Minimization

PHYS 250 (Autumn 2024) – Lecture 8

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Outline

Final Project Concept

As we discussed in Lecture 3 (& the syllabus), there will be a **final project for the course** (no exams of any kind).

Final project description

- **Individual project**
- **Focused on a specific physics question with a computational solution, model, calculation, and associated visualization**
  - Does **not** have to be one of the topics covered in the course
  - Needs to have a clear physics question and computational approach to its answer
  - Can be related to work outside of this class.
  - I encourage *connections* to other domains as well (statistics, mathematics, engineering, art, music, social science, finance)
- **Delivered in the form of a poster presentation**
  - "How to design an award-winning conference poster"
  - "Better" poster design

Final Project Ideas and Suggestions

A few seeds of an idea for a poster project:

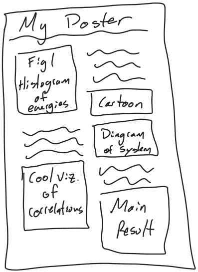
- **Randomness and emergent phenomena**
  - Develop your own cellular automata simulation (e.g. the Game of Life)
  - 3D Ising Model
  - Spin glass model
- **Numerical Differential equations**
  - Solutions of time-dependent Schroedinger equation for two particles
  - Projectile motion including air resistance / solar wind on satellite motion
- **Fourier Transforms**
  - Sound/image filtering using the FFT and eigenvector pruning
  - Analysis of similarities between artists, genres, songs using Fourier analysis
- **Chaotic systems**
  - Interactive plots and animations for realistic double pendulum
  - Dripping faucet

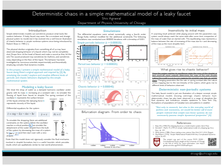
Final Project Timeline

Project Ideas Due this coming Tuesday!

Timeline

- **Week 5 – Tues 29 October:** 1 paragraph project descriptions and sketch of poster due (conceptual design incl. figure ideas)
- **Week 7 – Tues 12 November:** Progress report and updated outline of poster due
- **Week 10 – Tues 3 December:** Poster due for printing
- **Week 10 – Thur 5 December:** Poster session





Poster project example

Deterministic chaos in a simple mathematical model of a leaky faucet

Shiv Agrawal
Department of Physics, University of Chicago

Introduction

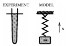
Simple deterministic models can sometimes produce what looks like random behavior. A leaky faucet may seem like a mundane and strange physical system to model, but it has evolved into a well known illustration of chaotic behavior in simple nonlinear systems since being introduced by Robert Shaw in 1985 [1].

The physical intuition originates from something all of us may have observed: dripping behavior of a faucet which may not be completely shut. Drops form at the head of faucet, and make a sound as they hit the sink. The sound produced may sometimes be rhythmic, and sometimes noisy, depending on the flow of the liquid. This behavior has been investigated by numerous scientists experimentally and theoretically employing complex fluid dynamics models.

In this project, I present a simple mathematical model of a leaky faucet along Shaw's original approach and inspired by [2]. By simulating the model, I explore and visualize different kinds of periodic and chaotic behaviors displayed by this simple mathematical system.

Modeling a leaky faucet

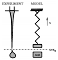
We treat the drop of water as a damped harmonic oscillator under gravity with its mass m increasing at a constant rate r, to simulate the flowing of liquid from faucet to droplet. The spring constant of the oscillator k represents the surface tension of the liquid, whereas the damping force b represents viscosity of the liquid.



Differential equations for the system:

$$\dot{v} = mg - kx - \dot{m}v - bv \qquad \dot{x} = v \qquad \dot{m} = r$$

To simulate the dropping, there are additional constraints. on the system. When the oscillator reaches a critical position $\boxed{x_c}$ we simulate the detachment of the water droplet from the bulk of the system by decreasing the mass of a system by $\boxed{\Delta m = \frac{v}{\beta + v}}$ and then start over with a new droplet.

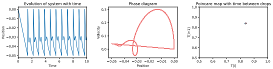


Note that this model does not rigorously consider the fluid mechanics involved in droplet formation, but is a useful heuristic which provides results which are qualitatively similar to real world phenomenon.

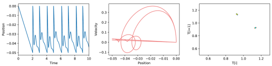
Simulations

The differential equations were solved numerically using a fourth order Runga Kutta method modified for the additional constraints. The following simulations was conducted over 800000 iterations with a timestep of 0.001.

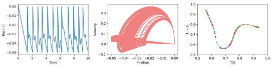
Simple periodic behavior (r = 0.000035)



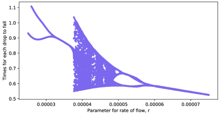
Period two behavior (r = 0.000025)



Chaotic behavior (r = 0.000045)

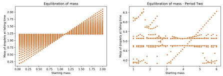


Bifurcation diagram- From order to chaos



Insensitivity to initial mass

A surprising result achieved while playing around with the parameters was system would always reach the same state after some time, irrespective of the mass of water that we started with. This equilibrating mass represents a balance between the rate of increasing of the mass due to r and decreasing of the mass as the more droplets form.



What gives rise to chaotic behavior?

Once the system reaches its equilibrium state, the mass of the droplet at each pinch-off event uniquely determines the mass of the next droplet, making this model a one-to-one mapping, the simplest map that can exhibit chaos. Changing parameters like the rate or spring constant alter the nature of this mapping due to the non-linearity of the system, which gives rise to different kinds of behaviors observed.

Deterministic non-periodic systems

The leaky faucet model is just one illustration of a deeper concept, simple mathematical models showing seemingly chaotic behavior. Such deterministic chaos has also been observed in a range of disciplines like fluid dynamics and turbulence, measles epidemics in New York City, fluctuations of populations of Canadian lynx and patterns in weather.

"Not only in research, but also in the everyday world of politics and economics, we would be better off if more people realized that simple non-linear systems do not necessarily possess simple dynamical properties" [4]

References

1. Shaw, R.S. (1984).The dripping faucet as a model chaotic system. *Aerial Press.*
2. Schmidt, T , Marhl, M. (1997). A simple mathematical model of a dripping tap. *Eur. J. Phys.*, 18, 377.
3. Gleick, James. (1988). Chaos: making a new science. New York, N.Y., U.S.A, Penguin
4. May, Robert. (1976). Simple Mathematical Models With Very Complicated Dynamics. *Nature.* 26. 457.

This project was part of the course PHYS 25000 - Computational Physics taught at the University of Chicago in the Fall of 2018. For more information visit: https://github.com/shiv-agr/PHSY250FinalProject

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Outline

Minimization is everywhere

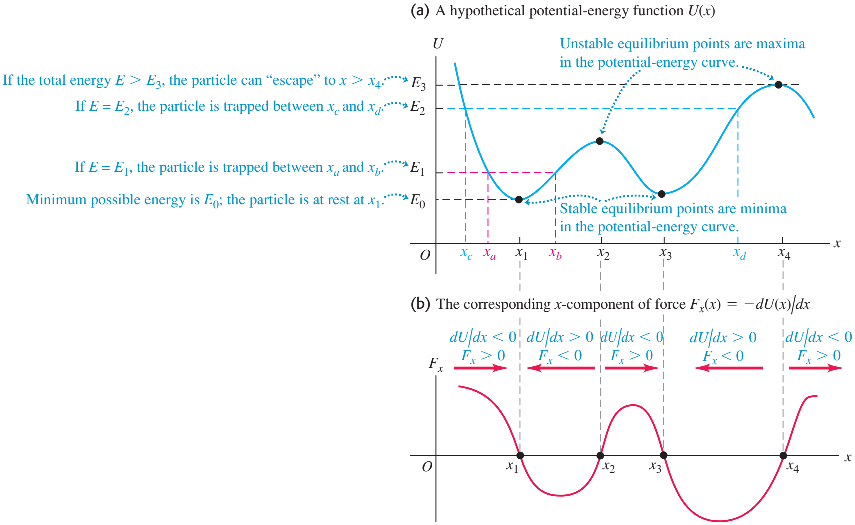
As physicists, we are **constantly attempting to minimize or maximize functions that describe the world around us**.

Examples of minimization

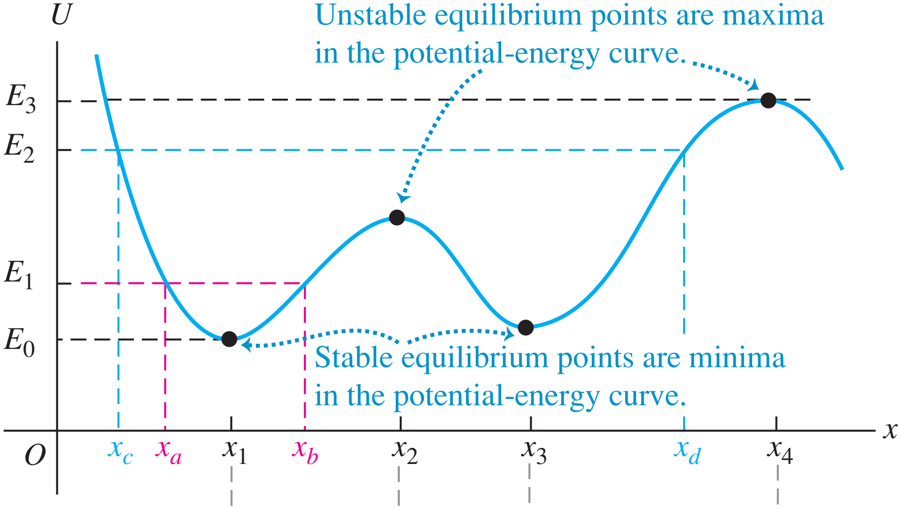
- **Fitting a model to data:** minimize differences between a model and data
- **Second law of thermodynamics:** minimize changes in entropy for a system in thermodynamic equilibrium
- **Conservation of momentum:** establish mechanical equilibrium by minimizing changes in momentum, $\frac{d\vec{p}}{dt} = 0$
- **Principle of least action:** obtain the equations of motion of a system by minimizing (or maximizing!) the variations of the action, S
- **Path integral formulation of quantum mechanics:** sort quantum mechanically possible trajectories by minimizing quantum action
- **Ising model:** minimization the energy of the spin configurations

Energy Minimization from your first year text books

7.24 The maxima and minima of a potential-energy function $U(x)$ correspond to points where $F_x = 0$.



Minimization can imply maximization → optimization



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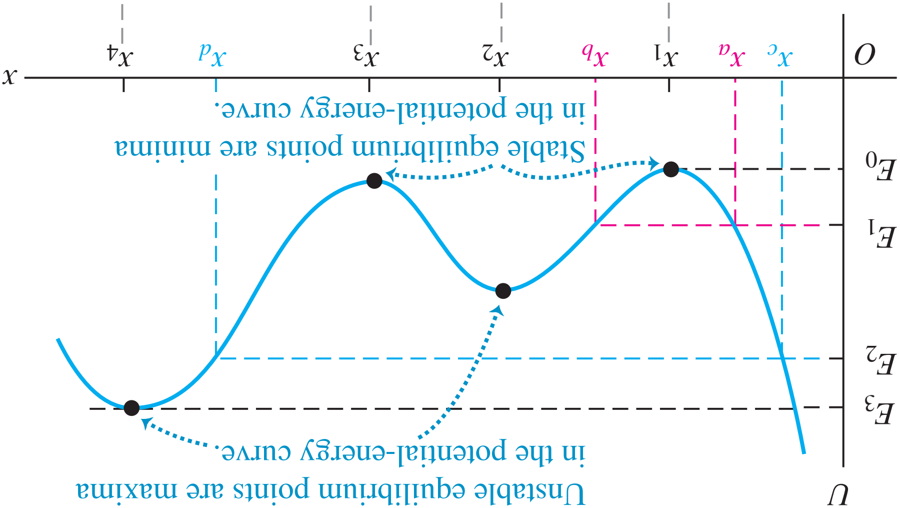


Optimization, or finding the extrema of a system

Since we are most often interested in maxima or minima of the evolution or behavior of a system as a function of some external parameter, the problem often boils down to the determination of **first and second derivatives** as a function of that parameter.

$$f(x) \approx f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots, \quad (1)$$

If we focus only on the first three terms, we can write this for a function of n variables $\vec{x} = \sum_{i=0}^{n} x_i$ as:

$$f(\vec{x}) \approx f(\vec{a}) + (\vec{x}-\vec{a})^{\mathrm{T}} \nabla f(\vec{a}) + \frac{1}{2!}(\vec{x}-\vec{a})^{\mathrm{T}} \mathbf{H}(\vec{a})(\vec{x}-\vec{a}) \quad (2)$$

where $\mathbf{H}$ is the **Hessian matrix**, describing the **curvature** of $f(\vec{x})$ by

$$\mathbf{H}_{i,j} = \frac{\partial^2 f(\vec{a})}{\partial x_i \partial x_j} \quad (3)$$

(Note: The determinant of $\mathbf{H}$ is also sometimes referred to as **the Hessian**.)

Optimization methods and approaches

There are many details associated with the **existence, feasibility, and constraints** on the optimization problem for finding and describing extrema.

Assuming that these are generally satisfied, we can categorize the approaches into two primary groups and specific implementations of each:

- **Evaluate second derivatives (Hessians):** Newton's method is the most famous and widely used
- **Evaluate first derivatives (gradients):** Gradient descent is perhaps the most widely used

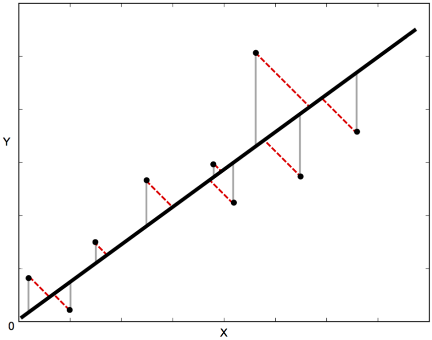
Then, there is a kind of "hybrid" approach which is referred to as **quasi-Newton** wherein the Hessian matrix is approximated using updates specified by gradient evaluations.

We will come back to these methods on Thursday, but for now, let's discuss a simple minimization: **Least squares**

Outline

Linear regression (II)

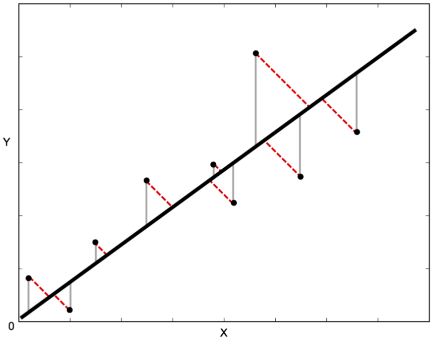
Suppose that you want to fit a set data points (x_i, y_i), where $i = 1, 2, \ldots, N$, to a straight line, $y = ax + b$.



The process of determining the best-fit line is called **linear regression**. This involves choosing the parameters a and b to minimize the sum of the squares of the differences between the data points and the linear function.

Linear regression (II)

Suppose that you want to fit a set data points (x_i, y_i), where $i = 1, 2, \ldots, N$, to a straight line, $y = ax + b$.



If there are only uncertainties in the y direction, then the differences in the vertical direction (the gray lines in the figure) are used. If there are uncertainties in both the x and y directions, the orthogonal (perpendicular) distances from the line (the dotted red lines in the figure) are used.

Using the χ^2 (again!)

For the case where there are only uncertainties in the y direction, there is an analytical solution to the problem.

If the uncertainty in y_i is σ_i, then the difference squared for each point is weighted by $w_i = 1/\sigma_i^2$. The function to be minimized with respect to variations in the parameters, a and b, is

$$\chi^2 = \sum_{i=1}^{N} w_i \left[y_i - (ax_i + b)\right]^2 . \tag{4}$$

The analytical solutions for the best-fit parameters that minimize χ^2 are those that satisfy $\dfrac{\partial(\chi^2)}{\partial a} = 0$ (and similarly for b).

Uncertainties

From the above equation for the χ^2, we can obtain a and b from:

$$a = \frac{\sum w_i \sum w_i x_i y_i - \sum w_i x_i \sum w_i y_i}{\sum w_i \sum w_i x_i^2 - \left(\sum w_i \sum w_i x_i\right)^2} \tag{5}$$

and

$$b = \frac{\sum w_i y_i \sum w_i x_i^2 - \sum w_i x_i \sum w_i x_i y_i}{\sum w_i \sum w_i x_i^2 - \left(\sum w_i \sum w_i x_i\right)^2}. \tag{6}$$

The uncertainties in the parameters are

$$\sigma_a = \sqrt{\frac{\sum w_i}{\sum w_i \sum w_i x_i^2 - \left(\sum w_i \sum w_i x_i\right)^2}} \tag{7}$$

$$\sigma_b = \sqrt{\frac{\sum w_i x_i^2}{\sum w_i \sum w_i x_i^2 - \left(\sum w_i \sum w_i x_i\right)^2}}. \tag{8}$$

All of the sums in the four previous equations are over i from 1 to N.