

The physics of randomness and emergent properties
PHYS 250 (Autumn 2024) – Lecture 3

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Outline

1 *Final Project*

- Concept
- Timing

2 *The physics of randomness and emergent properties*

- Coin flips
- Random walks
- Central limit theorem and analytic descriptions of random behavior

Final Project Concept

As mentioned in the first lecture and in 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

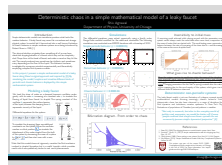
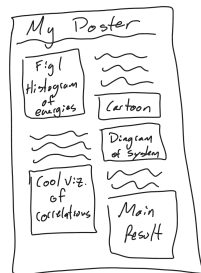
- **Chaotic systems**

- Interactive plots and animations for realistic double pendulum
- Dripping faucet

Final Project Timeline

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

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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:

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

To simulate the dripping there are additional constraints on the system. When the oscillator reaches a critical position x_c , we simulate the detachment of the water droplet from the bulk of the system by decreasing the mass of a system by $\Delta m = \frac{m}{10}$ and then start over with a new droplet.

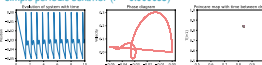
Note that this model does not rigorously consider the fluid mechanics involved in droplet formation, but is a useful heuristic which provides results which are qualitatively similar to real world phenomenon.



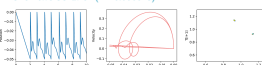
Simulations

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

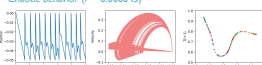
Simple periodic behavior ($r = 0.000035$)



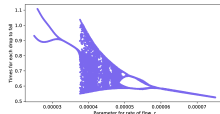
Period two behavior ($r = 0.000025$)



Chaotic behavior ($r = 0.000045$)

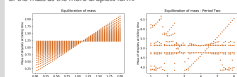


Bifurcation diagram- From order to chaos



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 discrete-time mapping. The smallest mass that can exist is m_{min} . 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

- Shaw, R.S. (1984). The dripping faucet as a model chaotic system. *Aerial Press*.
- Schmidt, T., Marhl, M. (1997). A simple mathematical model of a dripping tap. *Eur. J. Phys.* 18, 377.
- Gluck, James. (1988). *Chaos making a new science*. New York, N.Y. U.S.A. Penguin.
- 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: <http://github.com/shiv-agr/PHYS250FinalProject>



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Coin flips

See Sethna's text for more info

We began discussing random numbers last lecture. Let's continue on that topic and extrapolate to much deeper properties of physics.

Consider flipping a coin and recording the difference s_N between the number of heads and tails found. Each flip contributes $\ell_i = \pm 1$ to the total.

How big a sum

$$s_N = \sum_{i=1}^N \ell_i = (\text{heads} - \text{tails}) \quad (1)$$

do you **expect** after N flips? To answer the question regarding **expectations**, we need to be able to repeat the measurement many times and compute some statistics about what is going on.

Expectation values and statistics

The average of s_N is not a good measure for the sum, because it is zero (positive and negative steps equally likely). We could measure the average absolute value $\langle |s_N| \rangle$, but the root-mean-square (RMS) of the sum is better, $\sqrt{\langle s_N^2 \rangle}$. After each flip, the mean square is:

$$\langle s_1^2 \rangle = 0.5(-1)^2 + 0.5(1)^2 = 1 \quad (2)$$

$$\langle s_2^2 \rangle = 0.25(-2)^2 + 0.5(0)^2 + 0.25(2)^2 = 2 \quad (3)$$

$$\vdots \quad (4)$$

$$\langle s_N^2 \rangle = \langle (s_{N-1} + \ell_N)^2 \rangle = \langle s_{N-1}^2 \rangle + 2\langle s_{N-1}\ell_N \rangle + \langle \ell_N^2 \rangle \quad (5)$$

Since $\ell_N = \pm 1$, middle term cancels (equal probability of ± 1) and thus

$$\langle s_N^2 \rangle = \langle s_{N-1}^2 \rangle + \langle \ell_N^2 \rangle = N - 1 + 1 \quad (6)$$

$$= N \quad (7)$$

$$\sigma_s = \sqrt{\langle s_N^2 \rangle} = \sqrt{N} \quad (8)$$

Scale invariance and universality

The discussion above highlights an important point that we will revisit in the case of random “motion”, or random walks: **scale invariance and universality**.

- The rate of random $+1$'s and -1 's look no different when viewed a “few” at a time, or hundreds at a time
- On scales where the individual coin tosses are not observable, you cannot pick out any “preferred” features

To put this in slightly more concrete terms that will be best studied with random walks

- **Scale invariance:** the fluctuations of the system occur at all length scales.
- **Universality:** the behavior of the system is independent of the microscopic details of that system

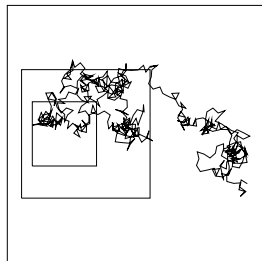
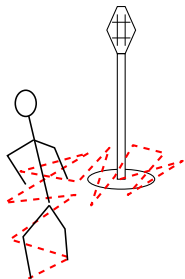
The latter is also deeply related to the **central limit theorem**.

Random walks

Random walks also arise as trajectories that undergo successive random collisions or turns; for example, the trajectory of a perfume molecule in a sample of air.

We will study this example using N fixed length steps:

- ℓ_N : sequence of N steps
- L : length of each step
- $\vec{\ell}_i$: step of length L in the i direction
- d : number of dimensions
- Assume exactly uncorrelated, random steps in each dimension d



How long of a walk?

This lack of correlation says that the average dot product between any two steps $\vec{\ell}_m$ and $\vec{\ell}_n$ is zero

$$\langle \vec{\ell}_m \cdot \vec{\ell}_n \rangle = L \langle \cos \theta \rangle = 0 \quad (9)$$

where θ is the angle between the two steps. This implies that the dot product of $\vec{\ell}_N$ with $\vec{s}_{N-1} = \sum_{m=1}^{N-1} \vec{\ell}_m$ is zero. Again, we can work by induction:

$$\langle \vec{s}_N^2 \rangle = \langle (\vec{s}_{N-1} + \vec{\ell}_N)^2 \rangle \quad (10)$$

$$= \langle \vec{s}_{N-1}^2 \rangle + \langle \vec{\ell}_N^2 \rangle \quad (11)$$

$$= \langle \vec{s}_{N-1}^2 \rangle + L^2 \quad (12)$$

$$= NL^2 \quad (13)$$

$$\sigma_s = \sqrt{\langle s_N^2 \rangle} = \sqrt{NL} \quad (14)$$

so the RMS distance moved is \sqrt{NL} .

Markov Chain Monte Carlo

A random walker is a specific subclass of a more general class of algorithms called **Markov chain Monte Carlo (MCMC)**.

A stochastic model describing a sequence of possible events in which the probability of each event depends only on the state attained in the previous event.

Some characteristics that distinguish this class of algorithms are:

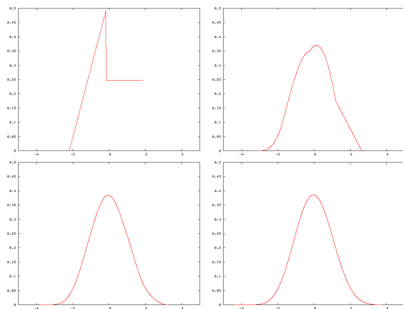
- Sequence of elements chosen from a fixed set using a probabilistic rule
- Chain is constructed by adding the elements sequentially
- Given the most recently added element, next element only depends on most recent addition

In the case of the random walker, the walker's position after N steps depends on the sequence of steps in the past, and cannot be predicted. However, a pattern emerges for an **ensemble** of positions after many such walks.

Central limit theorem

You're all likely familiar with the central limit theorem:

When independent random variables are added, their properly normalized sum tends toward a normal distribution, even if the original variables themselves are not normally distributed.



The picture on the right shows the end points of many separate random walks.

Diffusion equation

In cases in which simple behavior seemingly emerges from an ensemble of irregular, jagged random walks (in the continuum limit of long length and time scales) their evolution can be described by the diffusion equation:

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho = D \frac{\partial^2 \rho}{\partial x^2} \quad (15)$$

The diffusion equation can describe the evolving density $\rho(x, t)$ of a local cloud of perfume as the molecules **random walk** through collisions with the air molecules. Alternatively, it can describe the probability density of an individual particle as it **random walks** through space; if the particles are non-interacting, the probability distribution of one particle describes the density of all particles.

Random diffusion (I)

Consider a general, uncorrelated random walk where at each time step Δt the particle's position x changes by a step ℓ :

$$x(t + \Delta t) = x(t) + \ell(t). \quad (16)$$

Let the probability distribution for each step be $\chi(\ell)$, which in our case is a discrete probability (e.g. for the 2D random walk, $\chi(\ell) = \delta(|\ell| - L)$ with equal probability in $\pm x, \pm y$). We will assume that χ has mean zero and standard deviation a . The first few moments of χ are therefore:

$$\int \chi(z) dz = 1 \quad (17)$$

$$\int z \chi(z) dz = 0 \quad (18)$$

$$\int z^2 \chi(z) dz = a^2 \quad (19)$$

Random diffusion (II)

For the particle to go from x' at time t to x at time $t + \Delta t$, the step $\ell(t)$ must be $x - x'$. This happens with probability $\chi(x - x')$ times the probability density $\rho(x', t)$ that it started at x' . Integrating over original positions x' , we have:

$$\rho(x, t + \Delta t) = \int_{-\infty}^{+\infty} \rho(x', t) \chi(x - x') dx' \quad (20)$$

$$= \int_{-\infty}^{+\infty} \rho(x - z, t) \chi(z) dz \quad (21)$$

where we have changed variables $x' \rightarrow z = x - x'$. Now, perform a Taylor expansion in z :

$$\rho(x, t + \Delta t) \approx \rho(x, t) + \frac{1}{2} \frac{\partial^2 \rho}{\partial x^2} \int z^2 \chi(z) dz \quad (22)$$

$$\approx \rho(x, t) + \frac{a^2}{2} \frac{\partial^2 \rho}{\partial x^2} \quad (23)$$

Slow random diffusion

If the diffusion is also slow, such that the time derivative of ρ is approximately linear with respect to time and $\rho(x, t + \Delta t) - \rho(x, t) \approx (\frac{\partial \rho}{\partial t}) \Delta t$, then

$$\frac{\partial \rho}{\partial t} = \frac{a^2}{2\Delta t} \frac{\partial^2 \rho}{\partial x^2}. \quad (24)$$

This is the diffusion equation Eq. 15 with $D = \frac{a^2}{2\Delta t}$.

The point is that we obtained an analytical description of a random walk via the diffusion equation under minimal assumptions: the probability distribution is broad and slowly varying compared to the size and time of the individual steps.