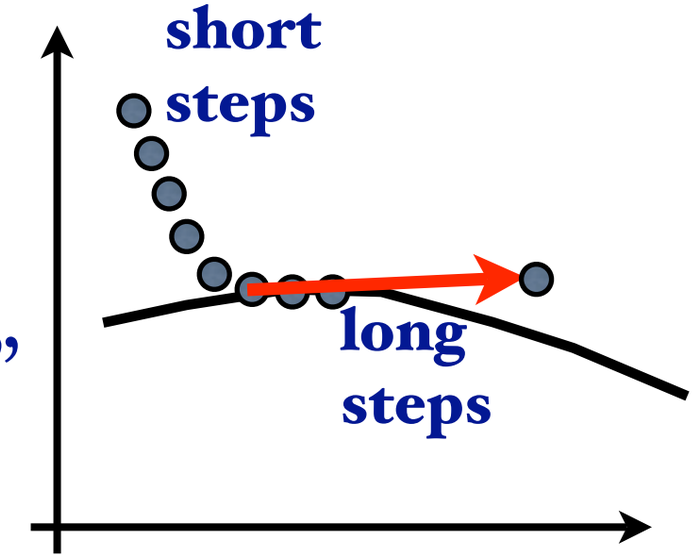

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Evolve x in time "**macroscopically**":

$$x_{n+1} = x_n + \Delta t\, f(x_n, y_{n,M})$$

Can be generalized to **higher-order schemes**.

Example:

$$\frac{dx}{dt} = y$$
$$\frac{dy}{dt} = \frac{1}{\epsilon}\left(-x + y - y^3\right)$$

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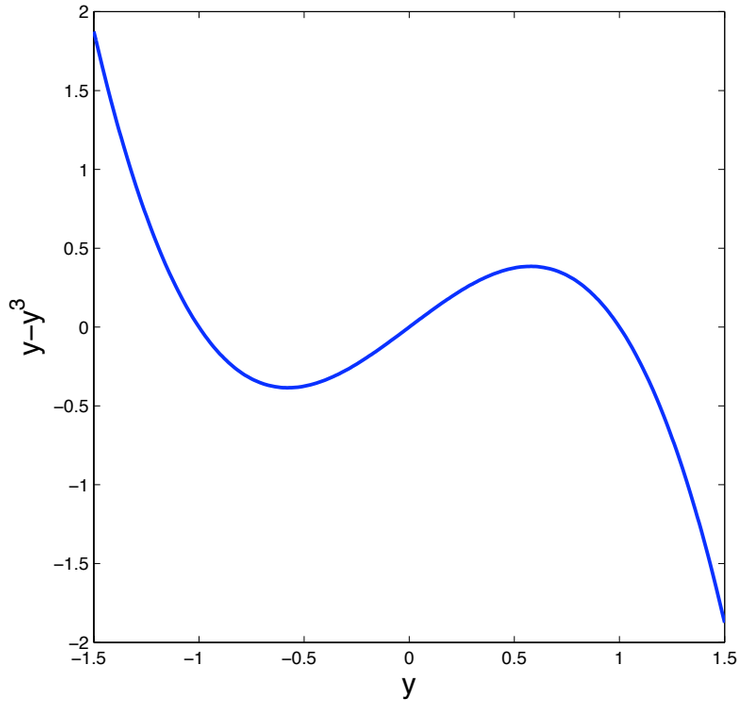

For $|x|<1/\sqrt{3}$ the y-equation is **bi-stable**. Suppose $x(0)<1/\sqrt{3}$ and y is near the positive fixed point. x grows until it exceeds $1/\sqrt{3}$, then y jumps to the negative branch and x decreased until it gets under $-1/\sqrt{3}$ and so on.

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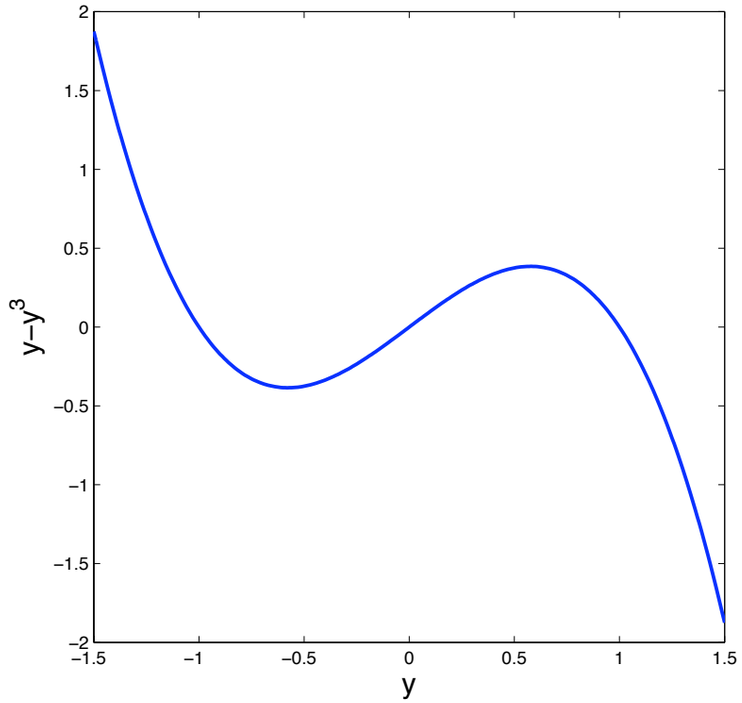

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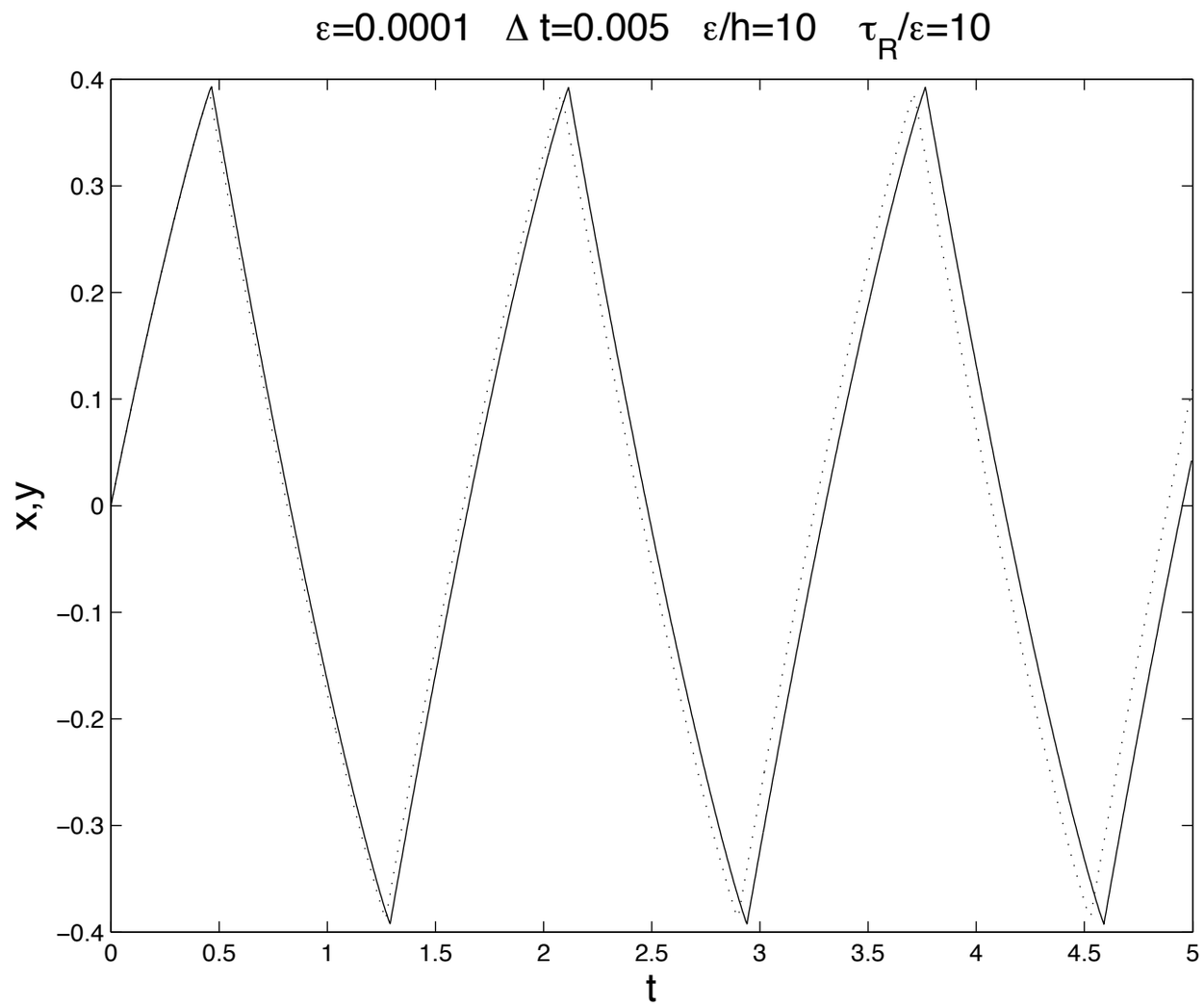
Projective integration:

$$y_{n,m+1} = y_{n,m} + \frac{\delta t}{\epsilon}\left(-x_n + y_{n,m} - y_{n,m}^3\right)$$

$$x_{n+1} = x_n + \Delta t\, y_{n,M}$$

Numerical results:



$\epsilon = 10^{-4}$ $\delta t = 0.1\epsilon$ $M\,\delta t = 10\epsilon$ $\Delta t = 0.005$

This idea can even be used in cases where **we do not know the parition of slow and fast variables** (but we know that such a partitions exists).

In many cases, no harm if we evolve x as well in the first (relaxation) phase, and then project forward both x and y (y will tend back to the invariant manifold in the following relaxation phase).

This idea was proposed by Gear and Kevrekidis as a mean to **accelerate** existing "**legacy codes**", by wrapping them with a projective integrator.

Equation-Free Closures

Kevrekidis and co-worker developed numerous algorithms on the premises that **one does not even have equations** (e.g., the legacy code), or, equivalently, that the equations are known but useless.

The assumption is that we have control of a numerical solver that we can use at will (e.g., initialize with various initial data), but only for **short time intervals** ("bursts").

The idea is to make a clever use of these short calculations to predict "coarse" properties of the system.

Example [Siettos *et al*. 2003]:
Liquid crystalline polymers are characterized by an orientation unit vector $\boldsymbol{u}$. The distribution $\psi(\boldsymbol{u},t)$ satisfies the (nonlinear) **Smoluchowski equation**:

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial \boldsymbol{u}} \cdot \left[\frac{1}{2} \frac{\partial \psi}{\partial \boldsymbol{u}} + \psi(\boldsymbol{u}) \frac{\partial}{\partial \boldsymbol{u}} V(\psi, \boldsymbol{u}) \right]$$

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potential intensity **averaging w.r.t ψ**

Goal: find the equilibrium value of a "**coarse order-parameter**" as function of the potential intensity α. (high dimensional problem)

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial \boldsymbol{u}} \cdot \left[\frac{1}{2} \frac{\partial \psi}{\partial \boldsymbol{u}} + \psi(\boldsymbol{u}) \frac{\partial}{\partial \boldsymbol{u}} V(\psi, \boldsymbol{u}) \right]$$

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- Step 1: **select** the "coarse" variables: $X = \langle u_z u_z \rangle - \frac{1}{3}$
- Step 2: given X, "**lift**" it to many "microscopic" states $\boldsymbol{u}$ that are consistent with the value of X.
- Step 3: **evolve** each macroscopic state for a short duration T (here, evolve the corresponding SDE, and approximate ensemble averages by empirical averages).
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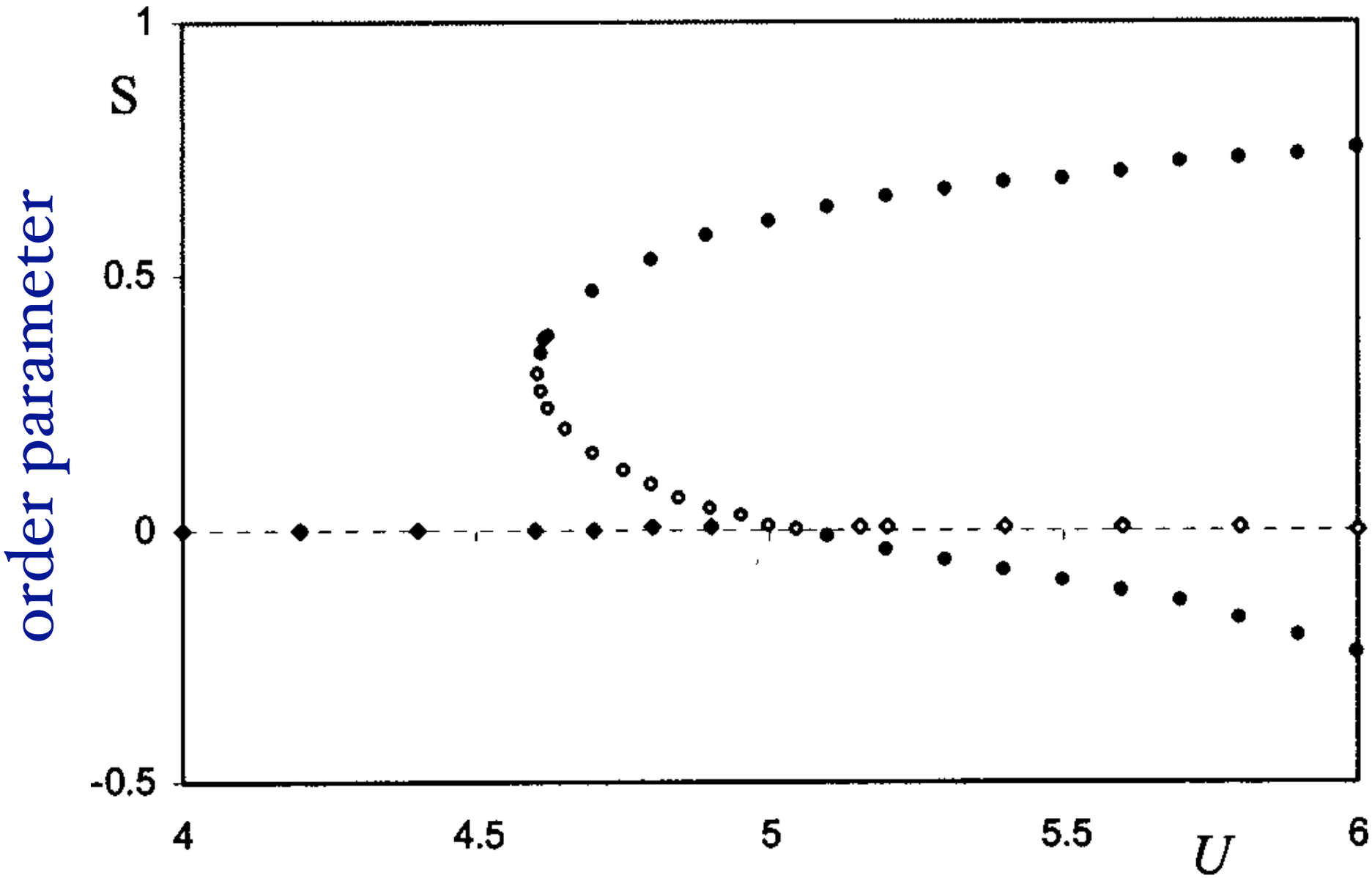
The **lift-evolve-project** cycle provides a "projective integrator" for the coarse variables (separation of scales implicity assumed).

Use it to do "**numerical analysis**" (e.g., find fixed points, bifurcation analysis, etc.)

Results: bifurcation diagram



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- We assume that the effective dynamics consist of rare transitions between **metastable states**.
- We model the transitions between essential conformations by a **continuous-time Markov process**.
- Unclear **what conformations are** (we observe points in a high-dimensional space) and how many.

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Assume skew symmetric dynamics:

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Goal: identity the meta-stable states in $\mathcal{X}$ and the corresponding Markov transition matrix.

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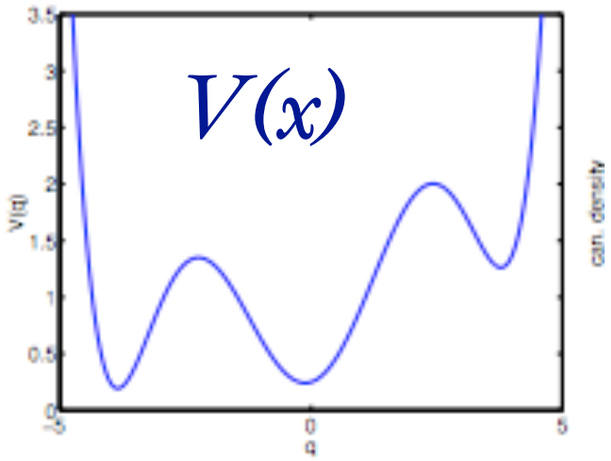
Algorithm: (1) partition into a finite (large) number of intervals. (2) construct the Markov transition matrix P_{ij} by empirical counting. (3) identify the cluster of e.v. close to 1. (4) identify the meta-stable states. (5) project P_{ij} onto the coarser partition.

Model example: a particle interacting with a “heat bath”

$$\frac{dx}{dt} = -V'(x) + \sum_{j=1}^{N} u_j$$

$$\frac{du_j}{dt} = -j\, u_j \qquad j = 1, \ldots, N$$



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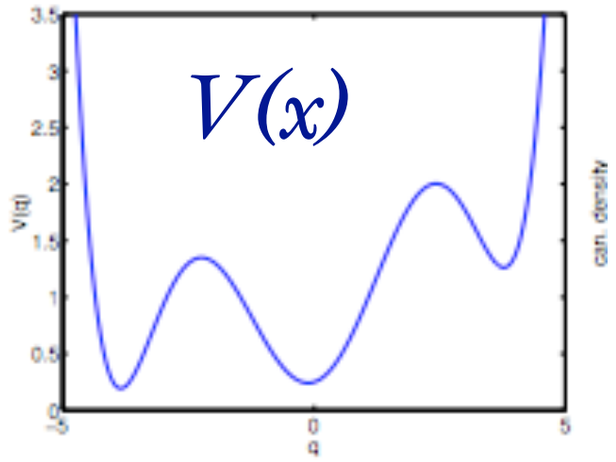

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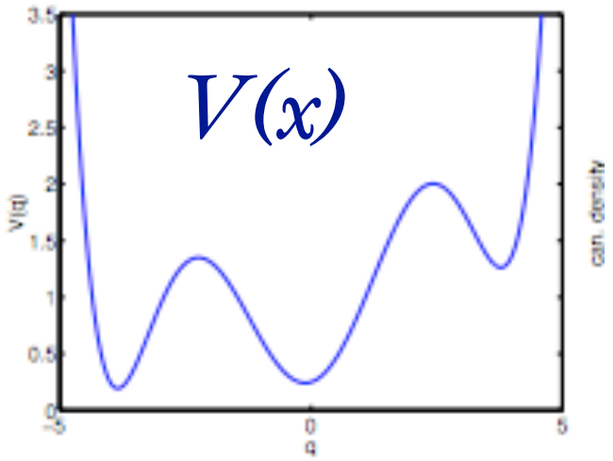

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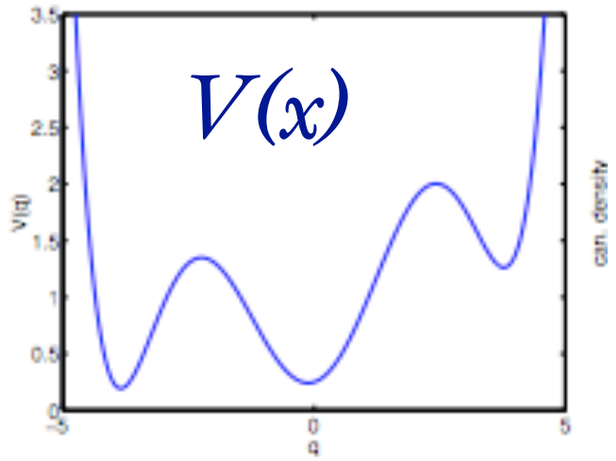

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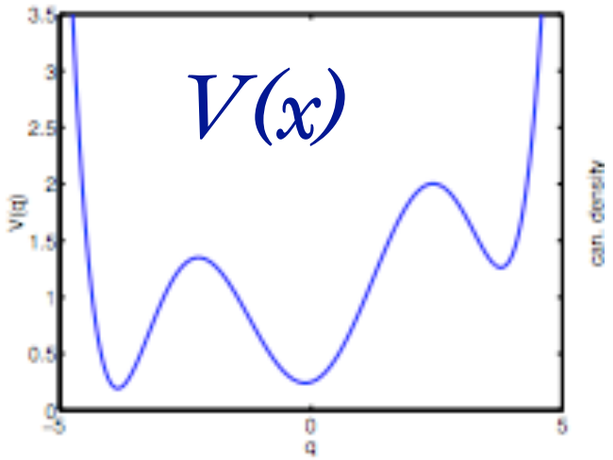

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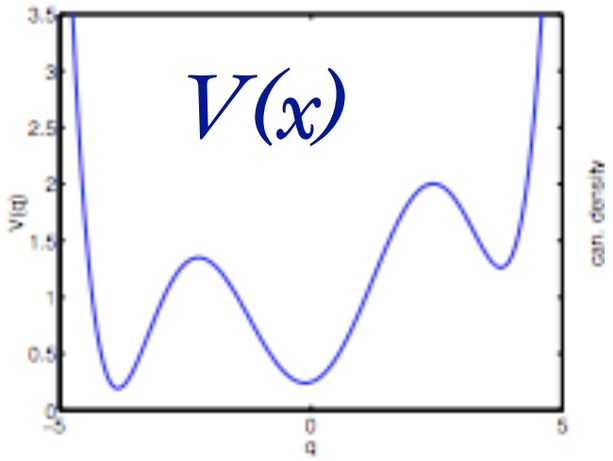

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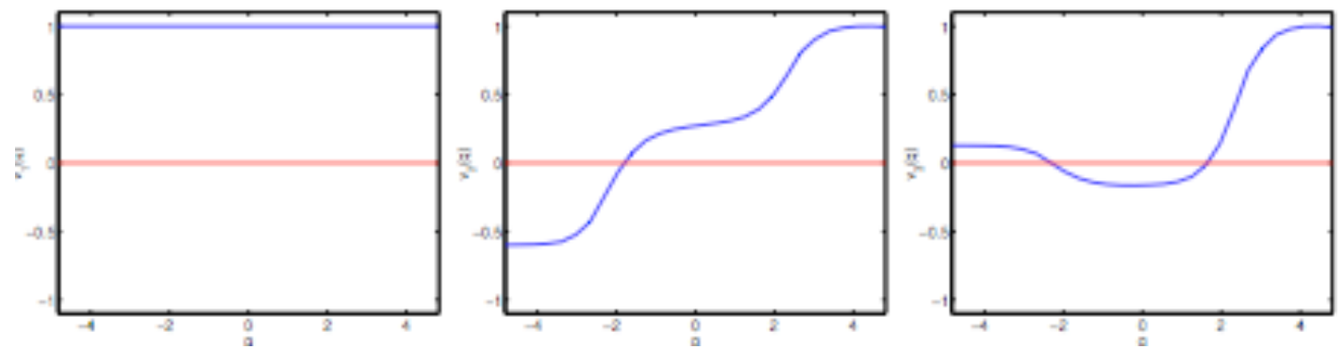
λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	...
1.000	0.950	0.915	0.387	0.227	0.125	...



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- Many open ends (e.g., what is the mathematical framework for equationsless closures?)