

# 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

# Science -II

## Requirements

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

Instructor: **Chittaranjan Hens**  
**CCNSB**

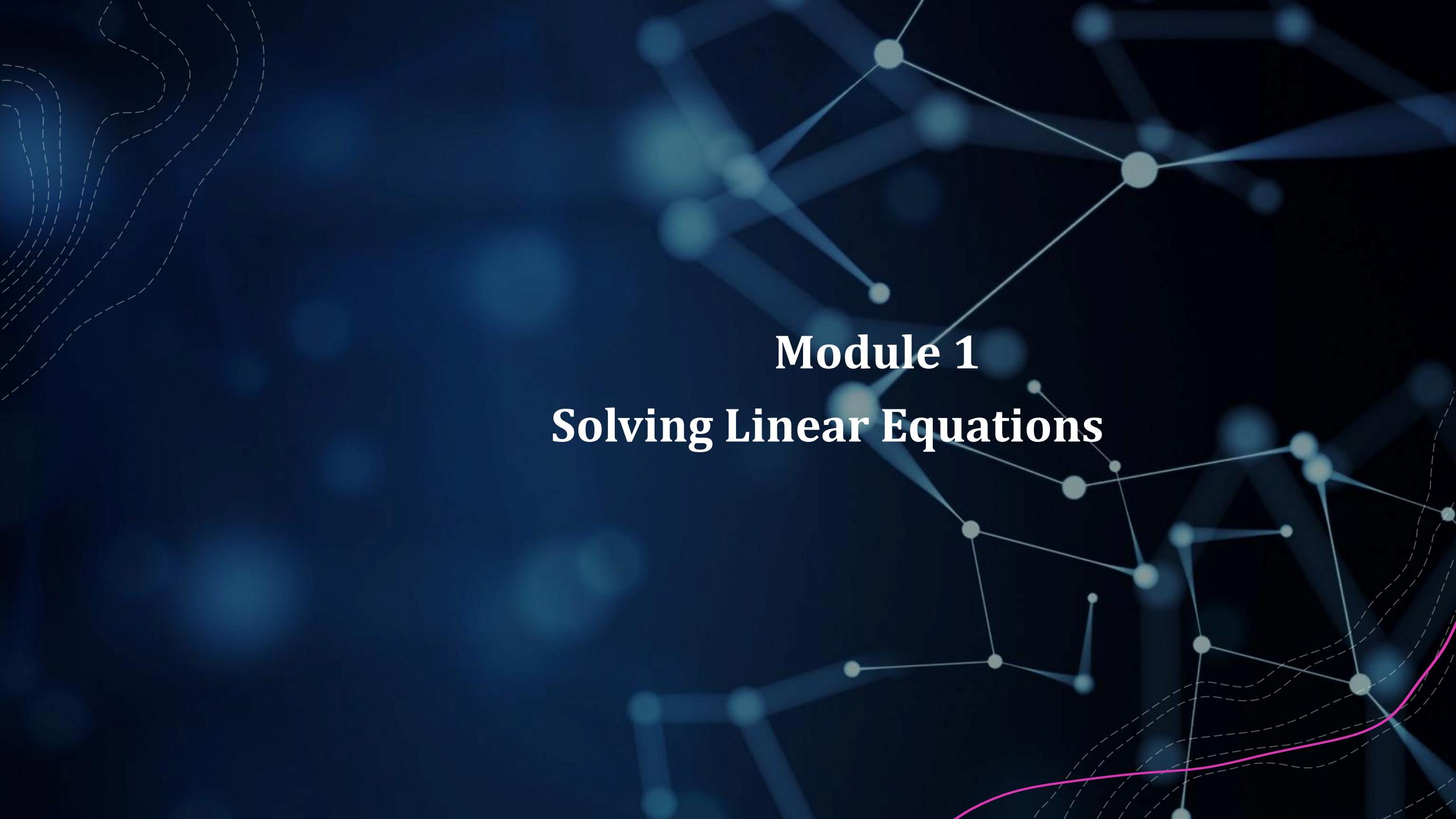
# Science -II

## 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)

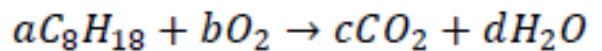
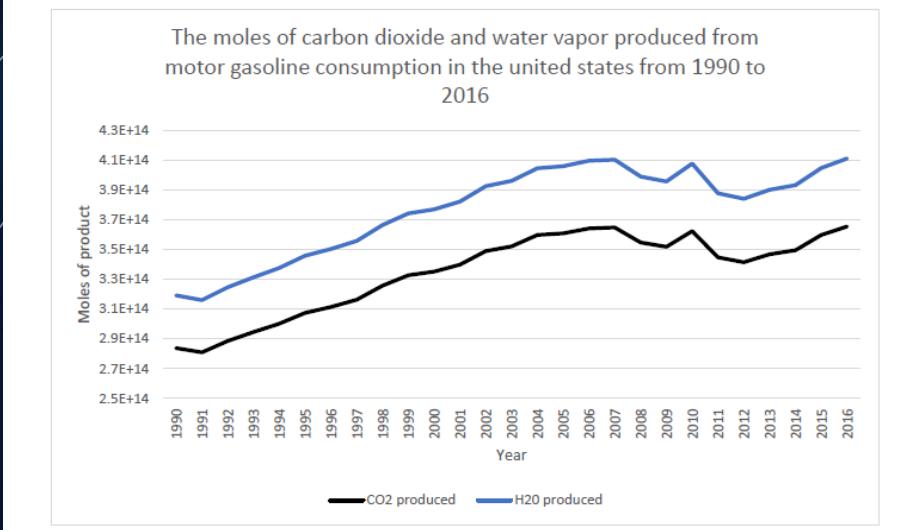




# Module 1

## Solving Linear Equations

# Balancing a chemical reaction



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



## Balancing Chemical Equations by Systems of Linear Equations

Ihsanullah Hamid

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## Module 1:Solving Linear Equations



Undergraduate Journal of Mathematical Modeling: One + Two

Volume 10 | 2019 Fall 2019

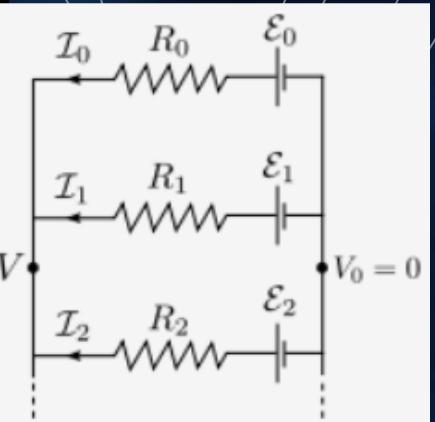
Article 5

2019

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

Emilee Barrett  
University of South Florida

# Electric Networks

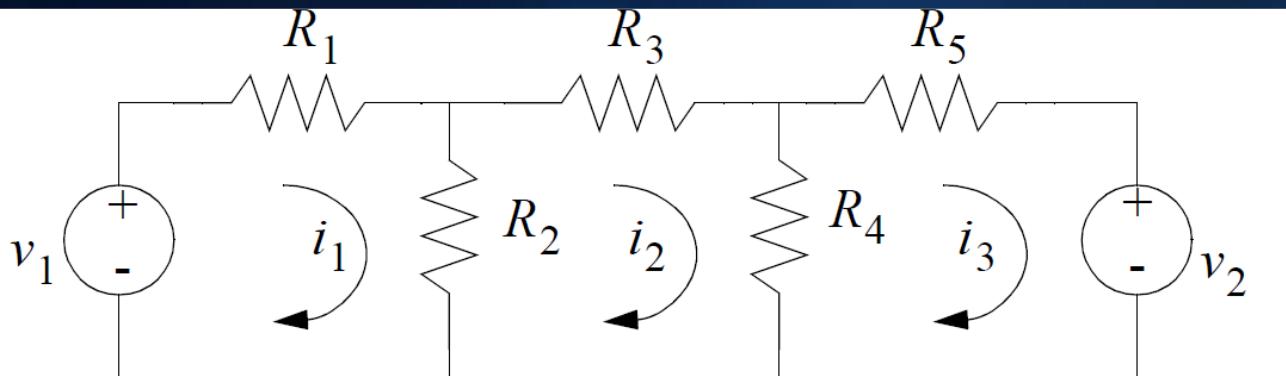


We can combine these  $N + 1$  equations into a matrix equation of the form  $\mathcal{A}\vec{x} = \vec{b}$

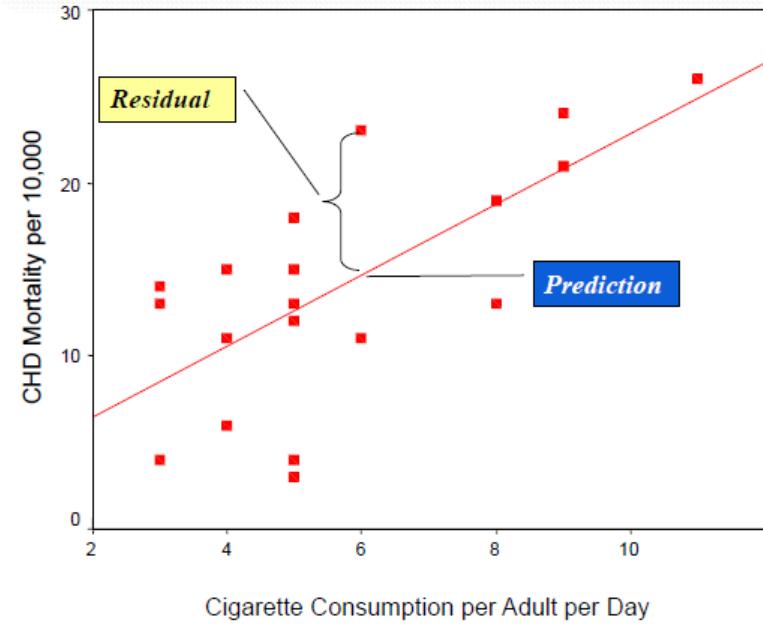
$$\begin{bmatrix} R_0 & 0 & \cdots & 0 & 1 \\ 0 & R_1 & \cdots & 0 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & R_{N-1} & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{bmatrix} \begin{bmatrix} \mathcal{I}_0 \\ \mathcal{I}_1 \\ \vdots \\ \mathcal{I}_{N-1} \\ V \end{bmatrix} = \begin{bmatrix}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

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

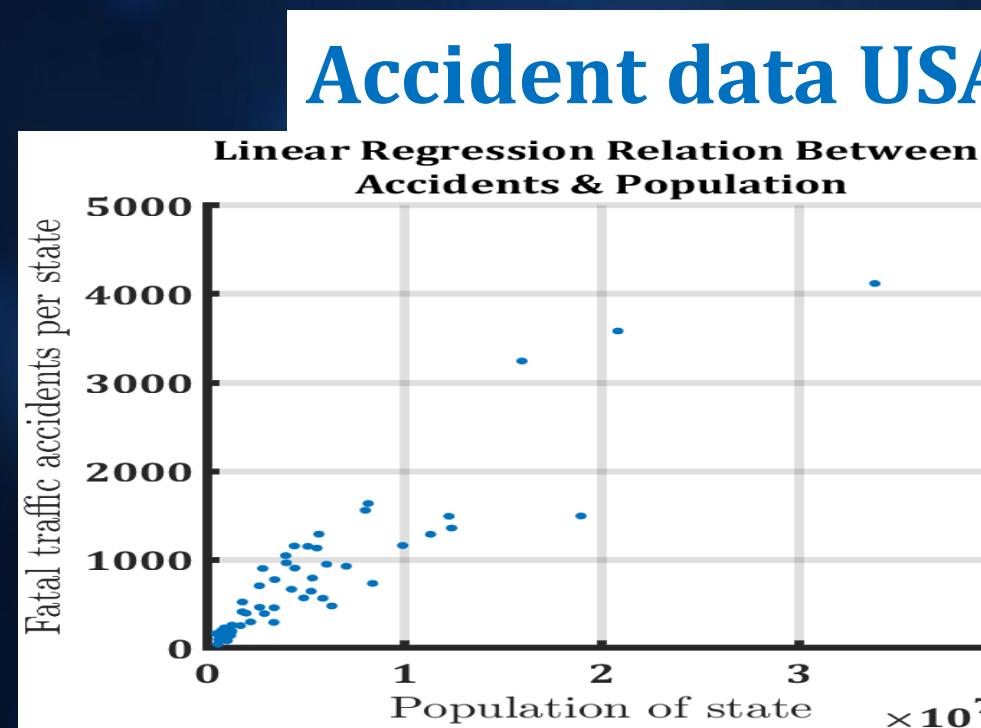
## Module 1: Solving Linear Equations



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



## Module 1:Linear Least Square Problem



- 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**

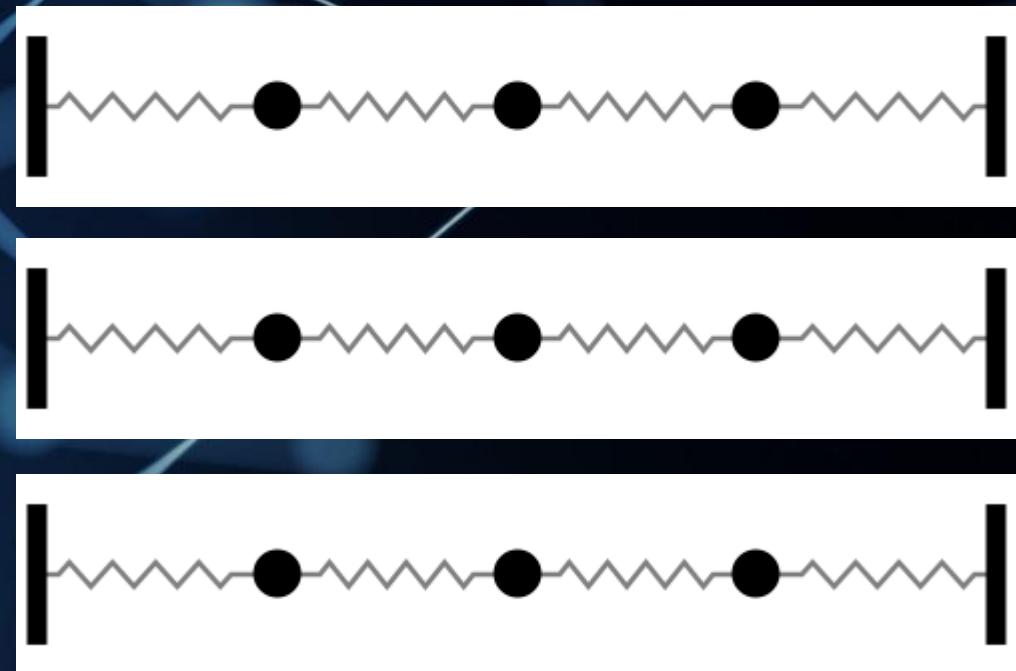
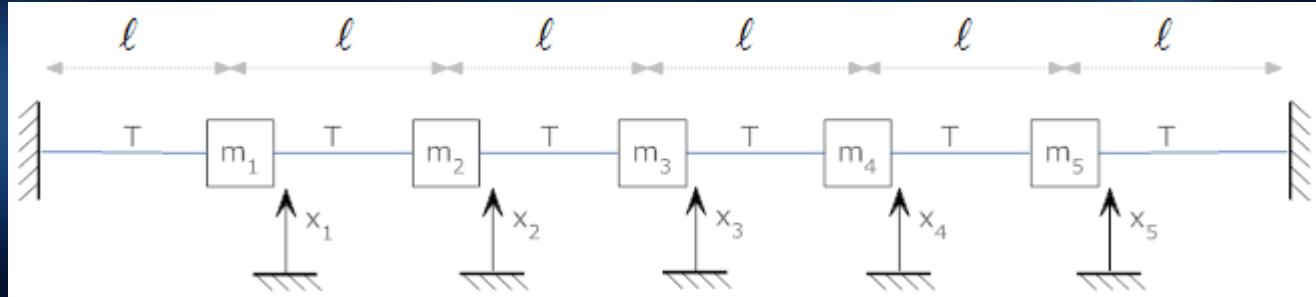
## **Algebra of matrices:**

### **contd.**

## Module 2

# Vibrating Systems with many DOF (Normal Modes)

# Vibrating Systems with many DOF (Normal Modes)



**Module 2: Matrix Algebra  
Eigenvalue analysis**

<https://ipsa.swarthmore.edu/MtrxFibe/Vibrations.html>

[https://www.brown.edu/Departments/Engineering/Courses/En4/Notes/vibrations\\_mdof/vibrations\\_mdof.htm](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)

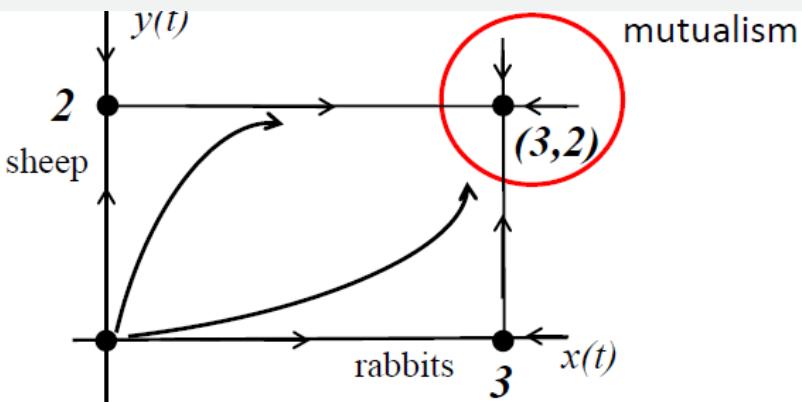
$$x'(t) = x(t) - 3, \quad y'(t) = y(t) - 2$$

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

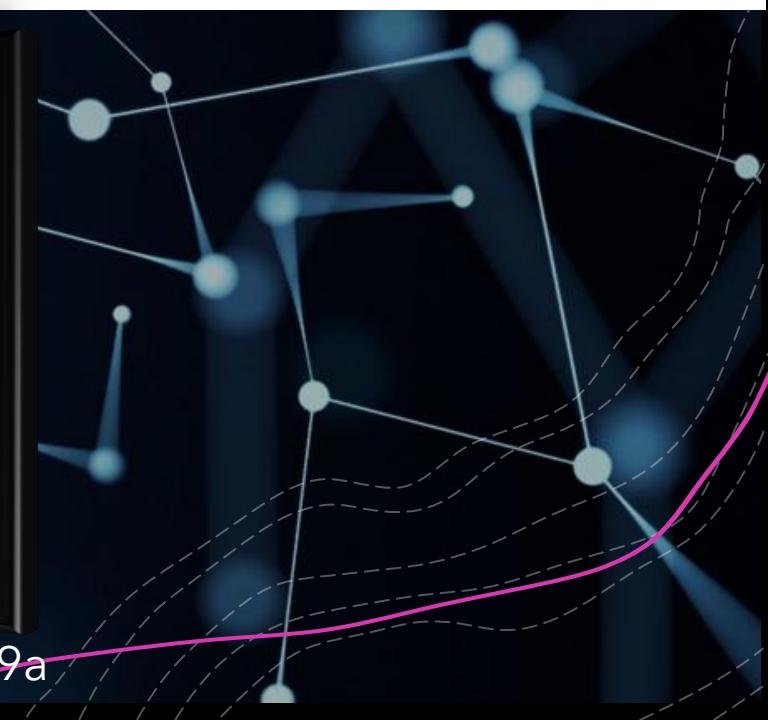
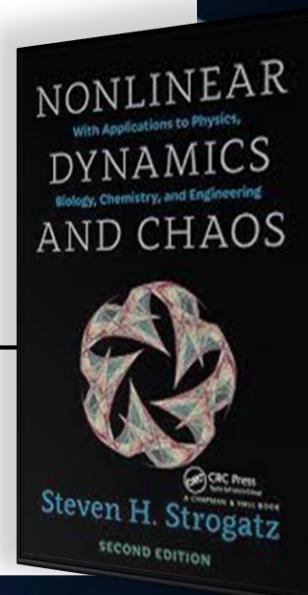
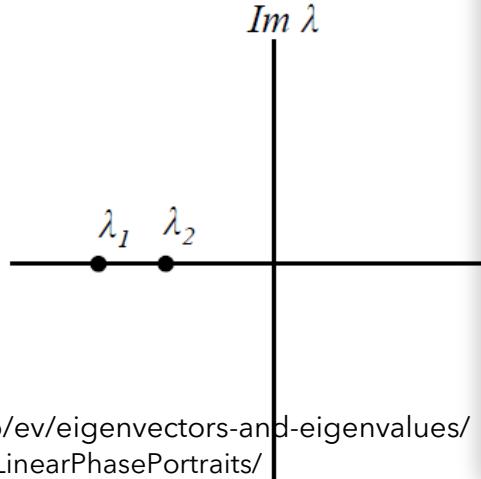
$$x'(t) = x'(0)e^{-\lambda_1 t}, \quad y'(t) = y'(0)e^{-\lambda_2 t}$$

two real eigenvalues:

$\lambda_1 = -3, \lambda_2 = -2$ , stable fixed point <https://setosa.io/ev/eigenvectors-and-eigenvalues/>  
<https://demonstrations.wolfram.com/EigenvaluesAndLinearPhasePortraits/>



## 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?**

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

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

deviations from the

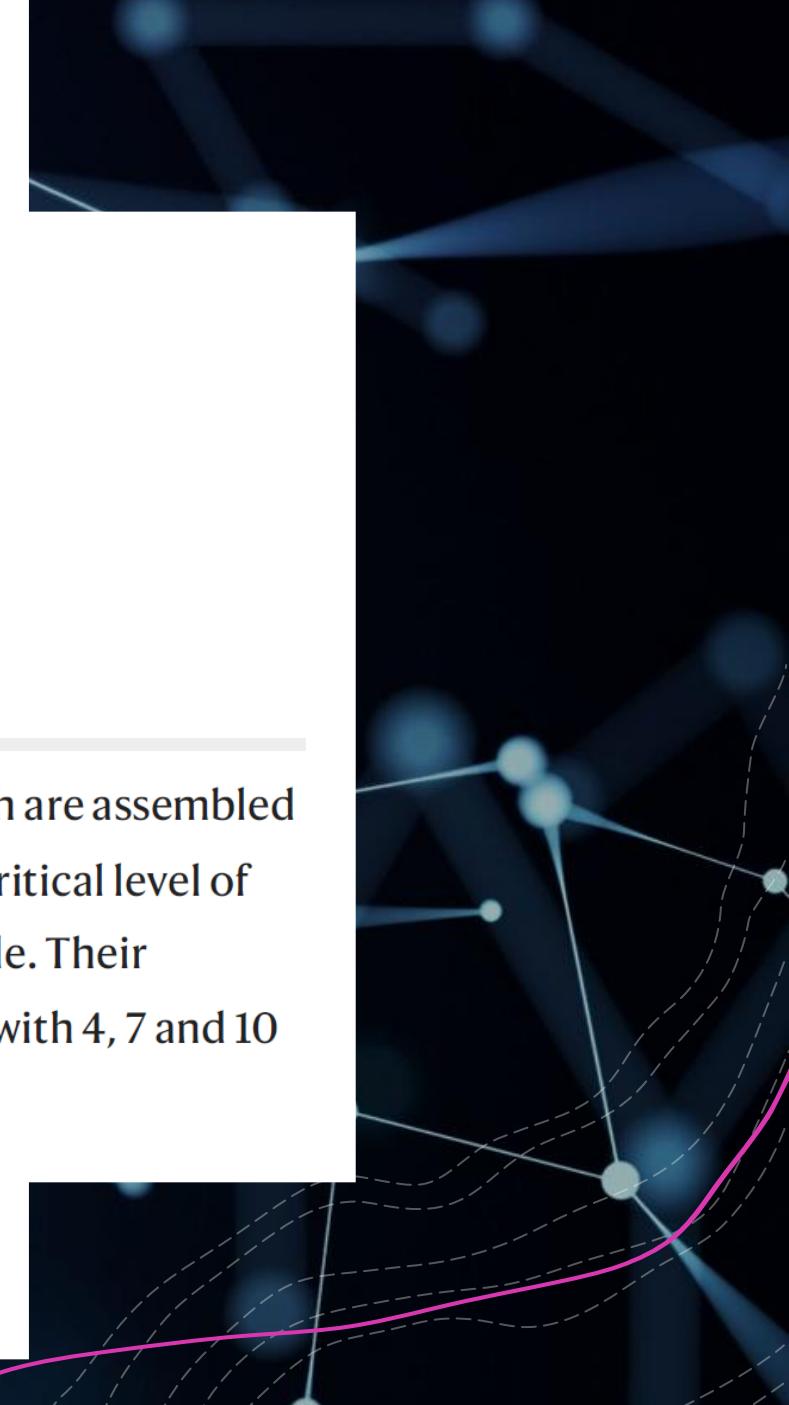
$$3. \tilde{A} \approx -\tilde{I} - \tilde{C}, \text{ where } \tilde{C}$$

mean for each element

### Abstract

The spectrum of the Jacobian matrix of a system of differential equations may be unstable if it contains eigenvalues with positive real parts. Gardner and Ashby<sup>1</sup> have suggested that large complex systems which are assembled of complex eigenvalues (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 Universal density conclusions were based on the trend of computer studies of systems with 4, 7 and 10 "Girko's Law" 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

# Matrix World

in  
Linear Algebra  
for Everyone

Matrix ( $m \times n$ )

1.4  $A = CR$   
row rank = column rank

$A = U\Sigma V^T$  7.1

Matrix Factorization

Appearing section

(in Linear Algebra for Everyone)

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

Square Matrix ( $n \times n$ )

Invertible  $\leftrightarrow$  Singular

$\det(A) \neq 0, \text{all } \lambda \neq 0$  at least one  $\lambda = 0, \det(A) = 0$

4.4  $A = QR$   
Gram-Schmidt

Triangularize  $A = LU$  2.3

$U$  has a zero row

$$A = \begin{bmatrix} 2 & 1 \\ 0 & 2 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix}$$

Diagonalizable

6.2  $A = X\Lambda X^{-1}$  Diagonalize

$A = XJX^{-1}$  A7  
 $J = \text{Jordan form}$

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix}$$

$$J = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

A5 Normal

$A^T A = AA^T$   
diagonalizable by orthogonal matrix

$$A = Q\Lambda Q^T$$

2.4 Symmetric

$S = S^T, \text{all } \lambda \text{ are real}$

Positive Semidefinite

$$S = Q\Lambda Q^T \quad 6.3$$

$$S = \begin{bmatrix} 1 & 2 \\ 2 & 0 \end{bmatrix}$$

Projection

$P^2 = P = P^T, \lambda = 1 \text{ or } 0$

$I$

$O$

Diagonal  $\Sigma = \begin{bmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{bmatrix}$

$$\Lambda = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}$$

Positive Definite 6.3

$\text{all } \lambda > 0$

Orthogonal 4.4

$Q^{-1} = Q^T$   
all  $|\lambda| = 1$

$$Q = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

Permutation 2.4

permutation of  $I$   
all  $\lambda$  are roots of 1

pseudoinverse for all  $A$

$$A^{-1} = V\Sigma^{-1}U^T$$

$$A^+ = V\Sigma^+U^T \quad 3.5, 7.4$$

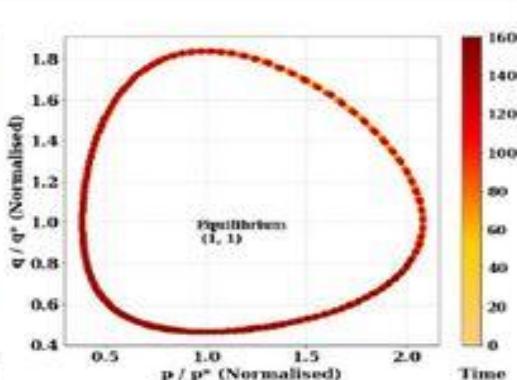
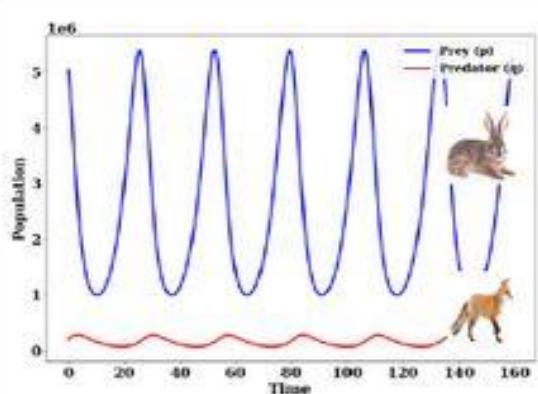
# Module 3 (Solving Differential Equations: numerical techniques)

# 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

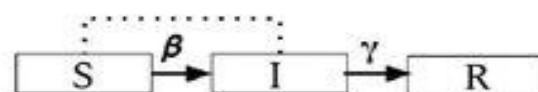
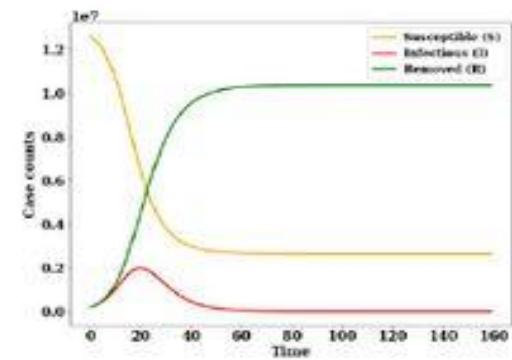
$d$  = Death Rate of Predator

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

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

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

(a) Lotka–Volterra



S = Susceptible

I = Infectious

R = Removed

N = Total population

$\beta$  = Transmission rate

$\gamma$  = Inverse Infectious period

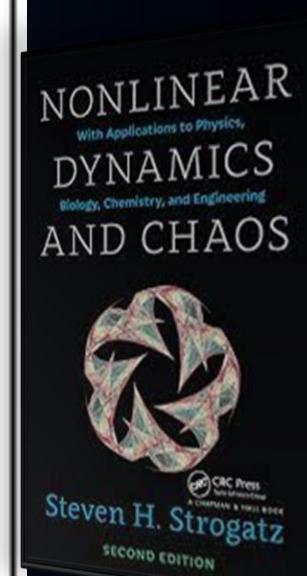
$$\dot{S} = -\frac{\beta SI}{N}$$

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

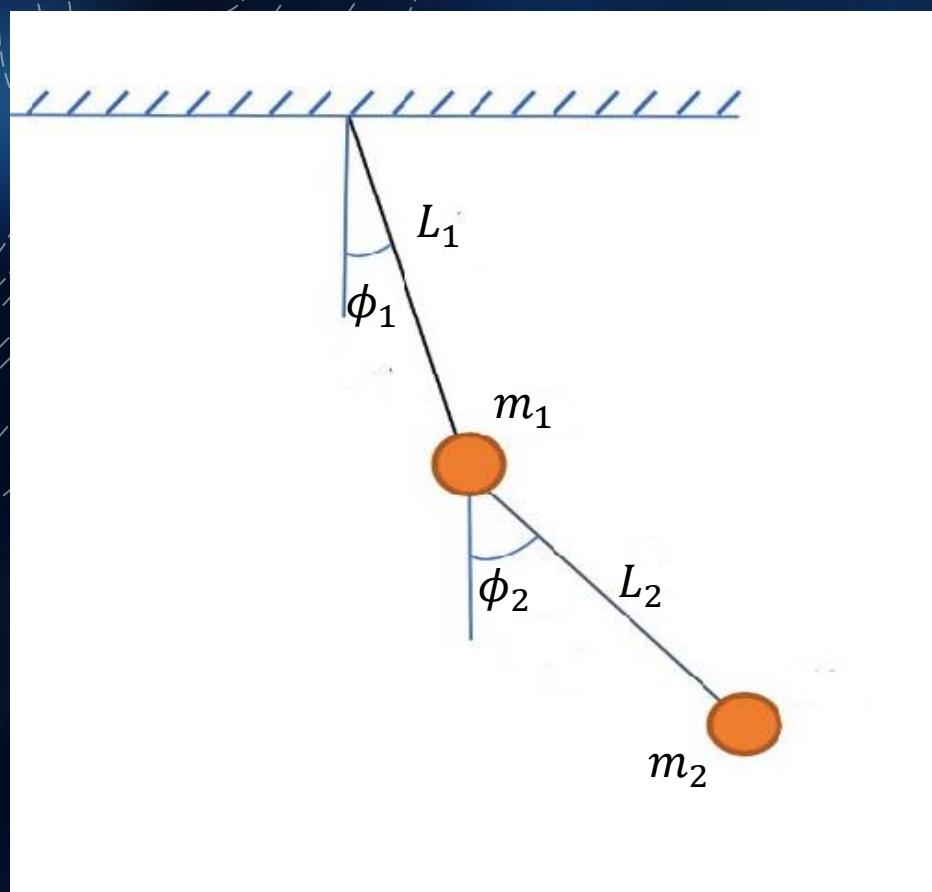
$$\dot{R} = \gamma I$$

$$S + I + R = N$$

(b) SIR (Constant  $\beta$ )

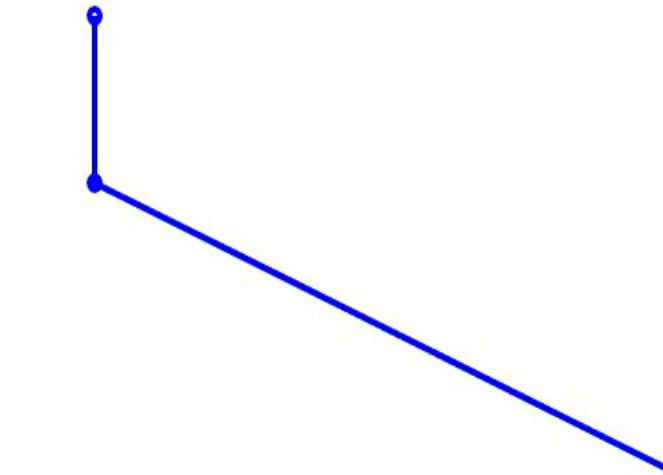


# Double Pendulum

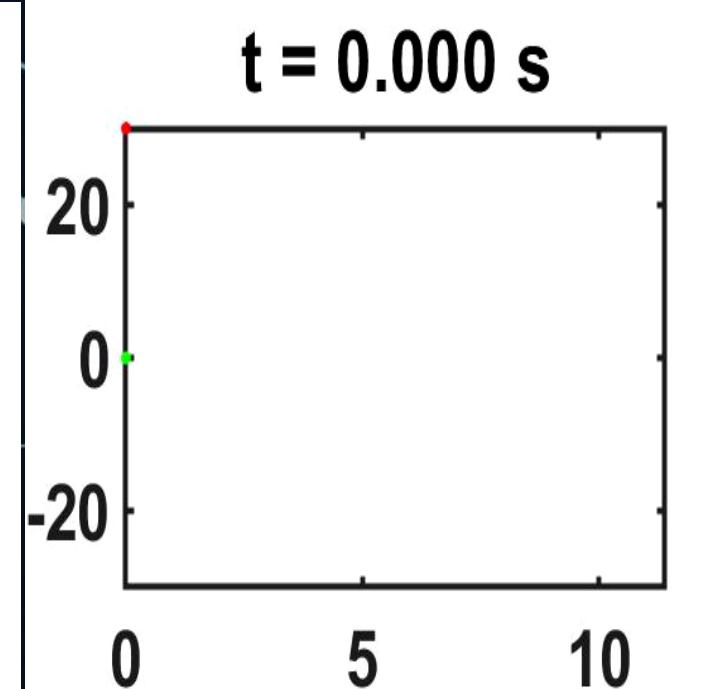


**Module 3: Solving  
Differential Equations**

**$t = 0.000 \text{ s}$**



**$t = 0.000 \text{ s}$**

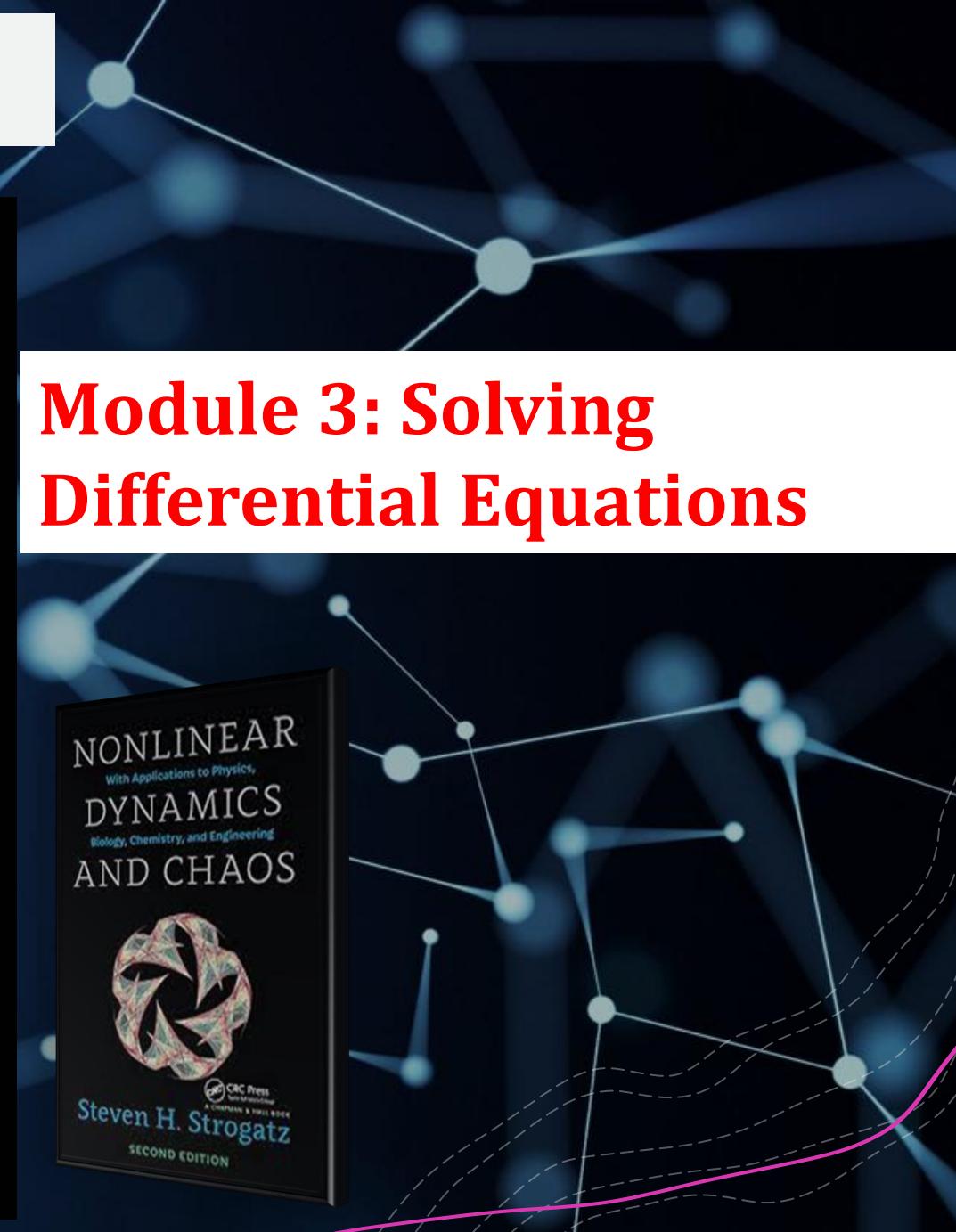


# Chaotic Double Pendulum

$t = 0.000 \text{ s}$



# Lorenz Oscillator



## **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 so differential equations
- Modelling and chaos in physics





# **Module 4**

## **(Monte Carlo Method and its application)**

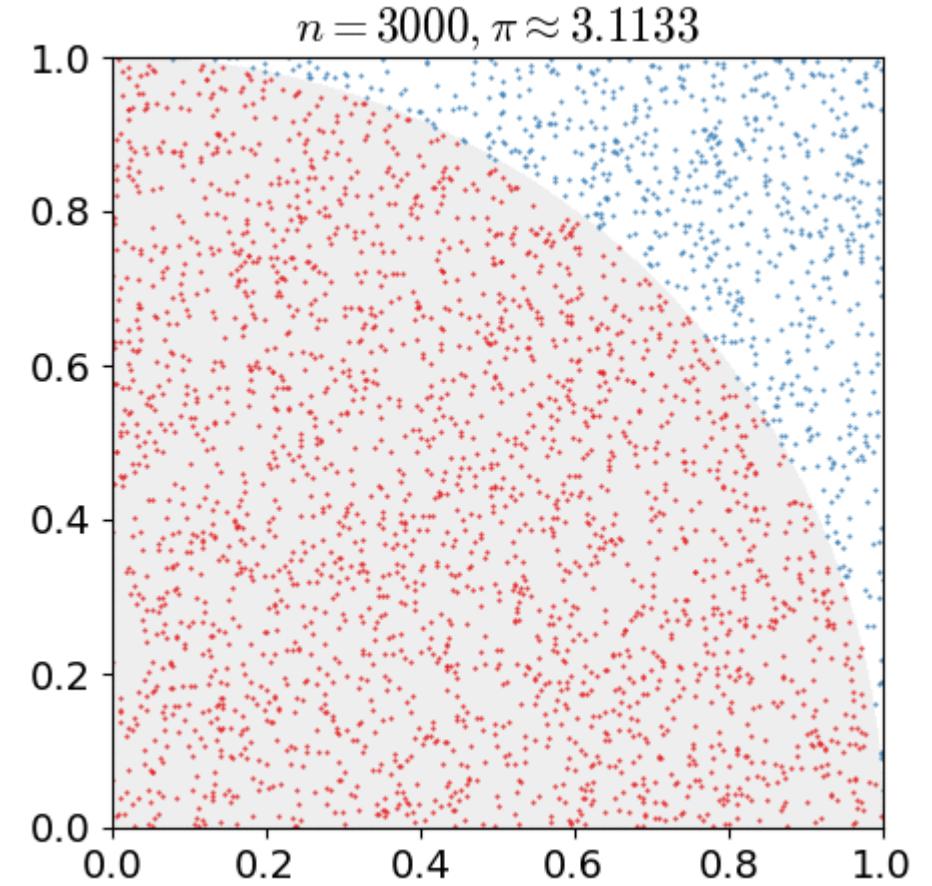
When you hear the words “Monte Carlo”, most people envision this



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**

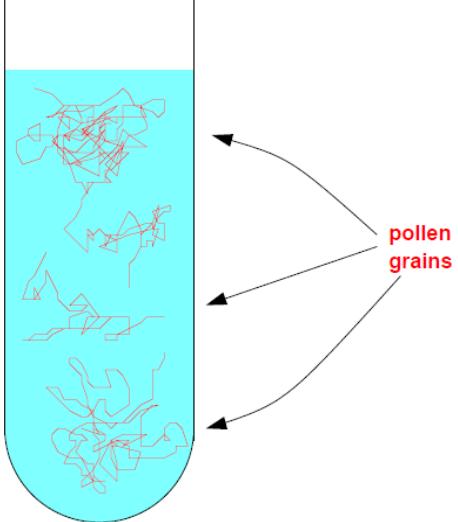
# Overall Targets

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

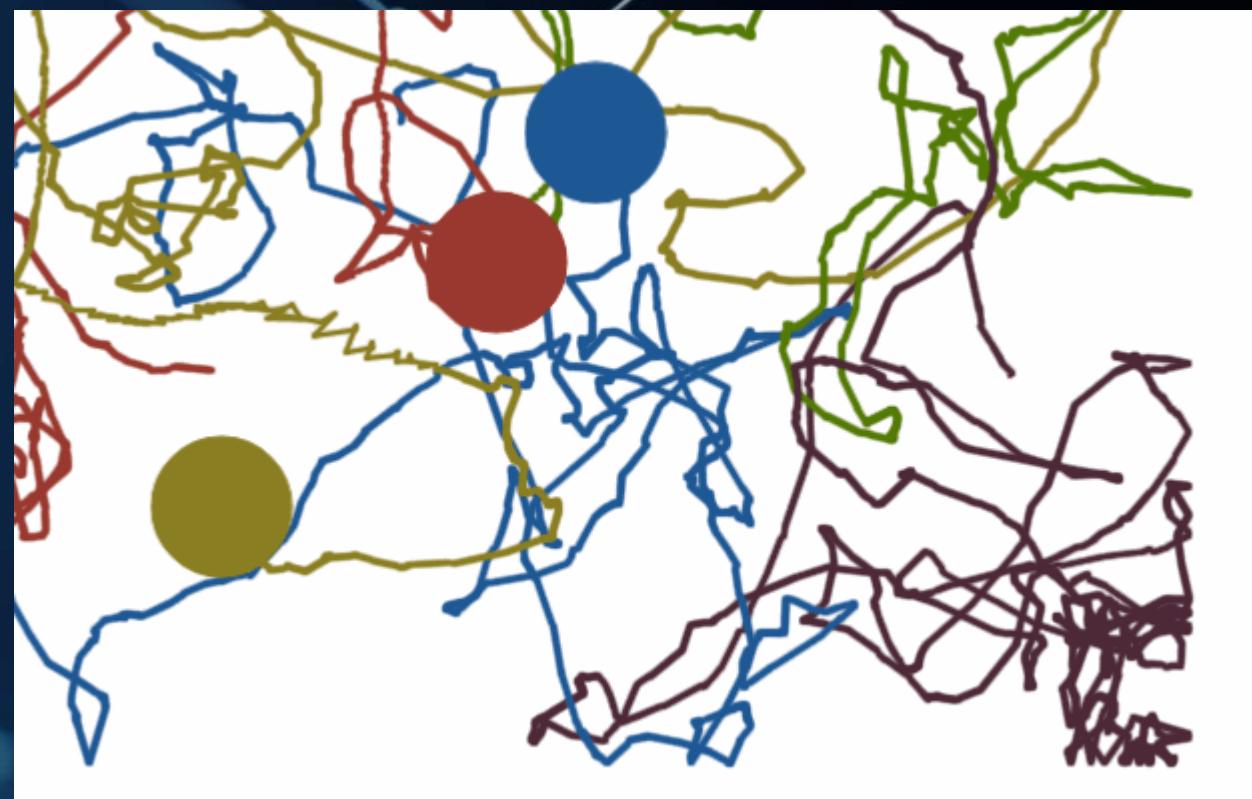


# Module 5

## (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

© 2001 Society for Industrial and Applied Mathematics

## 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†



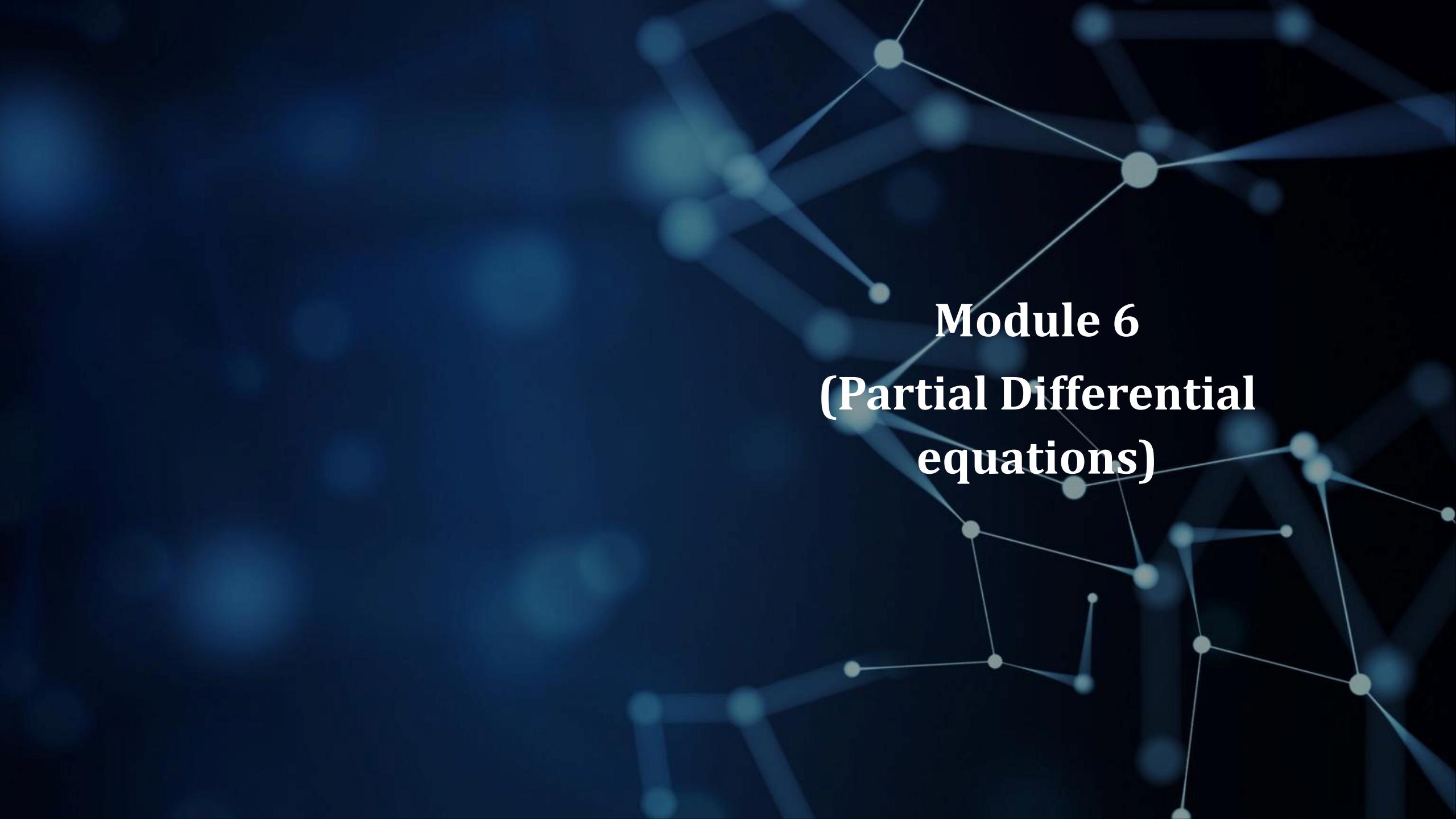
# Module 5 (Stochastic Differential Equations)

## **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

A dark blue background featuring a complex network of glowing blue nodes and connecting lines, creating a sense of data flow and connectivity.

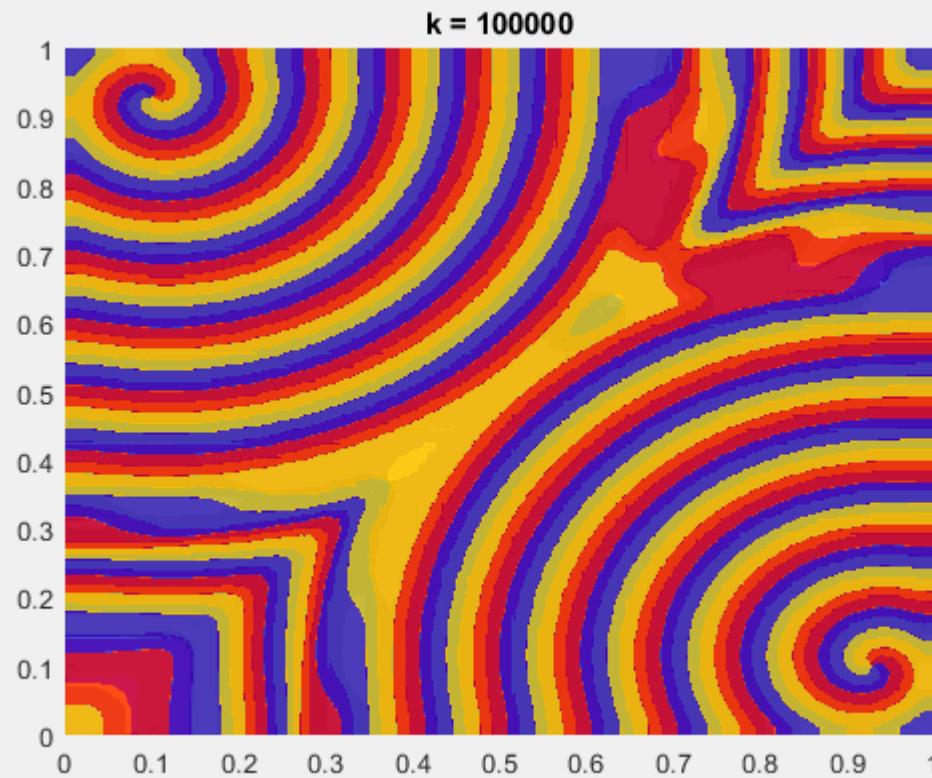
# Module 6

## (Partial Differential equations)

# *How the leopard gets its spots*

Alan Turing and the math behind biological development

By Albert Liu | Oct. 28, 2020

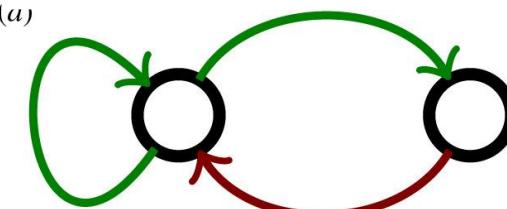


## Module 6 (Partial Differential equations)

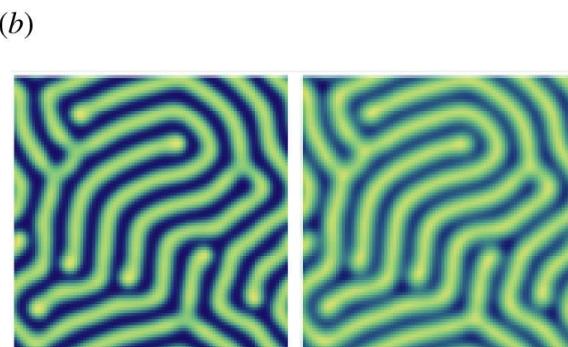
# How the leopard gets its spots

Alan Turing and the math behind biological development

By Albert Liu | Oct. 28, 2020



Gierer–Meinhardt model



(d)



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TRANSACTIONS A

[royalsocietypublishing.org/journal/rsta](https://royalsocietypublishing.org/journal/rsta)



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. Vittadello<sup>1</sup>, Thomas Leyshon<sup>3</sup>, David Schnoerr<sup>3</sup> and Michael P. H. Stumpf<sup>1,2</sup>

<sup>1</sup>School of BioSciences, and <sup>2</sup>School of Mathematics and Statistics, University of Melbourne, Melbourne, Victoria 3010, Australia

<sup>3</sup>Department of Life Sciences, Imperial College London, London, UK

STV, 0000-0002-4476-6732; MPH, 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>

## 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	

10<sup>th</sup> January: 2 to 2:45 pm (group A)  
10<sup>th</sup> 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).



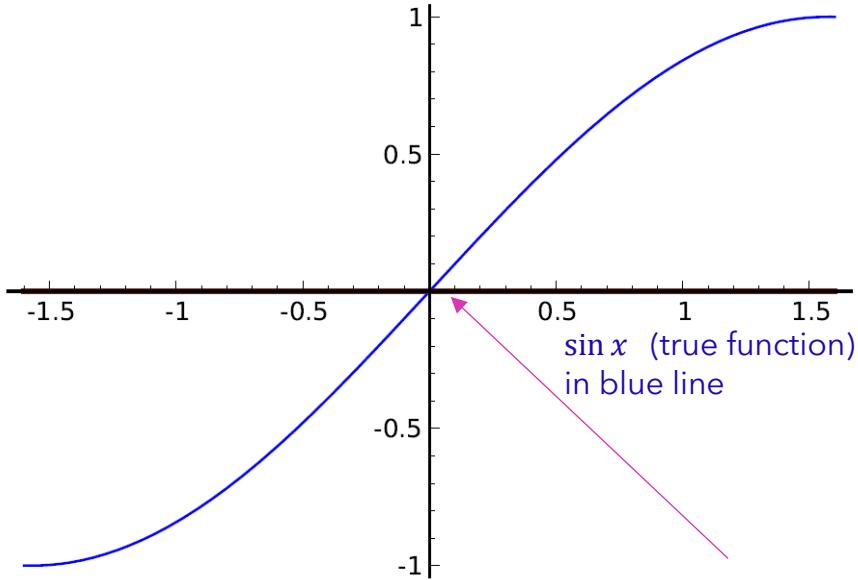
## Ninja techniques For Sleeping In Class

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

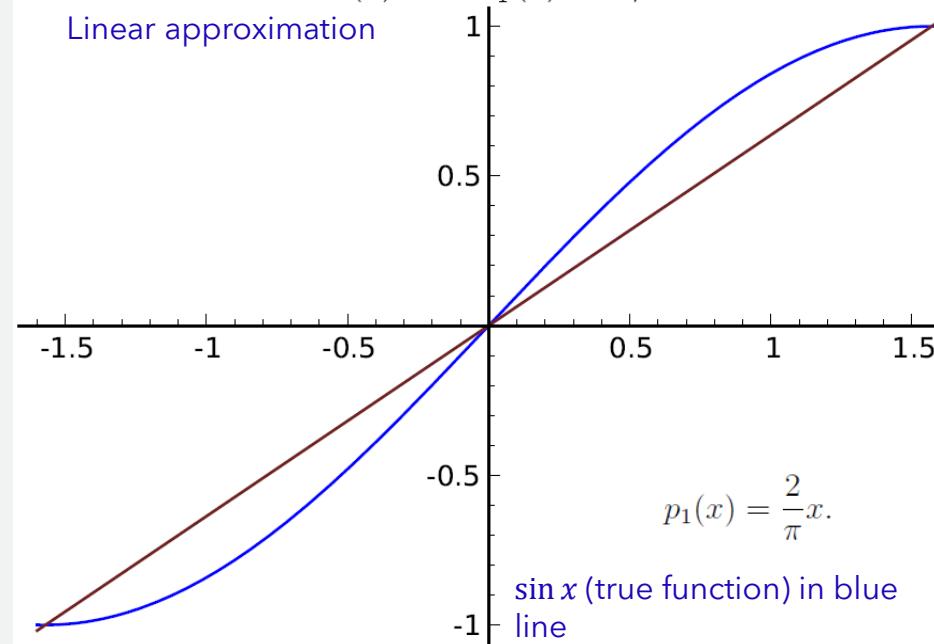


# Sinx as Polynomial

$\sin(x)$  and  $p_0(x) = 0$



Linear approximation



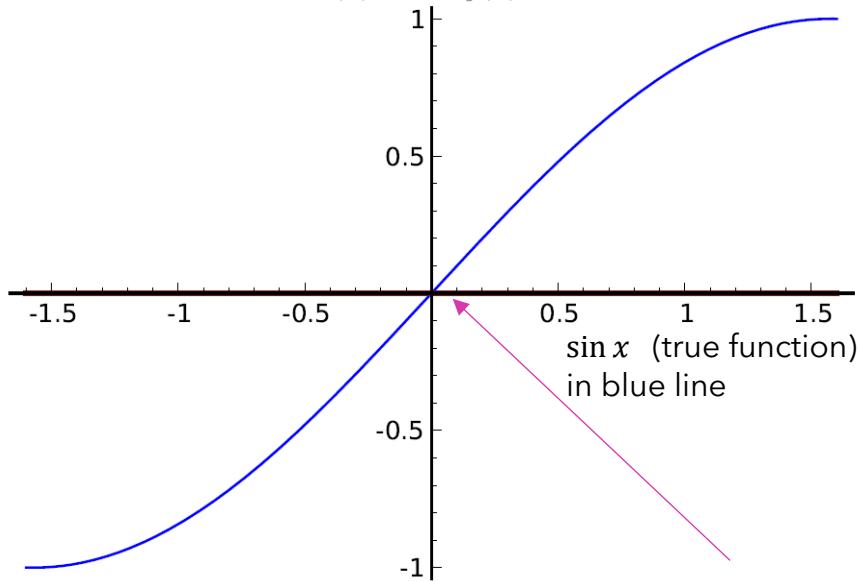
$$p_1(x) = \frac{2}{\pi}x$$

$\sin x$  (true function) in blue  
line

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

# Sinx as Polynomial

$\sin(x)$  and  $p_0(x) = 0$



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

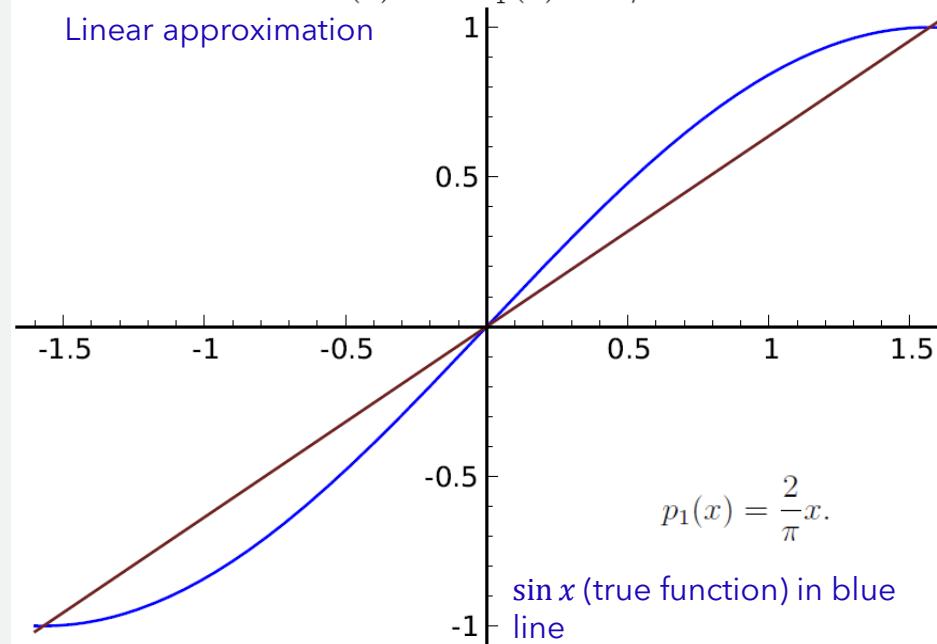
Take  $a = \pi$

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

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

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

Linear approximation

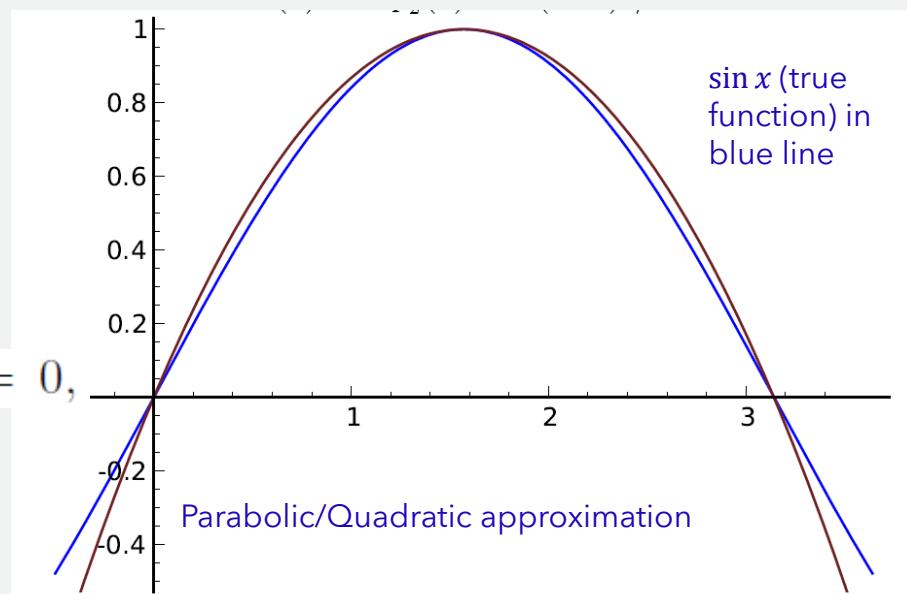


$$p_1(x) = \frac{2}{\pi}x.$$

$\sin x$  (true function) in blue line

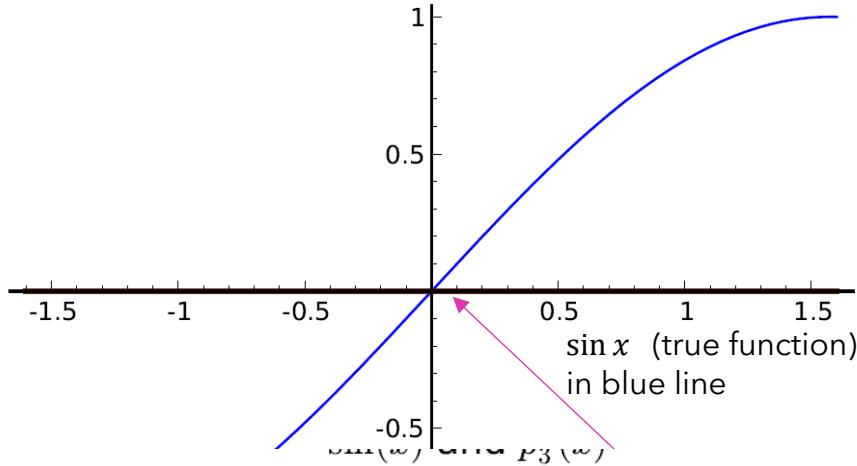
$\sin x$  (true function) in blue line

Parabolic/Quadratic approximation

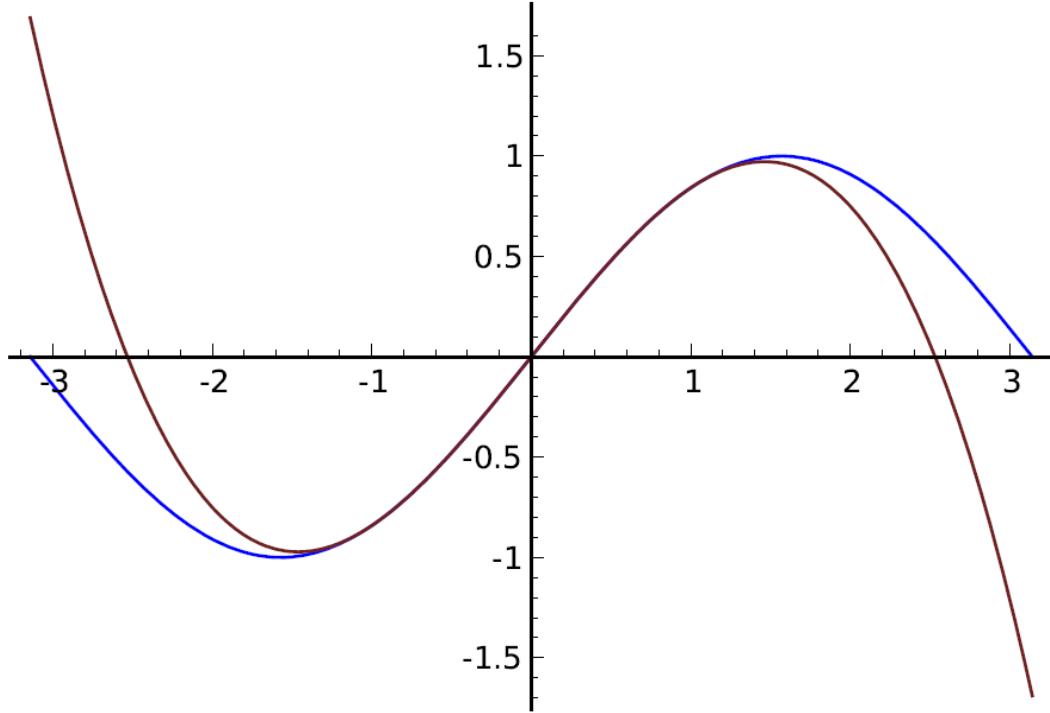


# Sinx as Polynomial

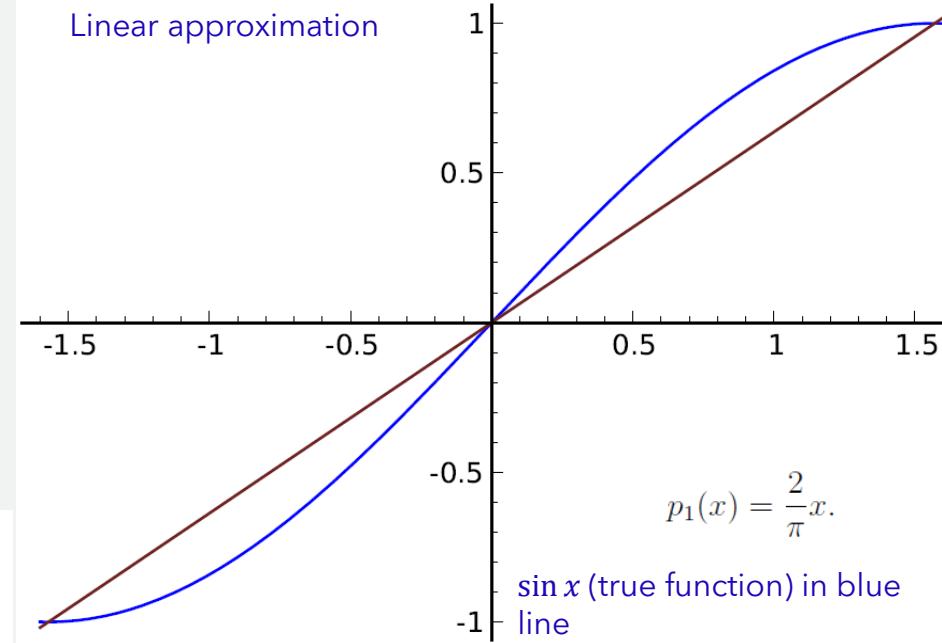
$\sin(x)$  and  $p_0(x) = 0$



$p_3(x)$



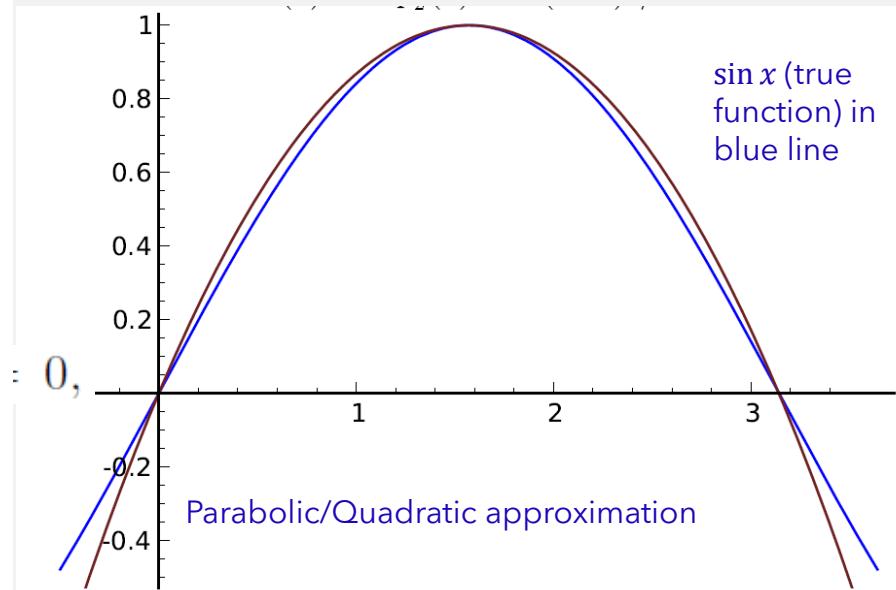
Linear approximation



$$p_1(x) = \frac{2}{\pi}x$$

$\sin x$  (true function)  
line

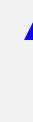
$\sin x$  (true  
function) in  
blue line



Parabolic/Quadratic approximation

# 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 Taylor 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

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

# Numerical techniques

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

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

```
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);
```

