

Science -II

Unit 1: Monte Carlo method: Its application in solving large dimensional integrals seen in statistical mechanics and quantum mechanics Unit 2: Solving linear systems: Huckel molecular orbital approximation for band structure in metallic bonding Unit 3: Algebra of matrices: Singular-Value Decomposition (SVD), Hessian matrix in normal mode analysis, and spectral decomposition Unit 4: Differential equations in sciences: Prey predator model, dynamics from Newton Laws, molecular dynamics simulation Unit 5: Stochastic differential equations: Diffusion, bistability of cellular processes Unit 6: Partial Differential equations in sciences: Heat equation and wave equation

Instructor: **Chittaranjan Hens**
CCNSB

Science -II

Requirements

- Newtonian Mechanics
- Basics of Matrix
- MatLab/Python/C++
- Graphical Plot (Must)
- Computational Complexity

Instructor: **Chittaranjan Hens**
CCNSB

Science -II

Requirements

- Newtonian Mechanics
- Lagrangian formulation /Classical Mechanics
- Basics of Matrix
- Statistical Mechanics
- Matlab/Python/C++
- Graphical Plot (Must)
- Computational Complexity

- “**Ludwig Boltzmann**, who spent much of his life Studying Statistical Mechanics, died in 1906 by his own hand”.
- “His student, **Paul Ehrenfest**, carrying on **Boltzmann**’s work, died similarly in 1933”.
- “*Now it is our turn to study statistical mechanics. Perhaps it will be wise to approach the subject cautiously*”.
- From the book “**States of Matter**” by David L. Goldstein (Dover, 1985)



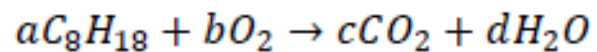
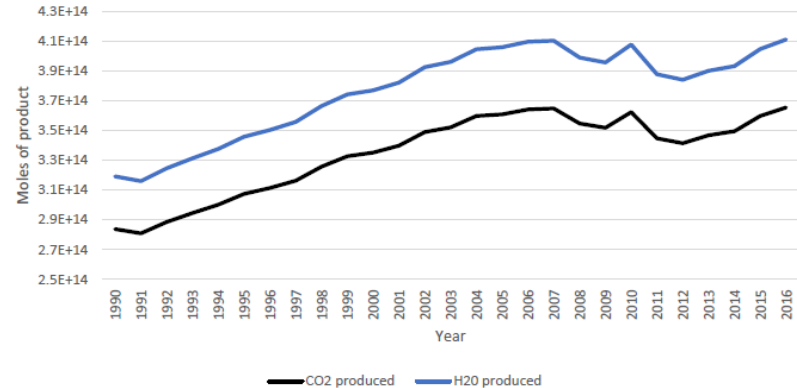


Module 1

Solving Linear Equations

Balancing a chemical reaction

The moles of carbon dioxide and water vapor produced from motor gasoline consumption in the united states from 1990 to 2016



The equation above is better now as the combustion of gasoline with available oxygen yields energy, carbon dioxide and water



Applied Mathematics, 2019, 10, 521-526
<http://www.scirp.org/journal/am>
ISSN Online: 2152-7393
ISSN Print: 2152-7385

Balancing Chemical Equations by Systems of Linear Equations

Ihsanullah Hamid

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Email: hamid@nu.edu.af

Module1:Solving Linear Equations

UJMM
ONE + TWO

Undergraduate Journal of Mathematical
Modeling: One + Two

Volume 10 | 2019 Fall 2019

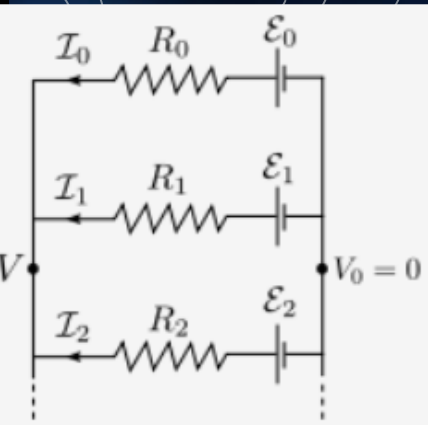
Article 5

2019

Using Matrices to Balance Chemical Reactions and Modeling the
Implications of a Balanced Reaction

Emilee Barrett
University of South Florida

Electric Networks

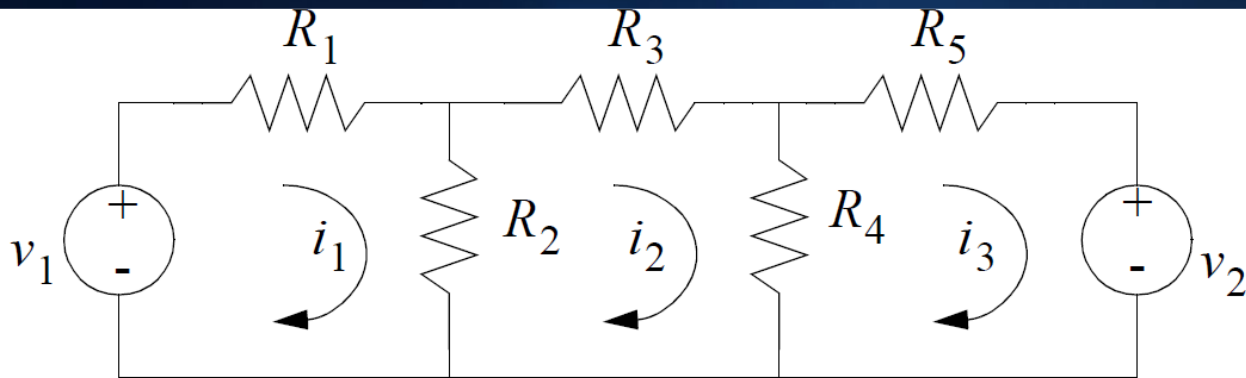


We can combine these $N + 1$ equations into a matrix equation of the form $\mathcal{A} \vec{x} = \vec{b}$

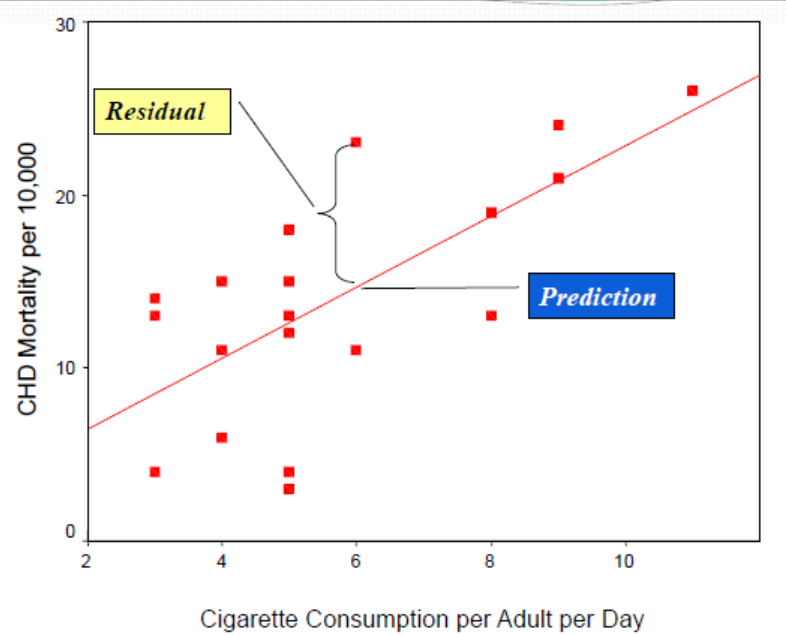
$$\begin{bmatrix} R_0 & 0 & \cdots & 0 & 1 \\ 0 & R_1 & \cdots & 0 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & R_{N-1} & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{bmatrix} \begin{bmatrix} \mathcal{I}_0 \\ \mathcal{I}_1 \\ \vdots \\ \mathcal{I}_{N-1} \\ V \end{bmatrix} = \begin{bmatrix} \mathcal{E}_0 \\ \mathcal{E}_1 \\ \vdots \\ \mathcal{E}_{N-1} \\ 0 \end{bmatrix}$$

Here, the unknown vector \vec{x} consists of the N currents passing through the branches of the circuit, and the potential V .

Module1: Solving Linear Equations

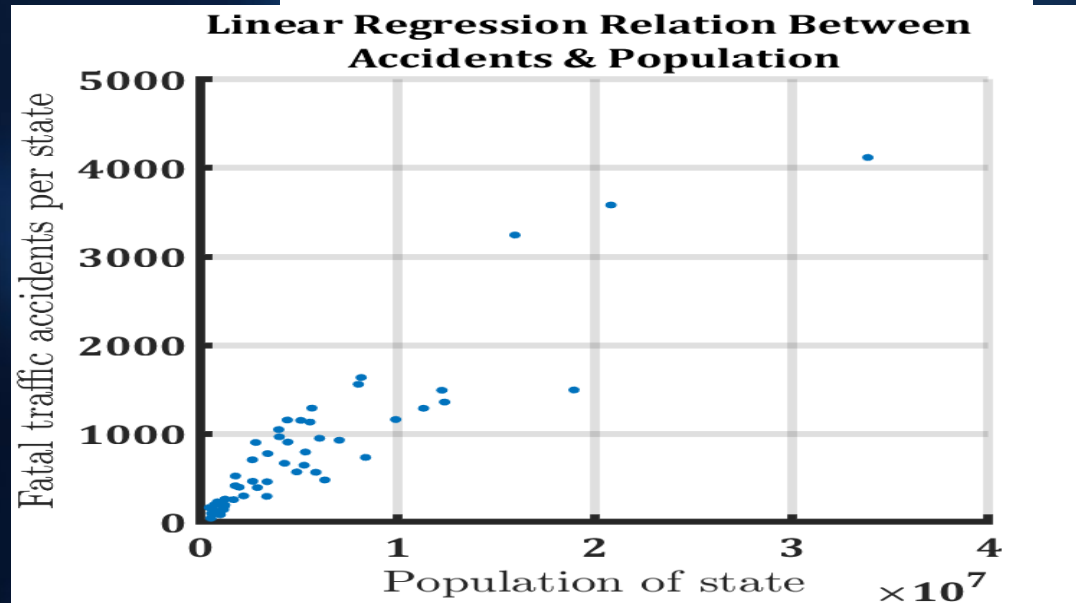


$$\begin{bmatrix} (R_1 + R_2) & -R_2 & 0 \\ -R_2 & (R_2 + R_3 + R_4) & -R_4 \\ 0 & -R_4 & (R_4 + R_5) \end{bmatrix} \begin{bmatrix} i_1 \\ i_2 \\ i_3 \end{bmatrix} = \begin{bmatrix} v_1 \\ 0 \\ -v_2 \end{bmatrix}$$



Module 1: Linear Least Square Problem

Accident data USA



- Useful for Multilinear Regression
- Useful for over determined systems

$$Ax \approx b$$

Module -1 (prerequisite)

- Basics of matrix
 - Basics of matrix
 - Computational Knowledge
 - Solving Linear Equations (Class 10 mode)
 - Algebra of matrices
-
- **Module -1 (Tools you will learn /or revisit)**
 - Gauss-Jordan Algorithm, LU decomposition in any linear equations, pseudo code
 - Linear Least square Problems : $Ax \approx b$; data fitting, Existence and uniqueness, Normal Equations,



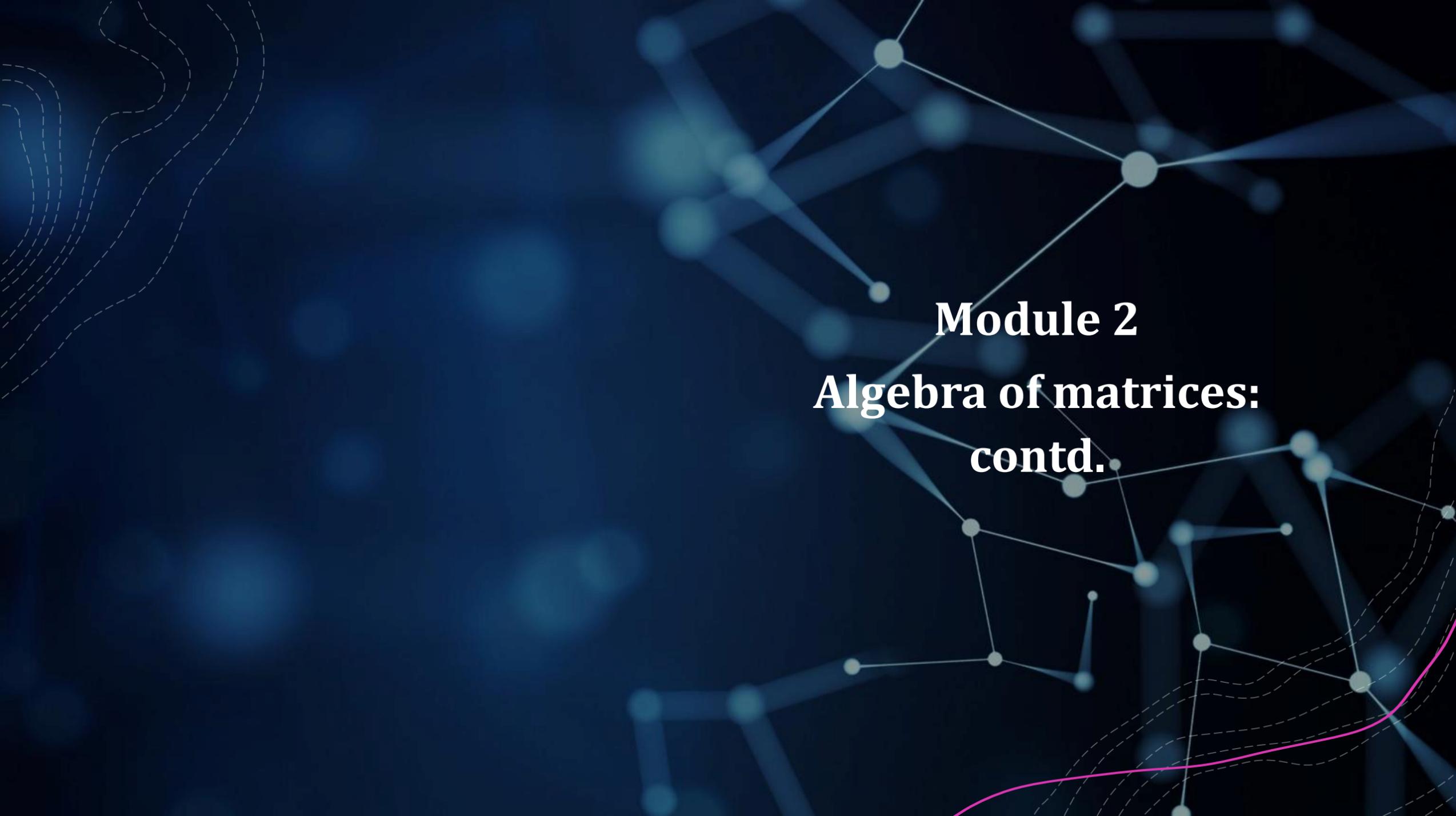
Overall Target

- *Know how systems of linear equations can be compactly represented in terms of matrix-vector multiplication*



- *Give examples of overdetermined and underdetermined systems, and systems with a unique /? solutions*

- *Application*

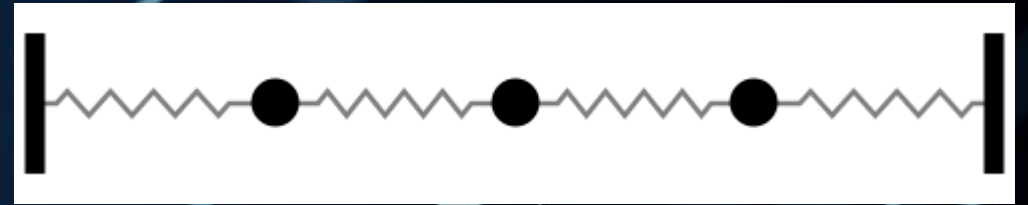
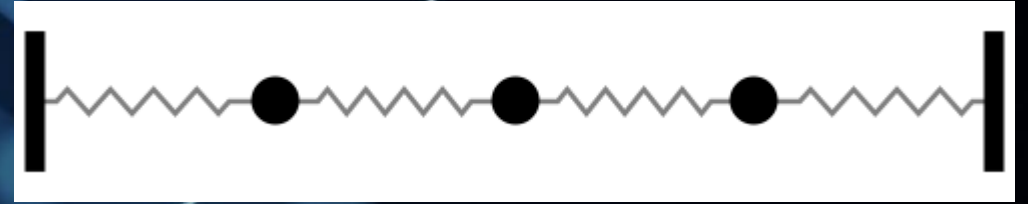
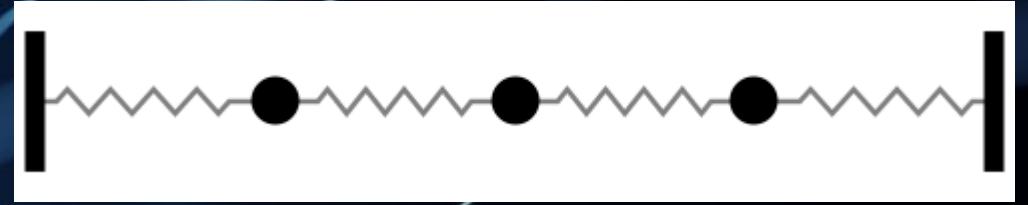
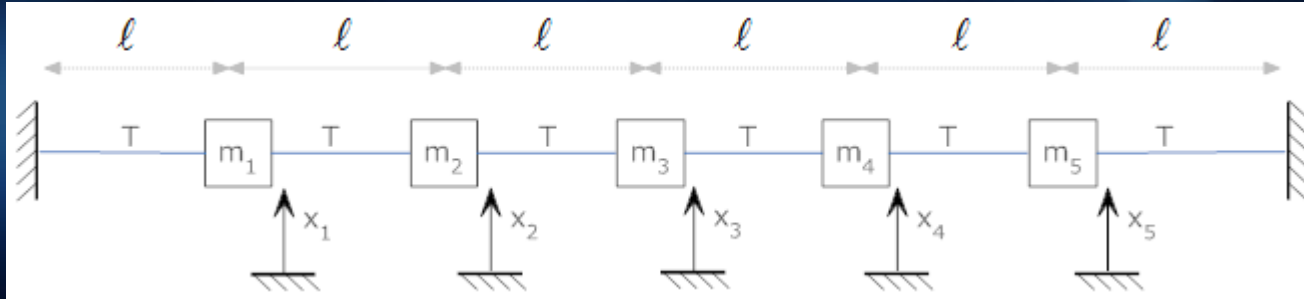


Module 2
Algebra of matrices:
contd.

Module 2

Vibrating Systems with many DOF (Normal Modes)

Vibrating Systems with many DOF (Normal Modes)



Module 2: Matrix Algebra Eigenvalue analysis

<https://lpsa.swarthmore.edu/MtrxVibe/Vibrations.html>

https://www.brown.edu/Departments/Engineering/Courses/En4/Notes/vibrations_mdof/vibrations_mdof.htm

<https://www.acs.psu.edu/drussell/Demos/multi-dof-springs/multi-dof-springs.html>

Eigenvector and Eigenvalue in ecology

*Eigenvectors and eigenvalues
in biology: rabbits vs. sheep*



$$\frac{dx}{dt} = 3x(1 - x/3)$$



$$\frac{dy}{dt} = 2y(1 - y/2)$$

*decoupled model:
two logistic equations*

linearize about the fixed point at (3,2)

$$x'(t) = x(t) - 3, \quad y'(t) = y(t) - 2$$

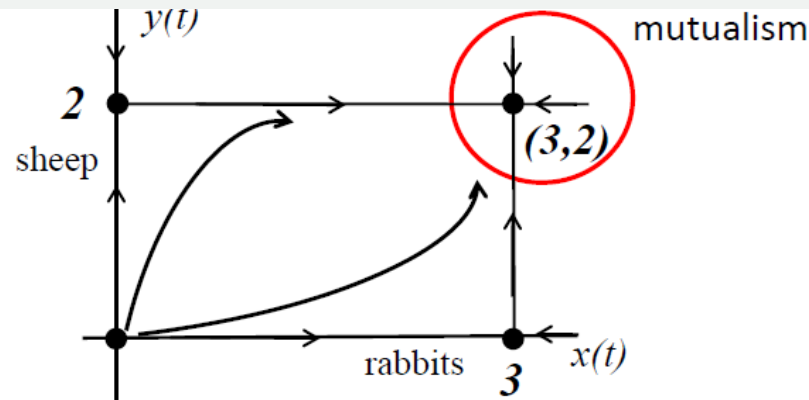
$$\begin{pmatrix} dx'(t)/dt \\ dy'(t)/dt \end{pmatrix} \approx \begin{pmatrix} -3 & 0 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} x'(t) \\ y'(t) \end{pmatrix}$$

$$x'(t) = x'(0)e^{-\lambda_1 t}, \quad y'(t) = y'(0)e^{-\lambda_2 t}$$

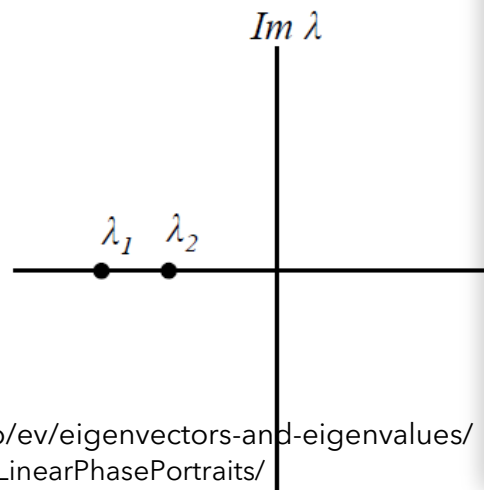
two real eigenvalues:

$$\lambda_1 = -3, \quad \lambda_2 = -2, \text{ stable fixed point}$$

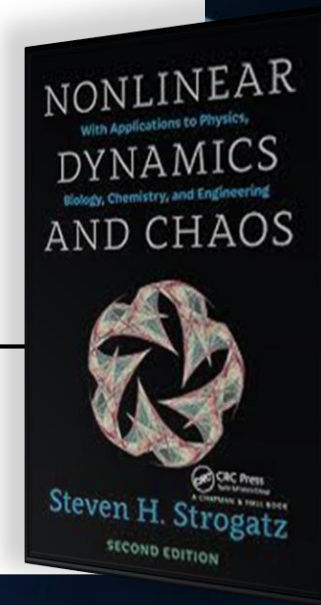
<https://setosa.io/ev/eigenvectors-and-eigenvalues/>
<https://demonstrations.wolfram.com/EigenvaluesAndLinearPhasePortraits/>



*x(t) = number of rabbits
y(t) = number of sheep*



Module 2: Eigenvalue analysis



Random matrix theory applied to N-species ecology models ($N \gg 1$)

1. Assume each species in isolation would obey a stable logistic equation

with stable eigenvalues **Will a Large Complex System be Stable?**

$$\frac{dx_i}{dt} = x_i(1 - x_i) \quad \text{ROBERT M. MAY}$$

2. $\frac{dx_i'(t)}{dt} \approx \sum_{j=1}^N A_{ij}$ [Nature](#) **238**, 413–414 (1972)

deviations from the

20k Accesses | **1604** Citations | **112** Altmetric | [Metrics](#)

3. $\vec{A} \approx -\vec{I} - \vec{C}$, with

mean for each element

Abstract

The spectrum of

of complex eigenvalues

in the complex plane

Universal density

"Girko's Law"

Gardner and Ashby¹ have suggested that large complex systems which are assembled (connected) at random may be expected to be stable up to a certain critical level of connectance, and then, as this increases, to suddenly become unstable. Their conclusions were based on the trend of computer studies of systems with 4, 7 and 10 variables.

Any ecological system becomes unstable for sufficiently large N !



Module -2 (prerequisite)

- Basics of matrix
- Module 1
- Introduction of Ordinary Differential Equations
- Newtonian Mechanics

Module -2(Learning outcome)

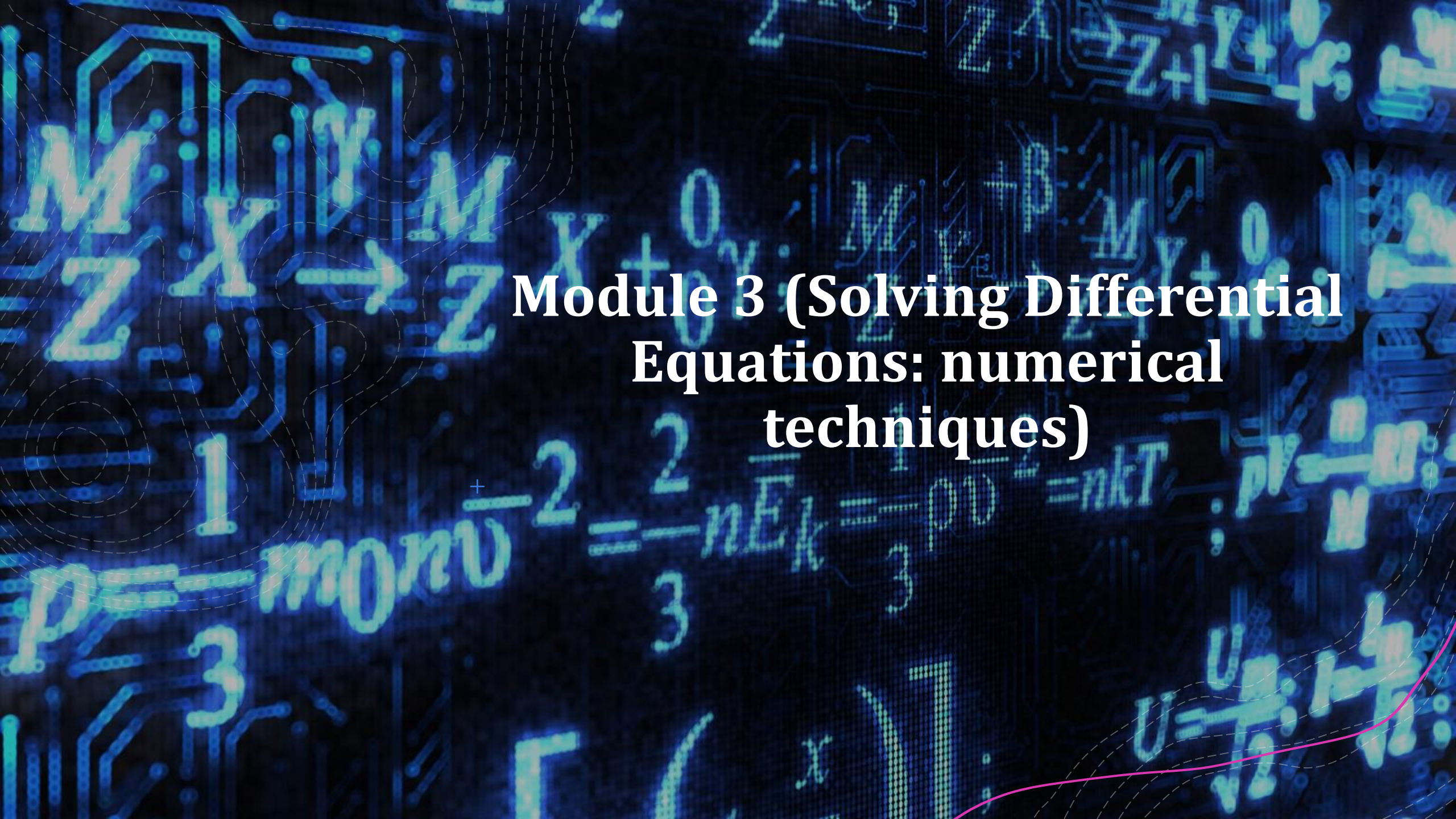
- Eigenvalue analysis
- Spring-mass systems: normal modes,
- Ecology: Predator-Prey system
- Eigenvalues of large matrix

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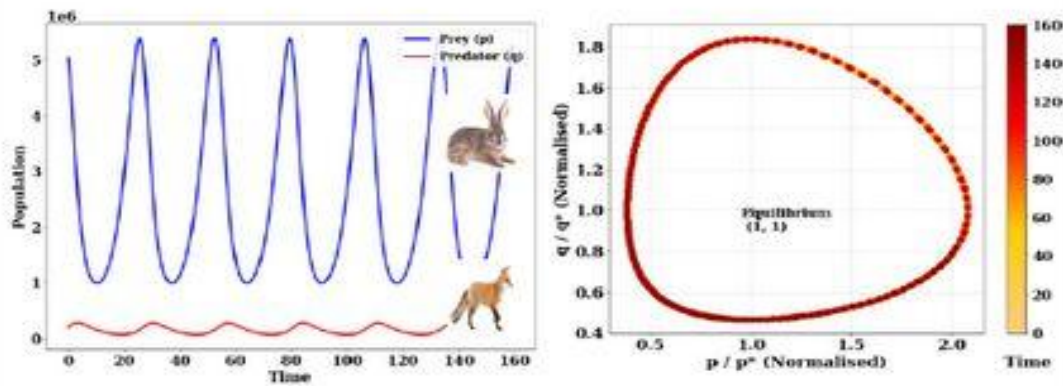


The background is a dark blue field filled with glowing, semi-transparent mathematical formulas and circuit-like patterns. Visible formulas include $M \rightarrow Z$, $X \rightarrow Z$, $1 = \frac{2}{3} n \bar{E}_k = \frac{1}{3} \rho \bar{v}^2 = nkT$, $p = \frac{1}{3} m_0 n \bar{v}^2$, $U = \frac{U_0}{\sqrt{2}}$, and x . There are also dashed white lines and a solid pink curve in the bottom right corner.

Module 3 (Solving Differential Equations: numerical techniques)

Nonlinear Dynamics Predator-Prey Epidemic model

Module 3: Solving Differential Equations



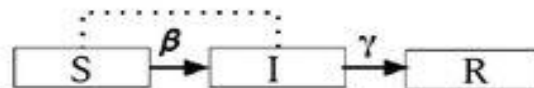
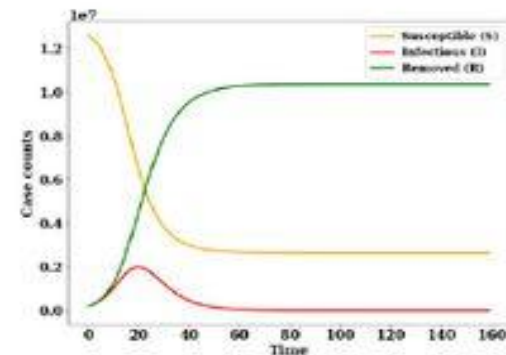
p = Prey
 q = Predator
 r = Growth Rate of Prey
 e = Rate of consumption of Prey
 b = Birth Rate of Predator
 d = Death Rate of Predator

$$\dot{p} = rp - epq$$

$$\dot{q} = bpq - dq$$

$$(p^*, q^*) = \left(\frac{d}{b}, \frac{r}{e} \right)$$

(a) Lotka–Volterra



S = Susceptible
 I = Infectious
 R = Removed
 N = Total population
 β = Transmission rate
 γ = Inverse Infectious period

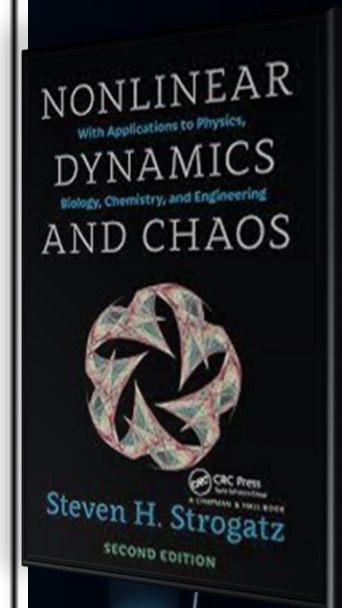
$$\dot{S} = -\frac{\beta SI}{N}$$

$$\dot{I} = \frac{\beta SI}{N} - \gamma I$$

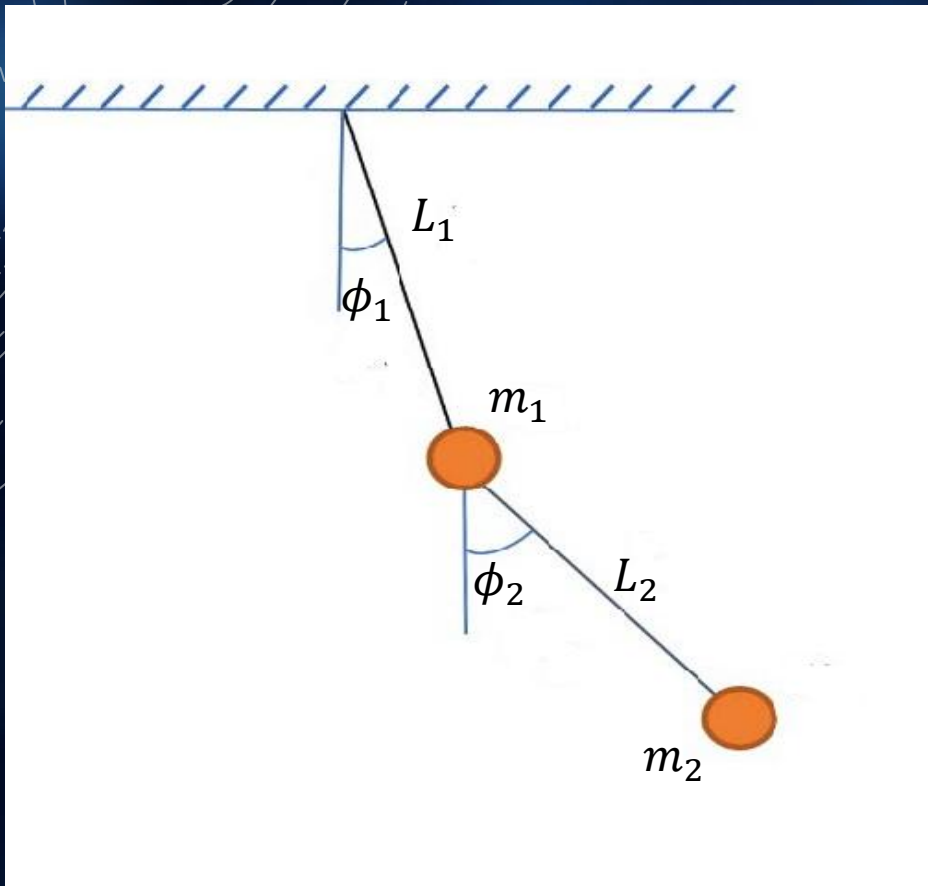
$$\dot{R} = \gamma I$$

$$S + I + R = N$$

(b) SIR (Constant β)

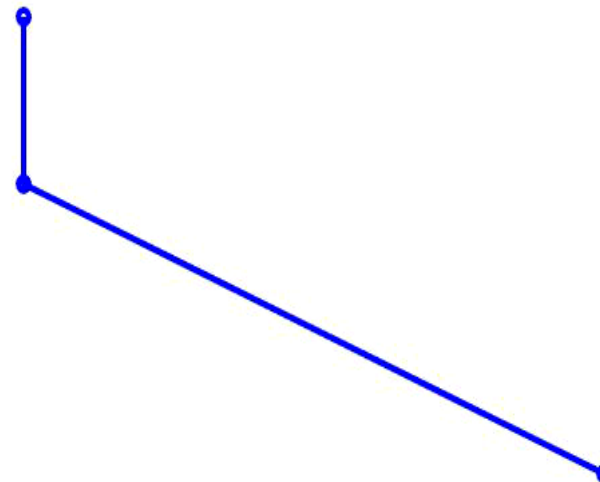


Double Pendulum

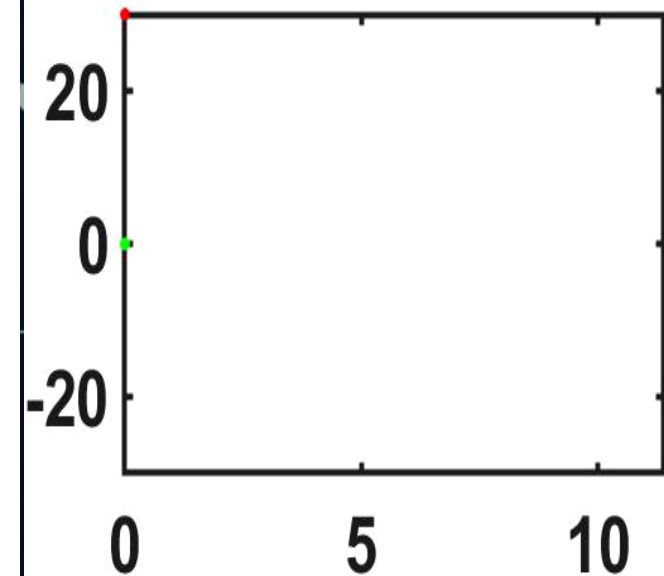


Module 3: Solving Differential Equations

$t = 0.000 \text{ s}$

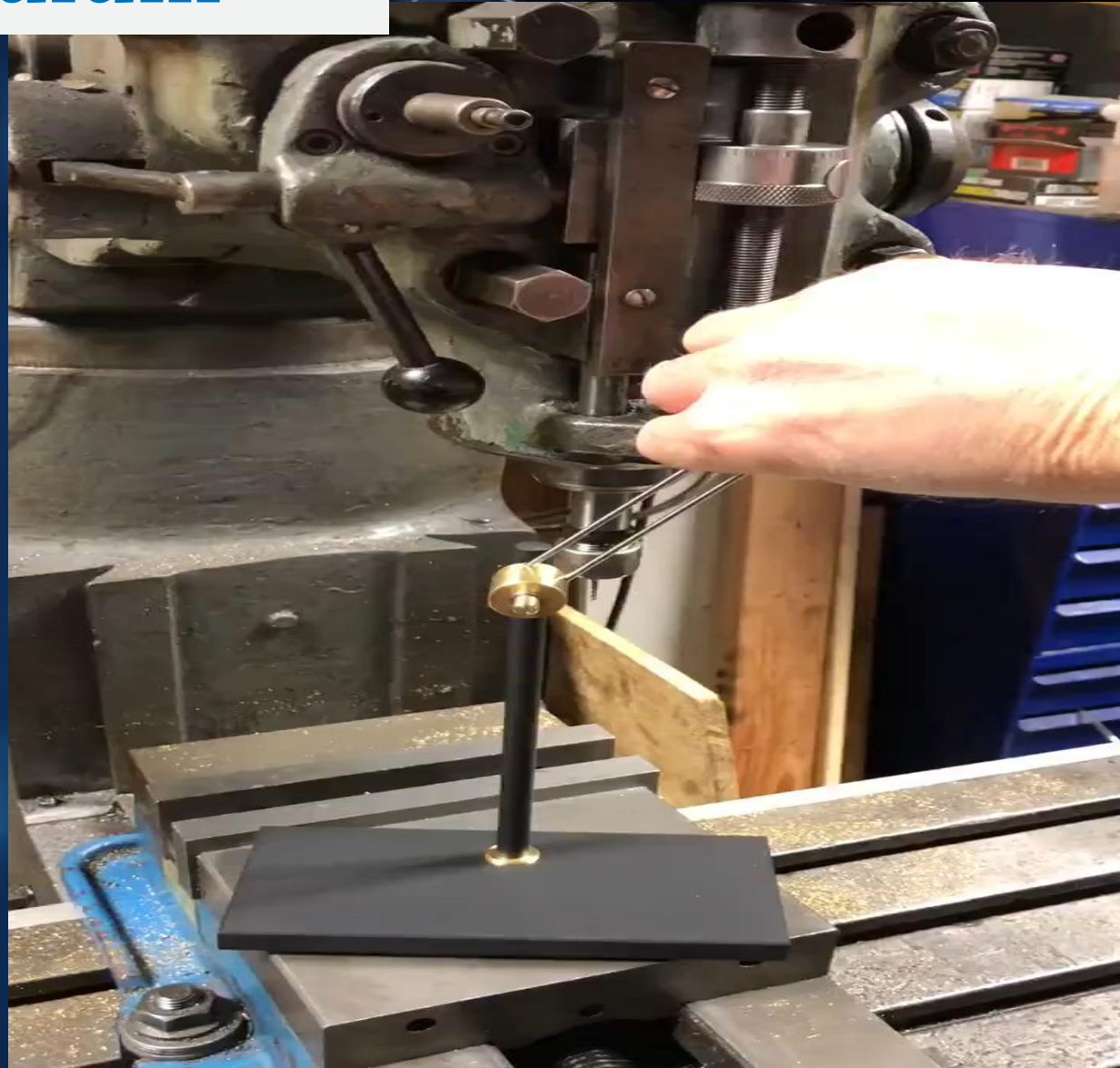


$t = 0.000 \text{ s}$



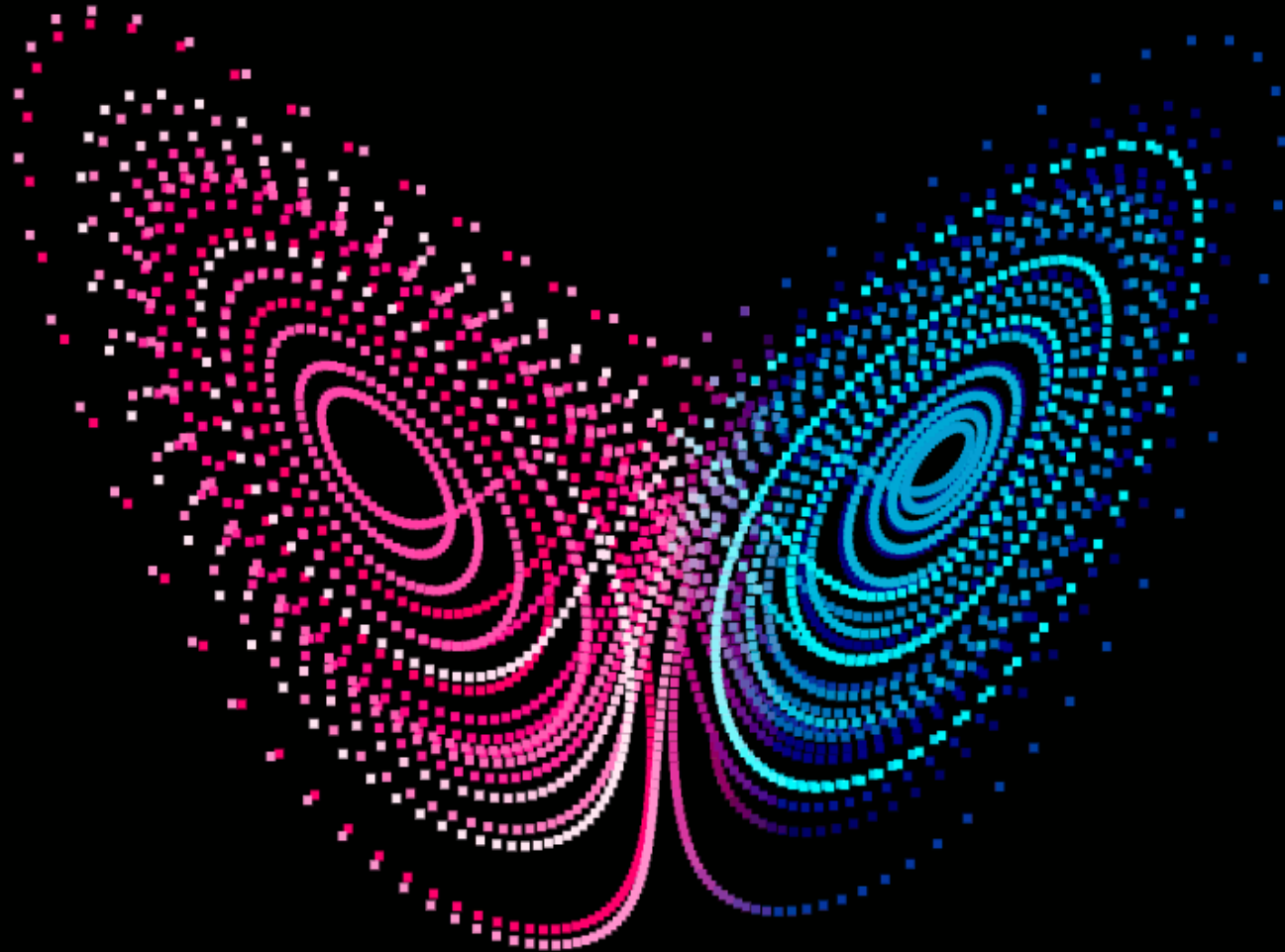
Chaotic Double Pendulum

$t = 0.000 \text{ s}$

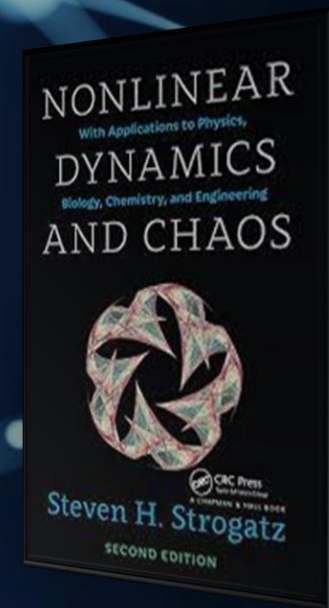


S

Lorenz Oscillator



Module 3: Solving Differential Equations



Module -3 (prerequisite)

- **Module 1,2**
- **Ordinary Differential Equations**
- **Newtonian Mechanics**

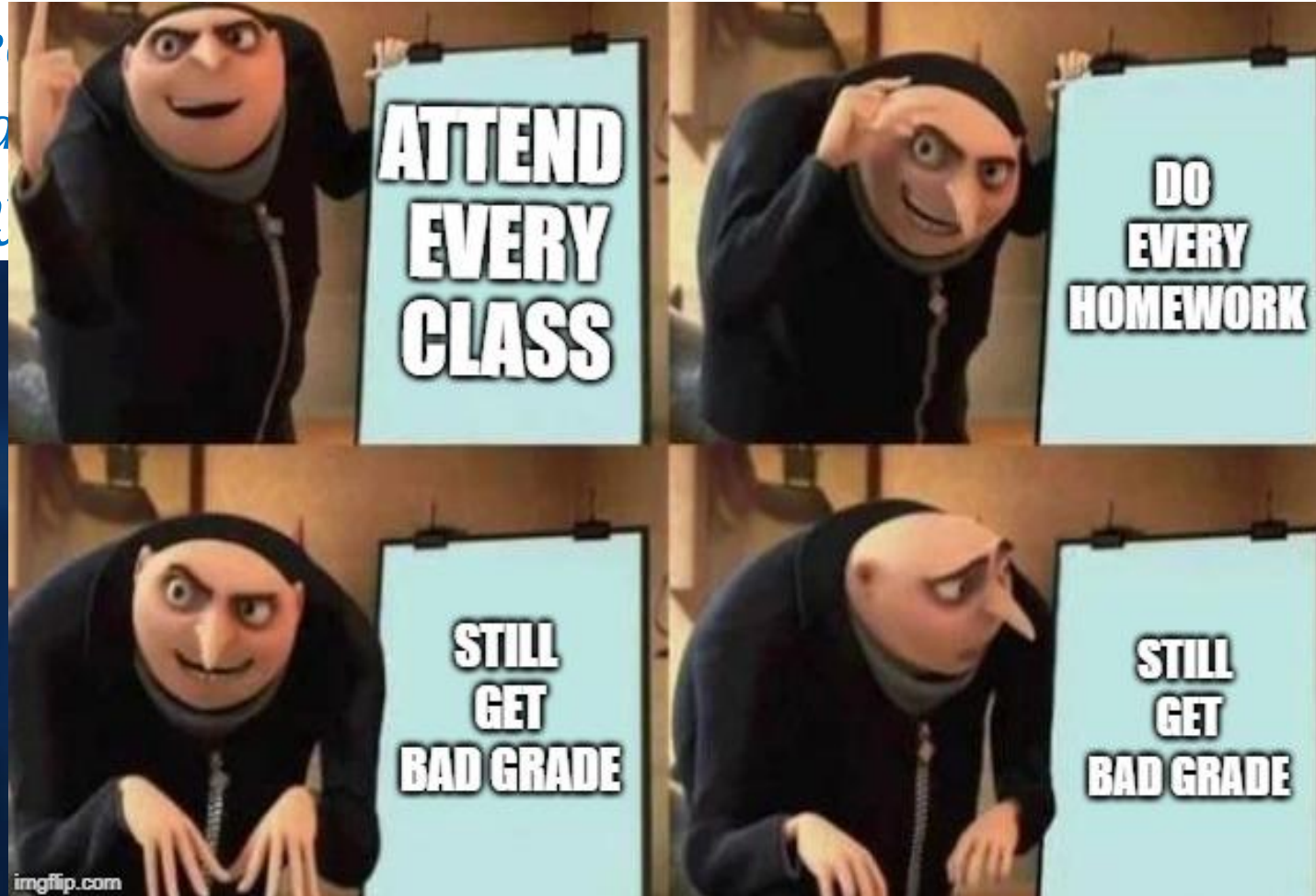
Module -3 (Learning outcome)

- **Learning of Non-linear Differential Equations**
- **Predator-Prey interactions and SIR model**
- **Numerical Methods-Euler, Runge-Kutta 4**
- **Double Pendulum, Lorenz Oscillator**

Chaos theory : A brief and general idea (sensitivity to IC)

Overall Target

- Numerical solution of differential equations
 - Modelling of chaos in physics
- Me after every single differential equations test.



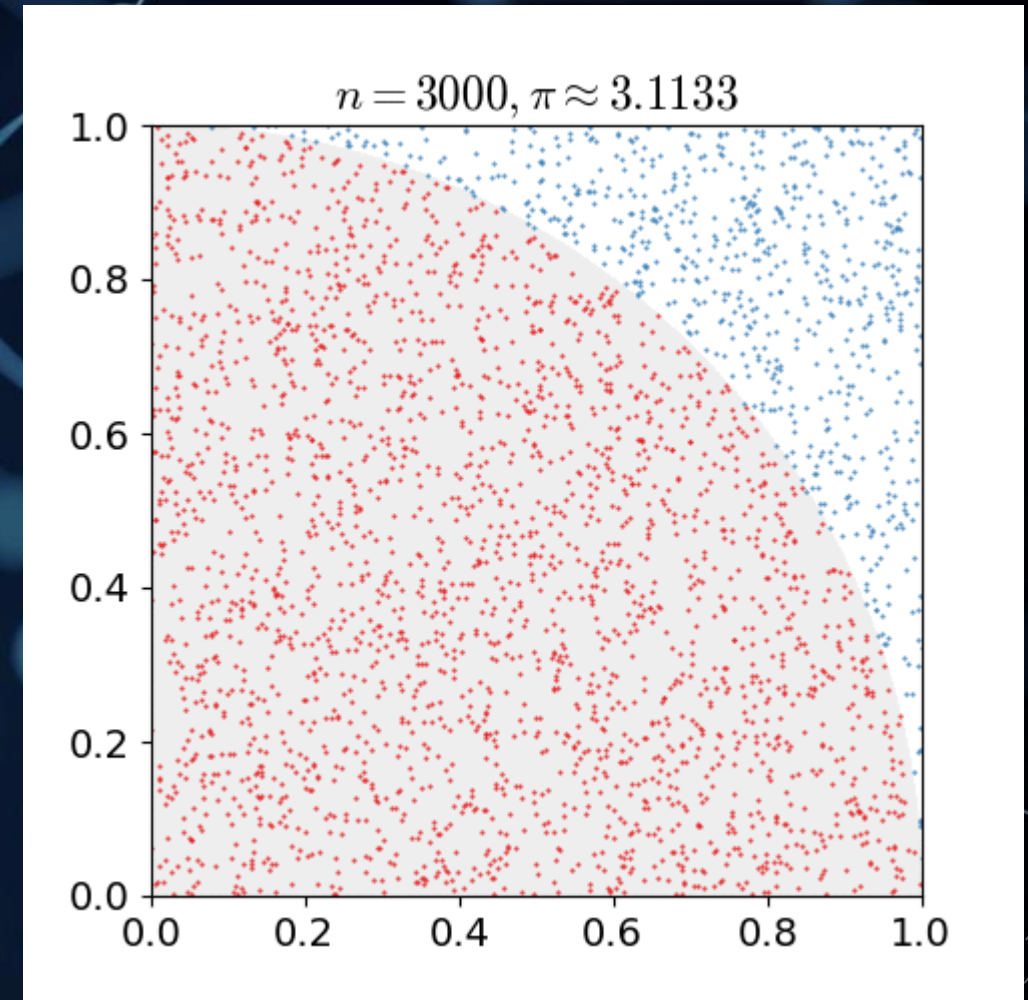


Module 4
**(Monte Carlo Method and
its application)**

When you hear the words “Monte Carlo”, most people envision this



But we will focus...



or this.....



Module 4: Monte Carlo Simulation

Module -4 (prerequisite)

- **Random Numbers**
- **Numerical Integration**
- **Probability and Statistics (knowledge on distribution)**

Module -4(Learning outcome)

- **Monte Carlo Method**
- **Importance sampling**
- **Random number generation techniques**
- **Non-uniformly distributed Random Number Generator**
- **Application to numerical integration**
- **Random Walks**

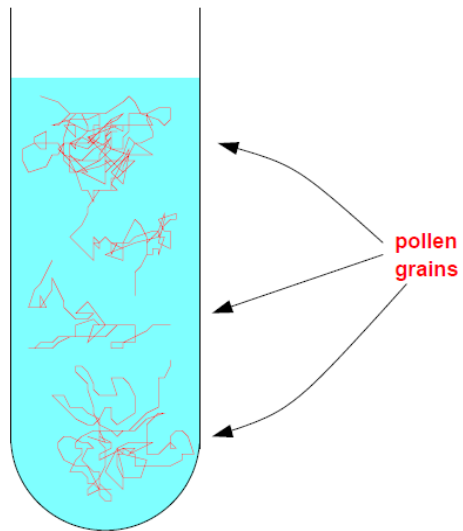
Overall Targets

- *Random Walk*
- *Integration*
- *Chemical rate equations*

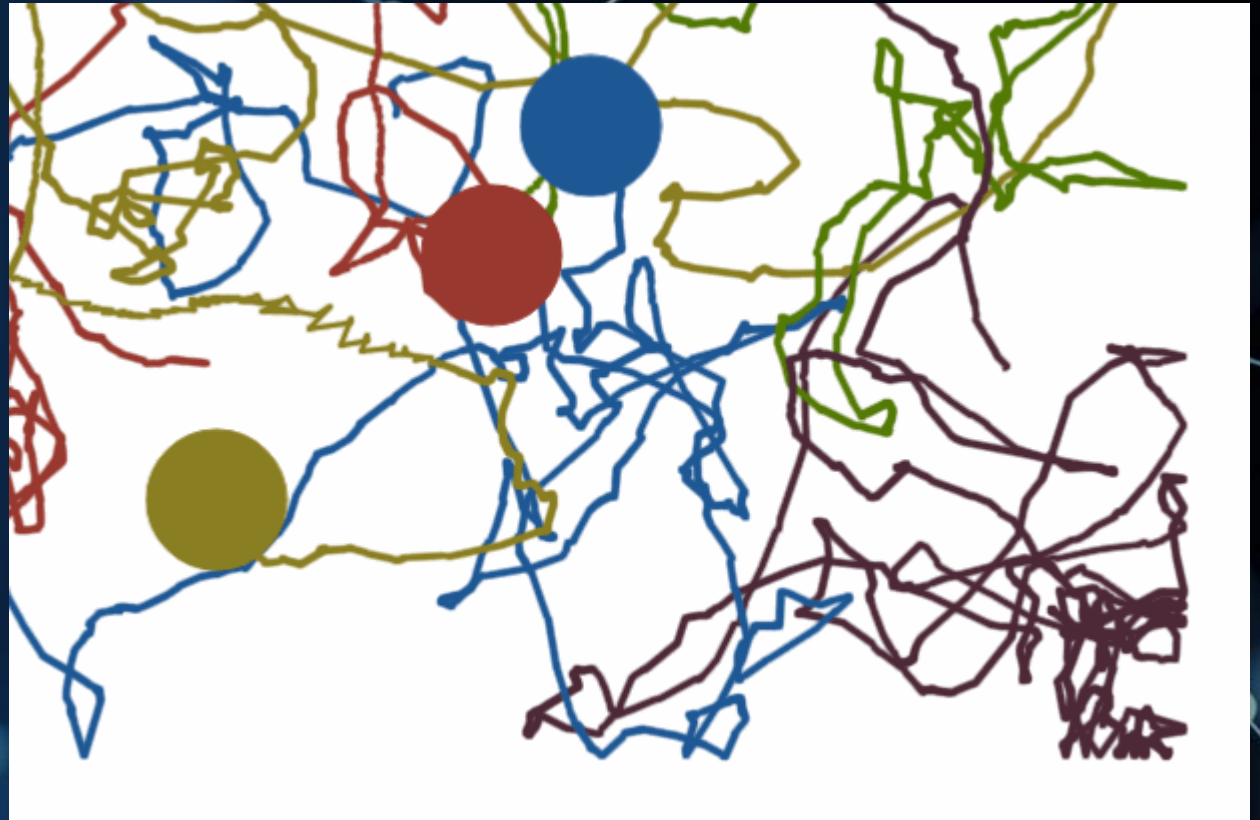


Module 5

(Brownian Motion)



In 1827 Robert Brown, a Scottish botanist and curator of the British Museum, observed that pollen grains suspended in water, instead of remaining stationary or falling downwards, would trace out a random zig-zagging pattern. This process, which could be observed easily with a microscope, gained the name of **Brownian motion**.



C.W. Gardiner

Handbook of Stochastic Methods

for Physics, Chemistry and the Natural Sciences

Second Edition
With 29 Figures

Module 5 (Brownian Motion)

SIAM REVIEW
Vol. 43, No. 3, pp. 525–546

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An Algorithmic Introduction to Numerical Simulation of Stochastic Differential Equations*

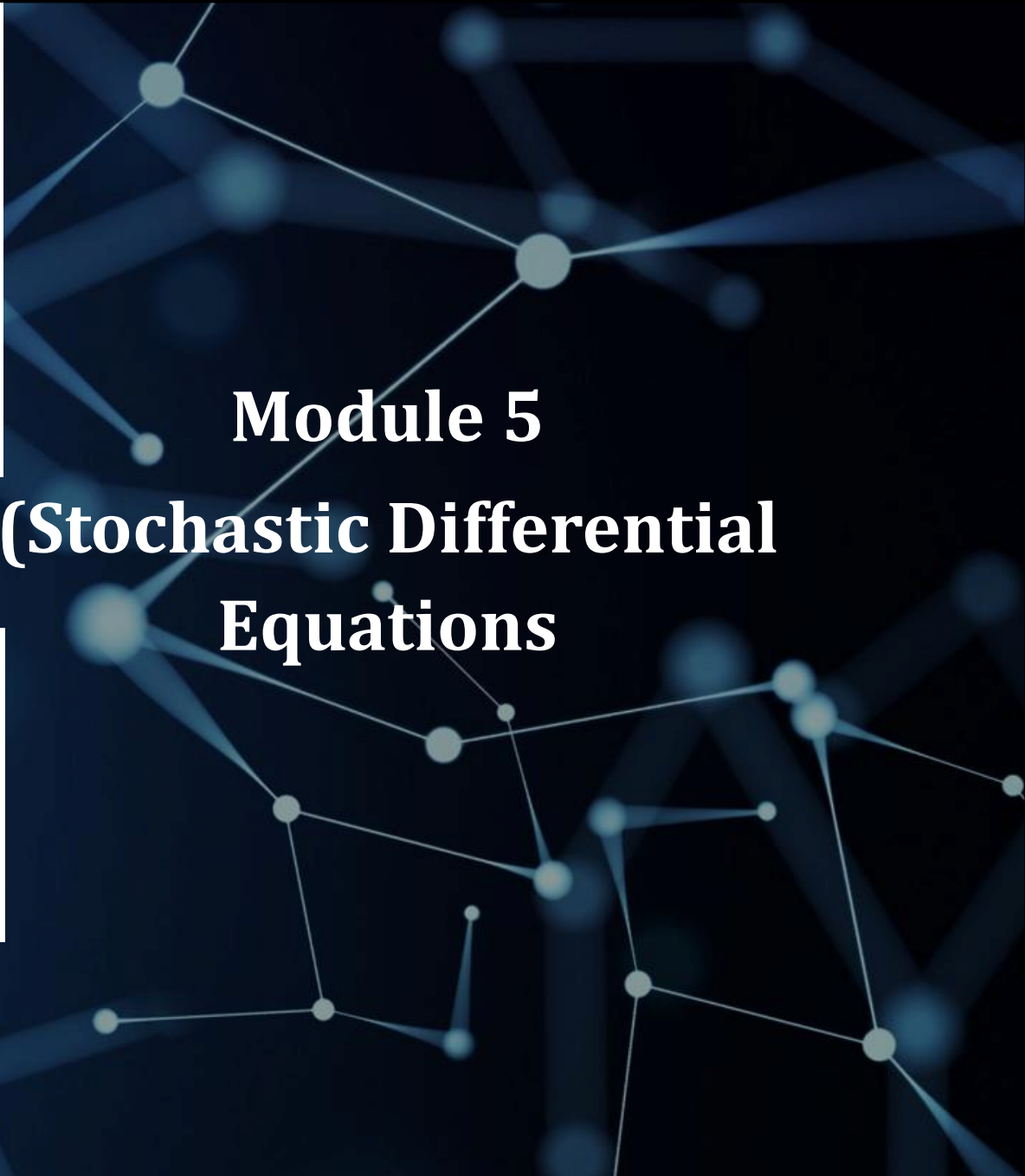
Desmond J. Higham[†]

SIAM REVIEW
Vol. 50, No. 2, pp. 347–368

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Modeling and Simulating Chemical Reactions*

Desmond J. Higham[†]



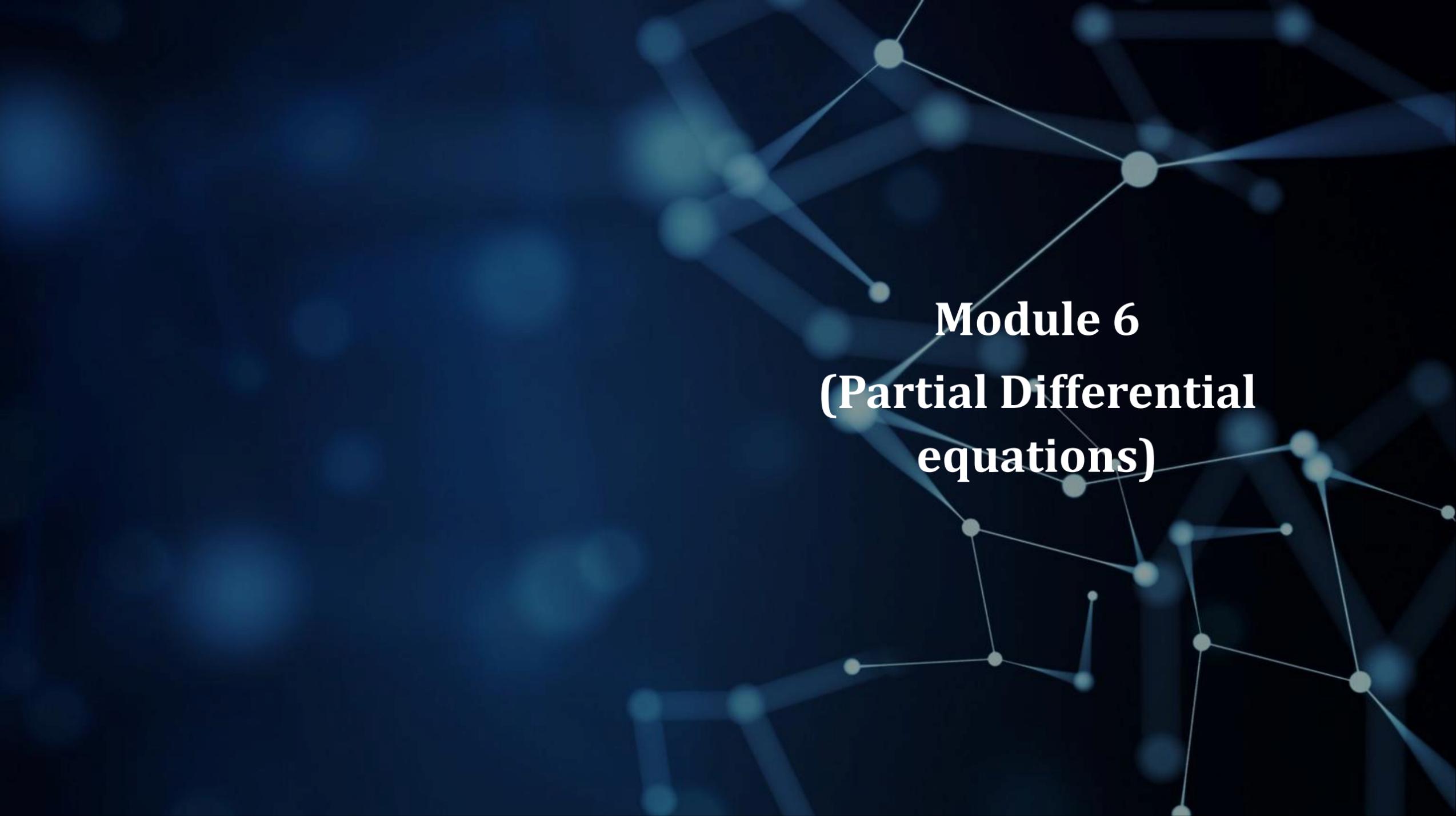
Module 5 (Stochastic Differential Equations)

Module -5 (prerequisite)

- **Numerical techniques for ODE (Module 3)**
- **Module 4**
- **Brownian Motion**

Module -5(Learning outcome)

- **Brownian motion simulation/Langevin equation**
- **Rate equations : Master Equations**
- **Gillespie Method**
- **SDE –Numerical solver**



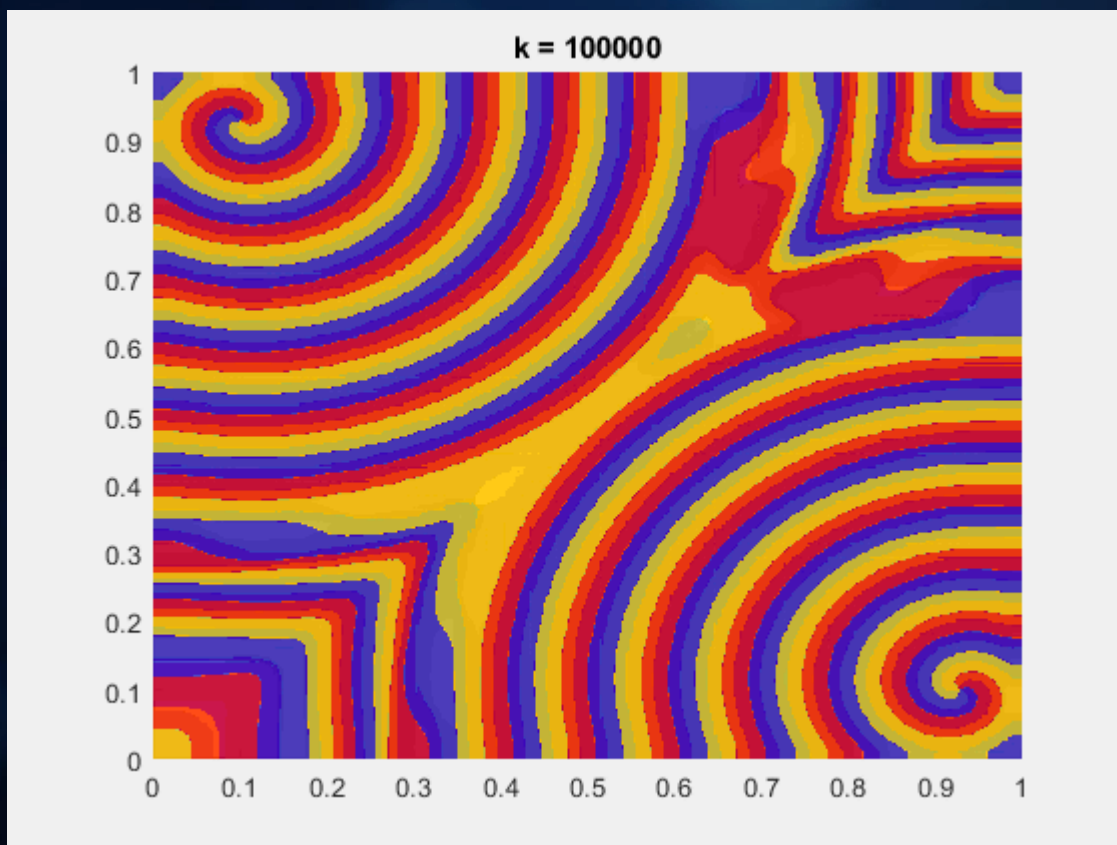
Module 6
(Partial Differential
equations)

SCIENCE

How the leopard gets its spots

Alan Turing and the math behind biological development

By Albert Liu | Oct. 28, 2020

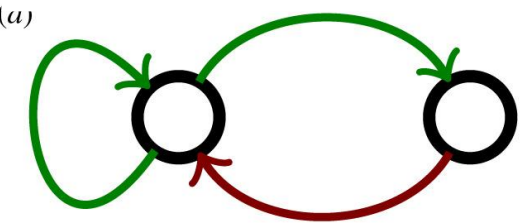


Module 6
(Partial Differential equations)

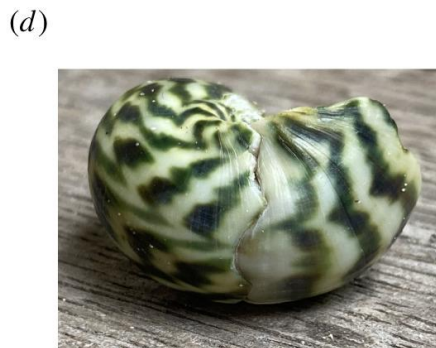
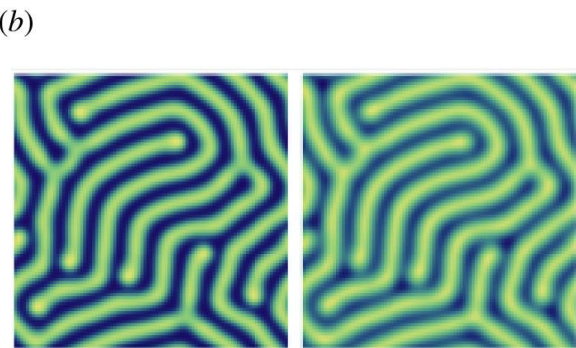
How the leopard gets its spots

Alan Turing and the math behind biological development

By Albert Liu | Oct. 28, 2020



Gierer–Meinhardt model



Review



Cite this article: Vittadello ST, Leyshon T, Schnoerr D, Stumpf MPH. 2021 Turing pattern design principles and their robustness. *Phil. Trans. R. Soc. A* **379**: 20200272. <https://doi.org/10.1098/rsta.2020.0272>

Accepted: 24 June 2021

One contribution of 11 to a theme issue 'Recent progress and open frontiers in Turing's theory of morphogenesis'.

Subject Areas:

mathematical modelling, cellular biophysics, biomathematics, computational biology

Keywords:

pattern formation, positional information, design principles

Turing pattern design principles and their robustness

Sean T. Vittadello¹, Thomas Leyshon³, David Schnoerr³ and Michael P. H. Stumpf^{1,2}

¹School of BioSciences, and ²School of Mathematics and Statistics, University of Melbourne, Melbourne, Victoria 3010, Australia

³Department of Life Sciences, Imperial College London, London, UK

id STV, 0000-0002-4476-6732; MPHS, 0000-0002-3577-1222

Turing patterns have morphed from mathematical curiosities into highly desirable targets for synthetic biology. For a long time, their biological significance was sometimes disputed but there is now ample evidence for their involvement in processes ranging from skin pigmentation to digit and limb formation. While their role in developmental biology is now firmly established, their synthetic design has so far proved challenging. Here, we review recent large-scale mathematical analyses that have attempted to narrow down potential design principles. We consider different aspects of robustness of these models and outline why this perspective will be helpful in the search for synthetic Turing-patterning systems. We conclude by considering robustness in the context of developmental modelling more generally.

This article is part of the theme issue 'Recent progress and open frontiers in Turing's theory of morphogenesis'.

<https://www.youtube.com/watch?v=8tArShb1fhw>

- Chemical basis of morphogenesis
- Patterns on snail and sea shells are one of the classical examples of Turing patterns in nature.

Module -6 (prerequisite)

- **Differential Equation**
- **Numerical methods for initial value problem**

Module -6(Learning outcome)

- **PDE –Numerical solver**
- **Heat equation**
- **Reaction-diffusion systems**
- **Spiral/stripe pattern in reality**

Science -II

Requirements

- **Newtonian Mechanics**
- **Lagrangian formulation**
- **Basics of Matrix**
- **Statistical Mechanics**
- **Matlab/Python/C++**
- **Graphical Plot (Must)**
- **Computational Complexity**
- **Error calculation**

Science -II

- Introduction to Computational Physics, Lecture of Prof. H. J. Herrmann
Swiss Federal Institute of Technology ETH, Zürich, Switzerland
Script by Dr. H. M. Singer, Lorenz Müller and Marco - Andrea Buchmann
Computational Physics, IfB, ETH Zürich
(Module 3, 4, and 6)
- Nonlinear Dynamics –Steven Strogatz (Module 2 and 3)
- Desmond Highham, plus PPTs (Module 5)
- Books: Gilbert Strang (Module 1 and 2)

Science –II (Evaluation)

Type of Evaluation	Weightage (in %)
Assignment 1 (January 18)	10
Quiz (January end)	15
Midsem Exam	25
Notes: Any Suggestions?	

Science -II (Weekly Plan)

		Comments
Class 1-2	Introduction of the course Module 1	
Class 3	Module 1, 2	
Class 4-5	Module 2/3	
Jan 22, 23	No class	
Class 6-9	Module 3/4	Class 6/7: Quiz
Class 10-13	Module 5-6	

10th January: 2 to 2:45 pm (group A)
10th January: 3 to 3:45 pm (Group B)
We can also use the tutorial slots

Science -II (Feedback)

course has lots of content not required by most people,



We spent too much time on basic details of eigenvectors. Probably, this portion should be completed faster



The flow of this course was the worst ever compared to other courses. **ZERO connection between topics whatsoever and none of the topics had any of their base built up.** Everything was expected to be known from beforehand. One of the worst courses overall ever. Neither the teaching style nor the content of the course was interesting.



Science -II (Your TAs)

- The TAs were extremely poor in their duties.



Science -II (Advice to the students)

- If you have to sleep, sleep. Don't talk or snore.
- You can leave (if you wish) after the attendance. But without using any type of noise (white, pink, blue, anything not allowed).

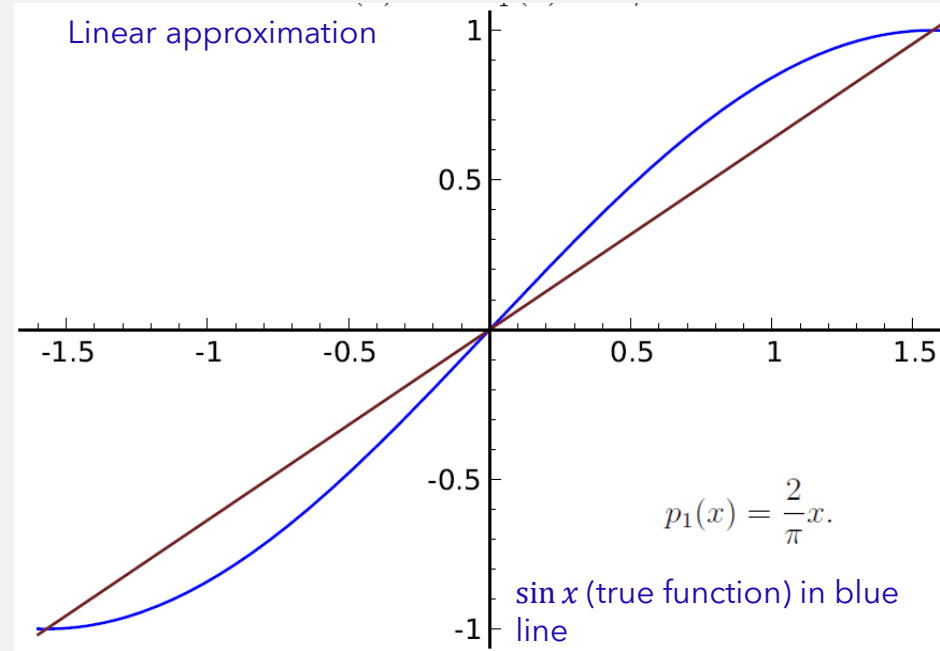
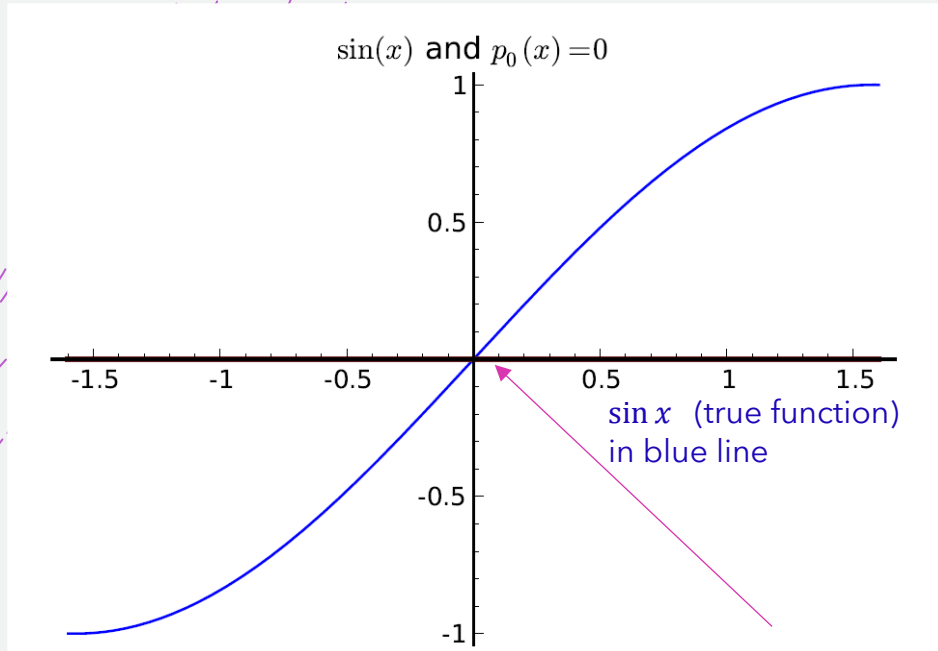


Ninja techniques For Sleeping In Class

<https://sites.imsa.edu/acronym/2012/09/03/techniques-for-sleeping-in-class-2/>

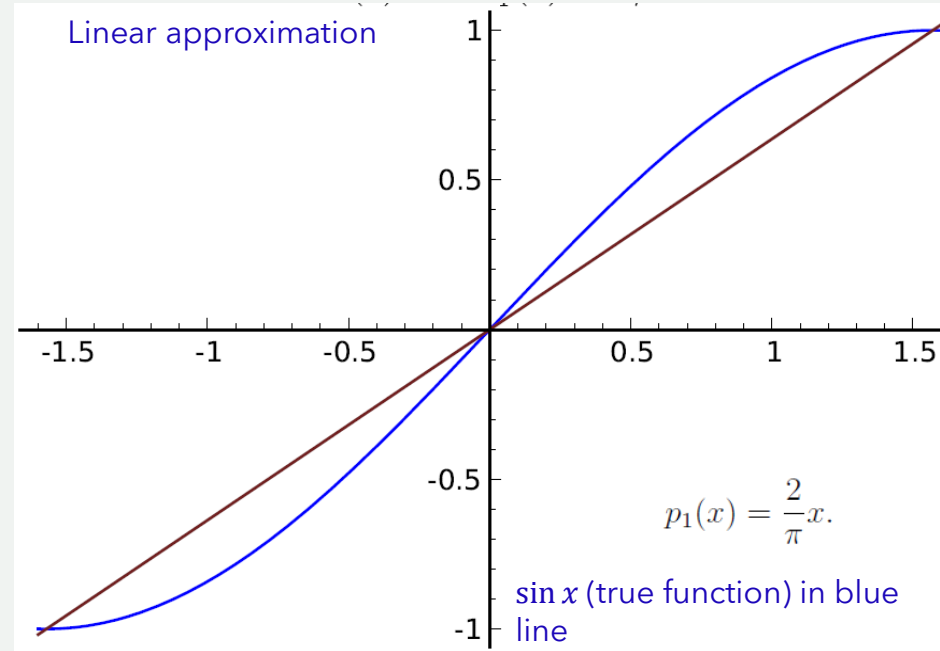
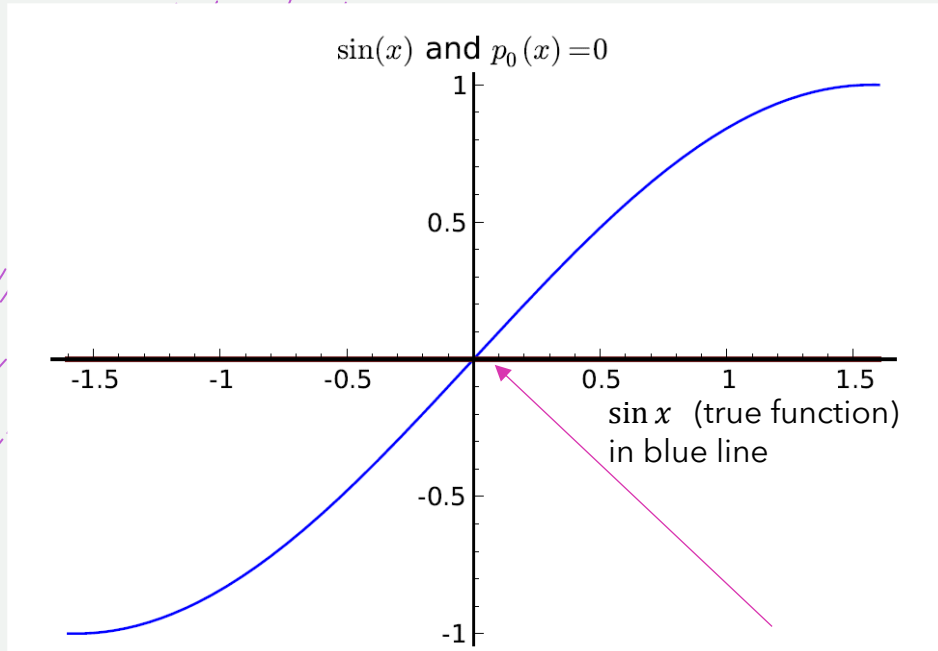


Sinx as Polynomial



What about $p_2(x) = -\frac{4}{\pi^2} x(x - a)$?

Sinx as Polynomial

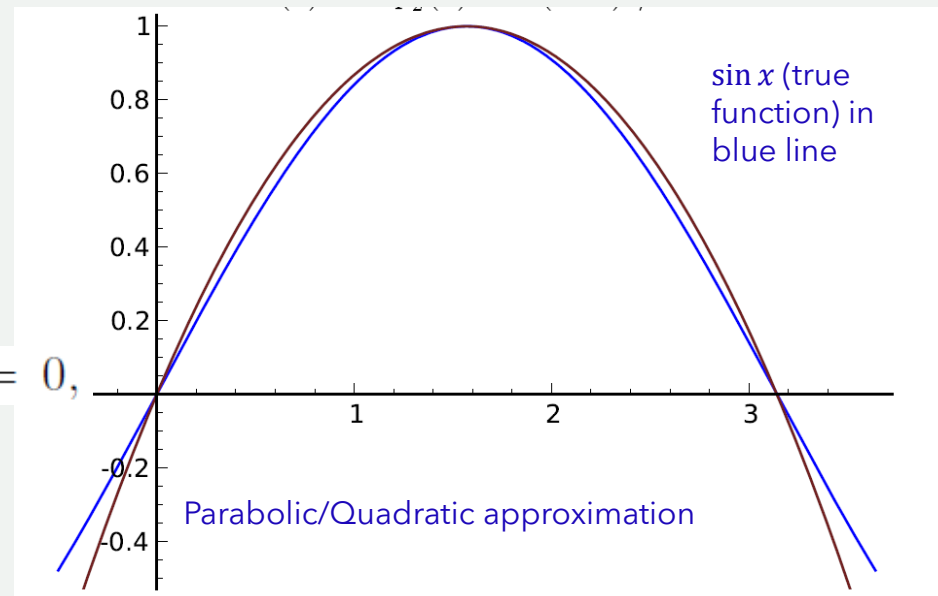


What about $p_2(x) = -\frac{4}{\pi^2}x(x - \pi)$?
Take $a = \pi$

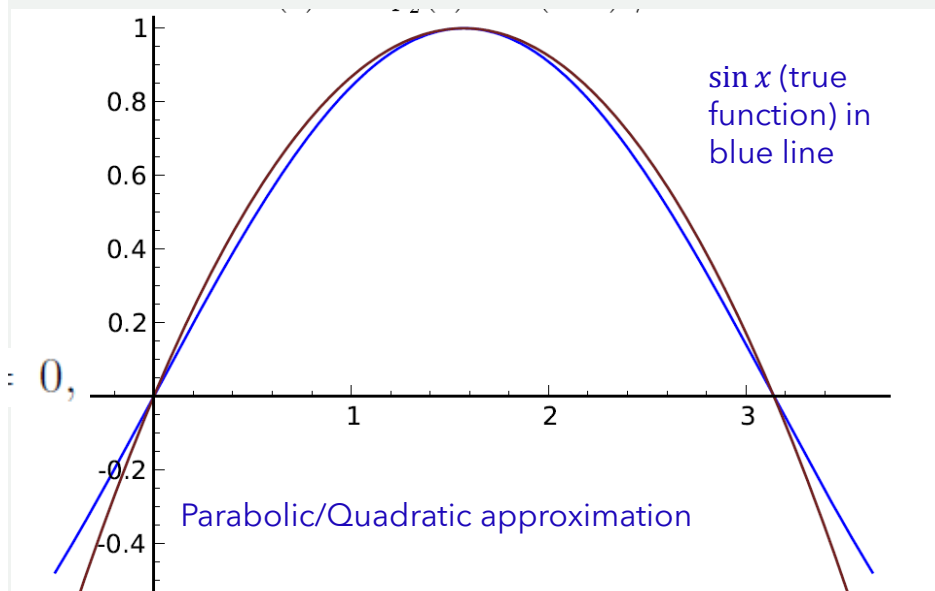
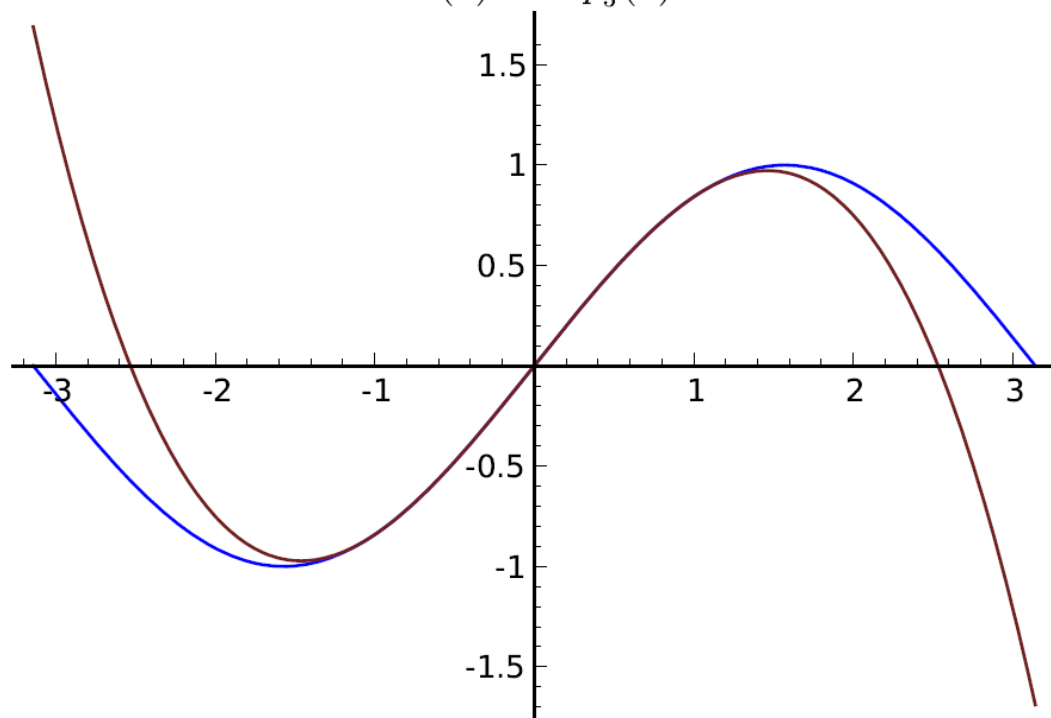
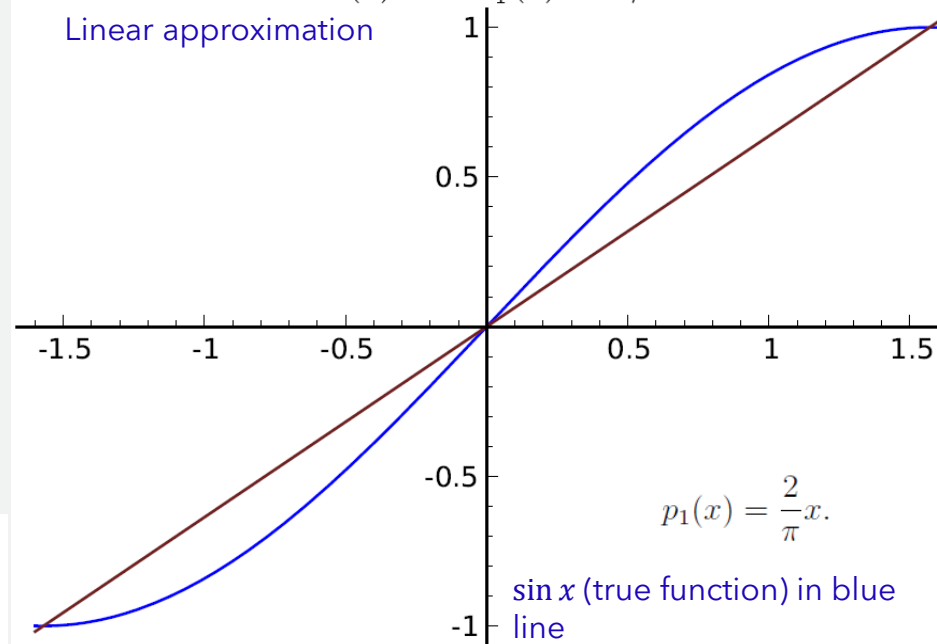
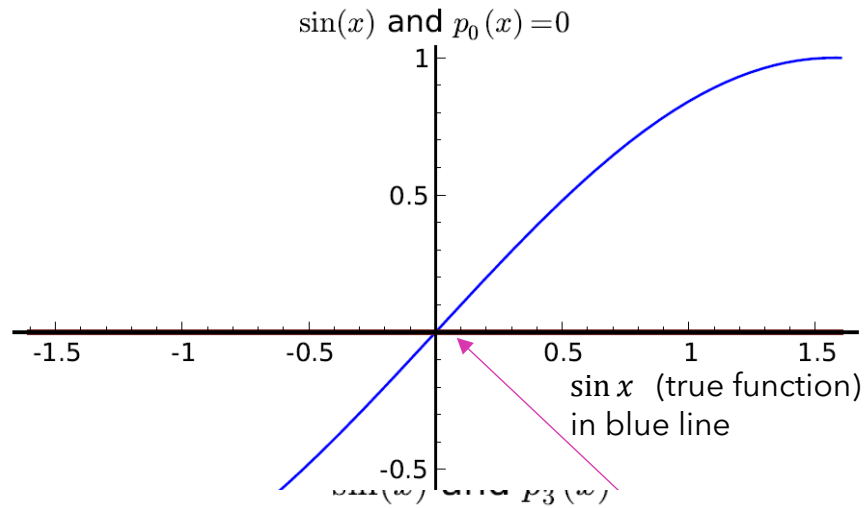
What about $p_3(x) = -px^3 + x$?

$$\sin(0) = 0, \sin'(0) = \cos(0) = 1, \sin''(0) = -\sin(0) = 0,$$

$$\sin'''(0) = -\cos(0) = -1.$$



Sinx as Polynomial



Numerical techniques

$$f(x_0 + h) = f(x_0) + h f'(x_0) + \frac{h^2}{2!} f''(x_0) + \cdots + \frac{h^n}{n!} f^n(x_0) + R_n(x)$$



Denotes the difference
between Talylor Polynomial
of degree n and the original
function

For the first derivative

$$f(x_0 + h) = f(x_0) + h f'(x_0) + R_1(x)$$



Small

$$\lim_{h \rightarrow 0} \frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0)$$

Numerical techniques

$$f(x_0 + h) = f(x_0) + h f'(x_0) + \frac{h^2}{2!} f''(x_0) + \cdots + \frac{h^n}{n!} f^n(x_0) + R_n(x)$$

$$\lim_{h \rightarrow 0} \frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0)$$

```
x=-2*pi:0.01:2*pi;  
h=0.01;  
f=sin(x);  
g= (sin(x+h)-sin(x))./h;  
plot(x,f,'-o');  
hold on;  
plot(x,g,'d');  
legend 'sin(x)' 'cos(x)'  
z=zeros(1,length(x));  
hold on;  
plot(x,z,'k','linewidth',3)  
;
```

