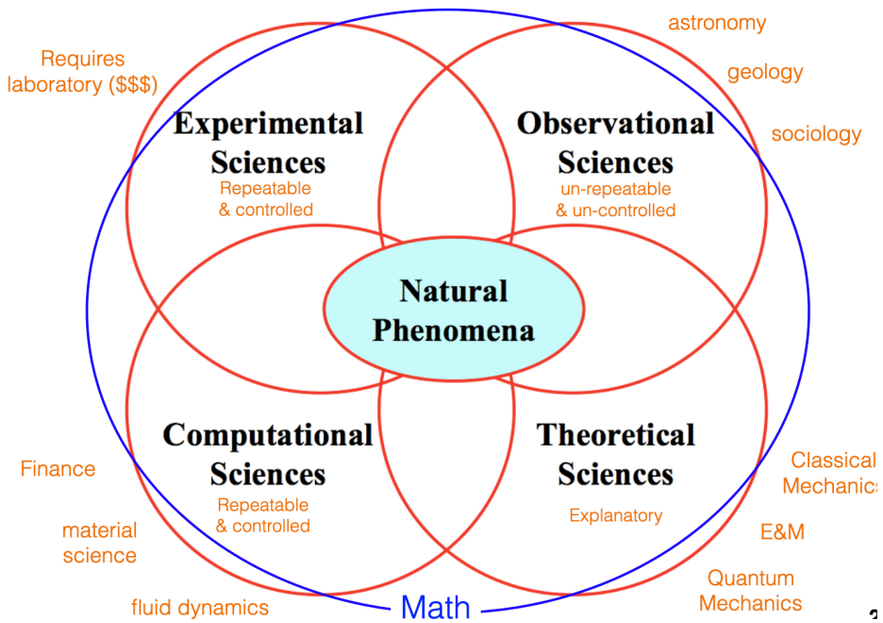
MODELING

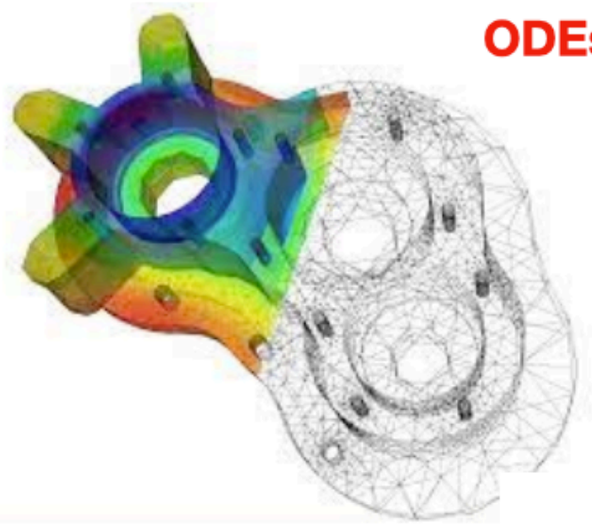
Topics

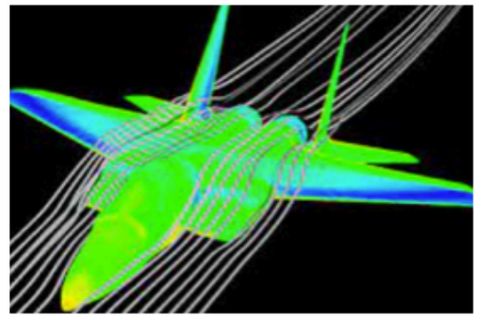
Mathematical Modeling



Differential modeling

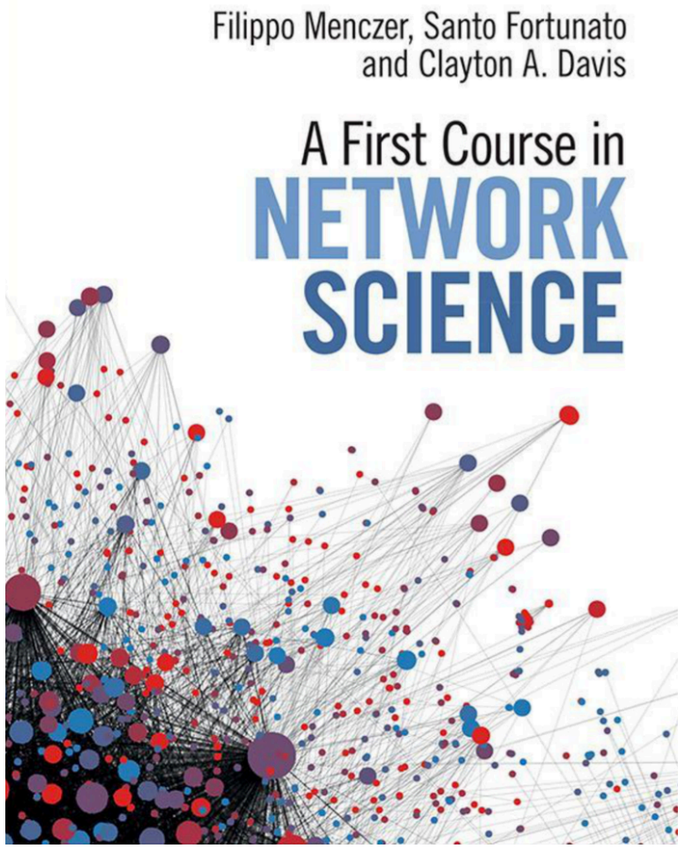
ODEs and PDEs





$$\mathbf{F} = m\mathbf{a} = m\frac{d\mathbf{r}}{dt}$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$



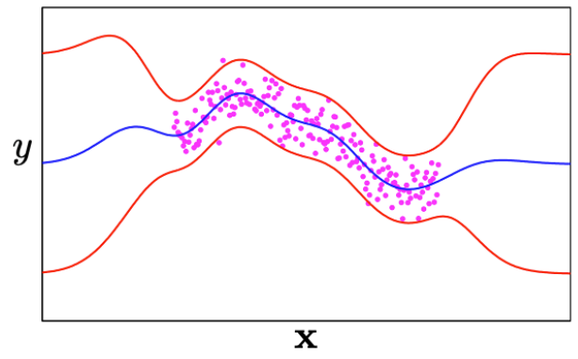
5 Network Models

- 5.1 Random Networks
- 5.2 Small Worlds
- 5.3 Configuration Model
- 5.4 Preferential Attachment
- 5.5 Other Preferential Models
- 5.6 Summary

Model categories

Non-Parametric

Gaussian processes
Gaussian process classifiers
Dirichlet process mixtures
infinite HMMs
infinite latent factor models



Other Frameworks

- Particle modeling
- Monte Carlo methods
- Cellular automaton
- Reinforcement simulations
- Network modeling

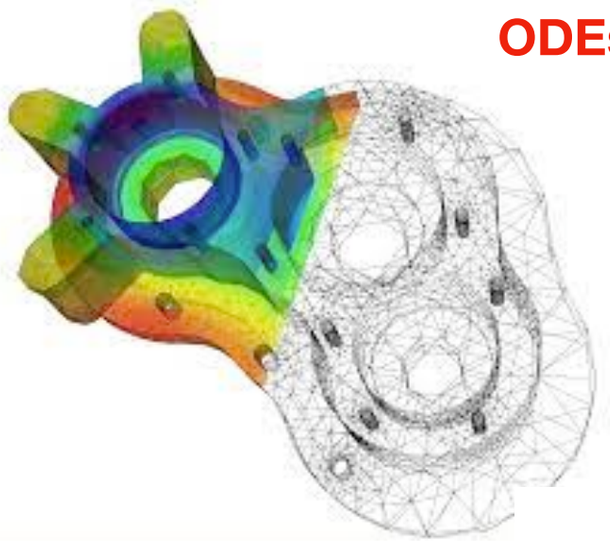
Mathematical Modeling

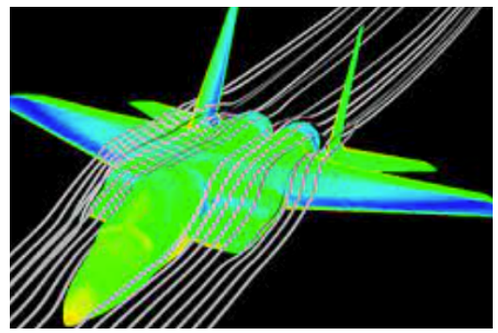
Parametric

polynomial regression
logistic regression
mixture models, k-means
hidden Markov models
factor analysis / pPCA / PMF
linear regression
Artificial neural networks

Differential modeling

ODEs and PDEs





$$\mathbf{F} = m\mathbf{a} = m\frac{d\mathbf{r}}{dt}$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

http://mlss.tuebingen.mpg.de/2015/slides/ghahramani/gp-neural-nets15.pdf
https://en.wikipedia.org/wiki/Mathematical_model

Complexity: data vs models

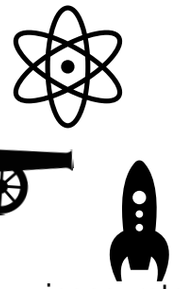
- **Less variables**
- **Few assumptions**
- **Reliable models**

Complexity

Fundamental physics

$$\mathbf{F} = m\mathbf{a} = m\frac{d\mathbf{r}}{dt}$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$



noise —> inaccurate sensors

When you find a problem or improvement with the models you might get a Noble Prize



Applied physics
Engineering
Chemistry

Nature, Biology ,Genetics

Social phenomena
Economics
Stock market prediction

Toolset is always
Mathematics

- **many variables**
- **More assumptions**
- **complex phenomena**
- **hard to determine generating function**
- **larger difference between reality and models**

Models match ground truth almost perfectly:

- Excellent qualitative and quantitative agreement between data and models (Little or no error between)
- Models provide explanatory power to why things are happening
- Very accurate predictions for both extrapolation and interpolation

Models typically match ground truth well:

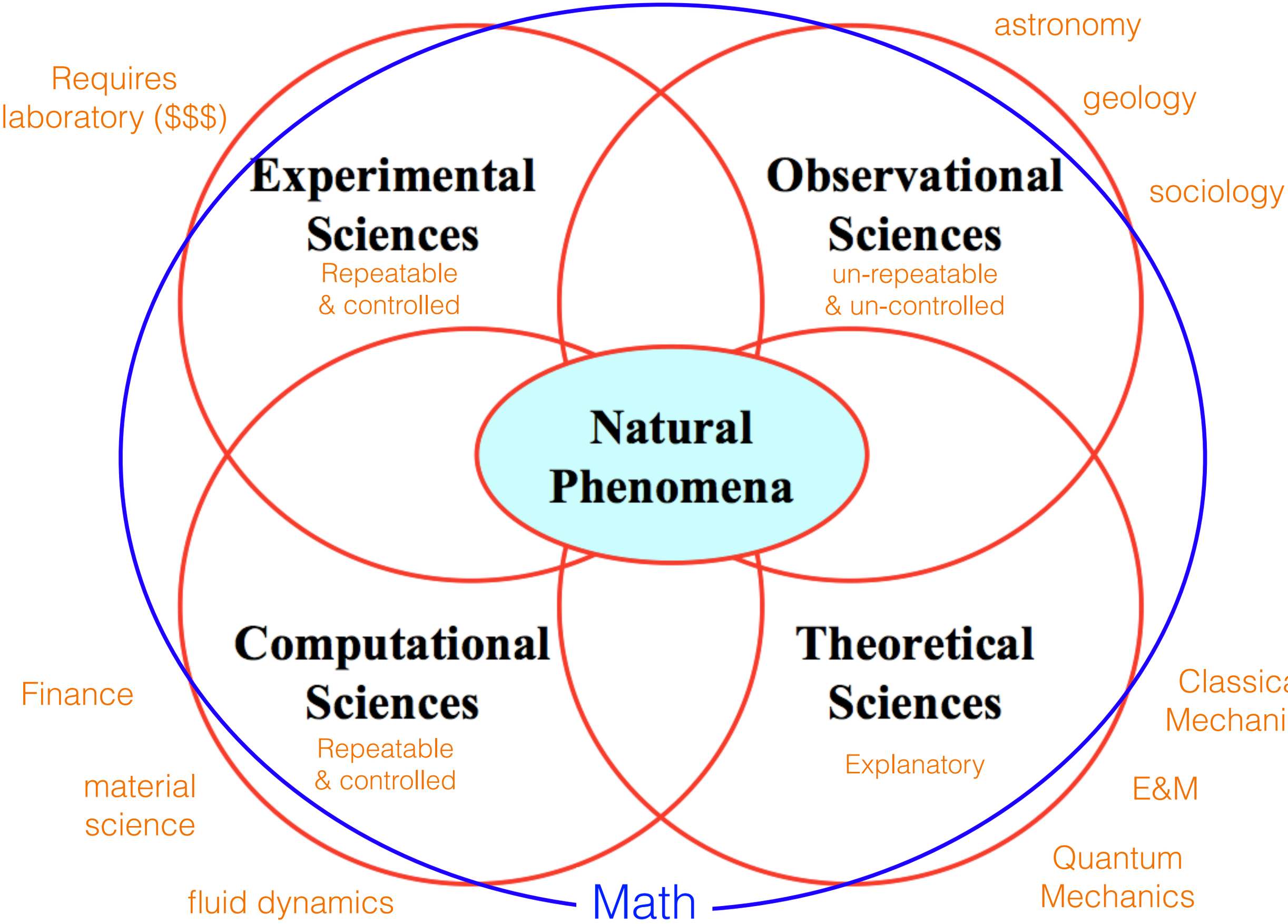
- Reasonable qualitative and quantitative agreement between data and models
- More assumptions
- Acceptable level of error between model and data
- Phenomena maybe too complex to perfectly capture all effects however primary effects are captured
- Decent predictions for both extrapolation and interpolation

Data starts to get extremely complex: unclear whether a given model will capture the ground truth behavior or not

- May have qualitative or some quantitative agreement between data and models
- Possibly high level of error between model and data
- Likely many “hidden” or un-accounted for variables
- Phenomena almost certainly too complex to perfectly capture all effects/contributions
- Likely have acceptable interpolation but extrapolation is a wild card

“All models are wrong, but some are useful”
~ George E. P. Box

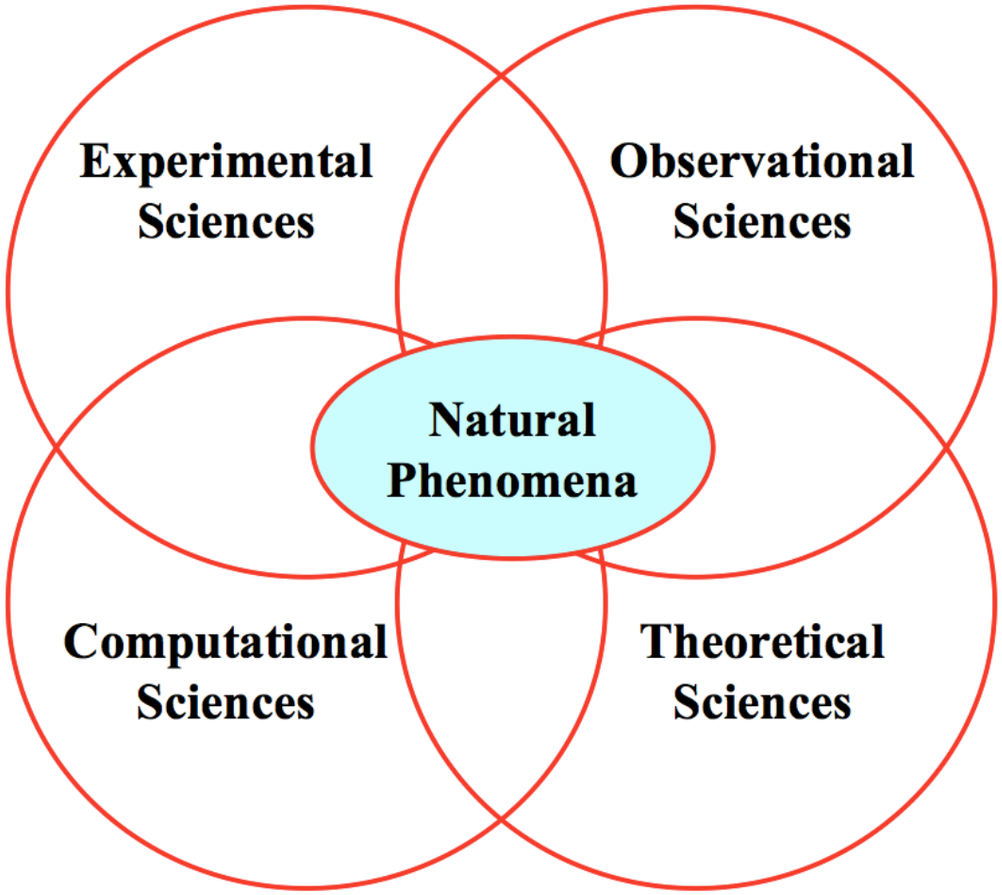
Science categories



Methodologies

Experimental sciences

- Instrumentation
- Physical experimentation
- Testing of theories



Observational sciences

- Instrumentation
- Hypothesis formulation
- Testing of theories

Computational sciences

- Methodology development
- Computational experimentatior
- Correlation with experiments
- Testing of theories (hypothesis,

Theoretical sciences

- Abstract science development
- Modeling physical phenomena
- Correlation with experiments

Tools

- Modeling and Simulation
- Numerical Methods
- Data Analysis
- Databases / Data mining
- Visualization
- High Performance Computing

Disciplines

Traditional Computational Sciences

Computational Physics
- Molecular dynamics
- Particle physics
- Material science

Computational Biology
- Drug design
- Protein folding
- Cellular signaling pathways
- Genome analysis

Computational Astrophysics
- Galactic collisions
- Solar physics
- Cosmology

Computational Mathematics
- Computational geometry
- Computational topology

Multi-disciplinary computational sciences

Computational climate dynamics
- Fluid mechanics, radiation transport, ecology, geography, image analysis, …

Computational social sciences
- Economics, psychology, …

Computational medicine
- Biomechanics, anatomy, physiology, cell biology, image analysis, …

Computational blast dynamics
- Fluid mechanics, structural dynamics, fracture mechanics, optimization techniques, databases, …

Modeling vs simulation

Modeling

- A model tries to reproduce the salient features of a system
- The objective of modeling is not to produce an exact copy of the system
- Since models are based on approximations, it is understood that models are imperfect representations of the system
- Models are valid only in some regimes and conditions and are always imprecise by a certain amount
- Models can be mathematical, experimental, computational, statistical, …

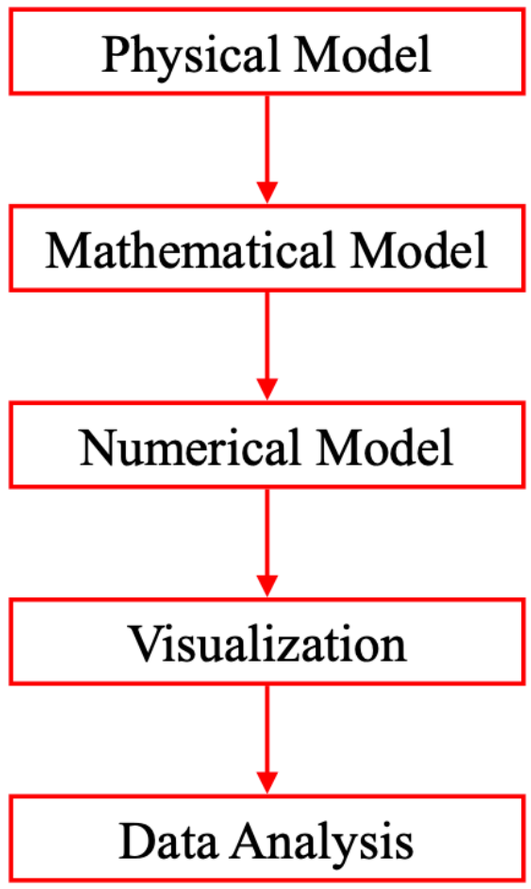
Simulation

- Attempts to imitate the dynamic behavior of a system and to predict or calculate subsequent events
- A simulation realizes a model for a particular choice of physical parameters, object geometry, initial and boundary conditions

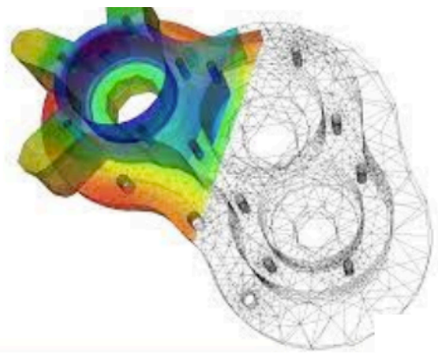
Model Classification

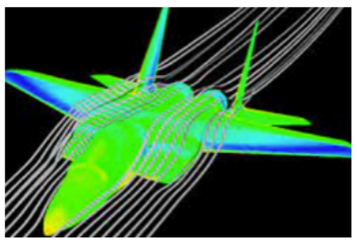
- Deterministic or Stochastic
- Dynamic or Steady
- Continuous or Discrete

Modeling Process



DIFFERENTIAL MODELING





$$\mathbf{F} = m\mathbf{a} = m\frac{d\mathbf{r}}{dt}$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

Instead of fitting models to data (regression). We instead use fundamental knowledge about how the phenomena changes (i.e. ordinary differential equations ODE) and where the system started (initial conditions) to predict the progression of the system (ODE solutions)

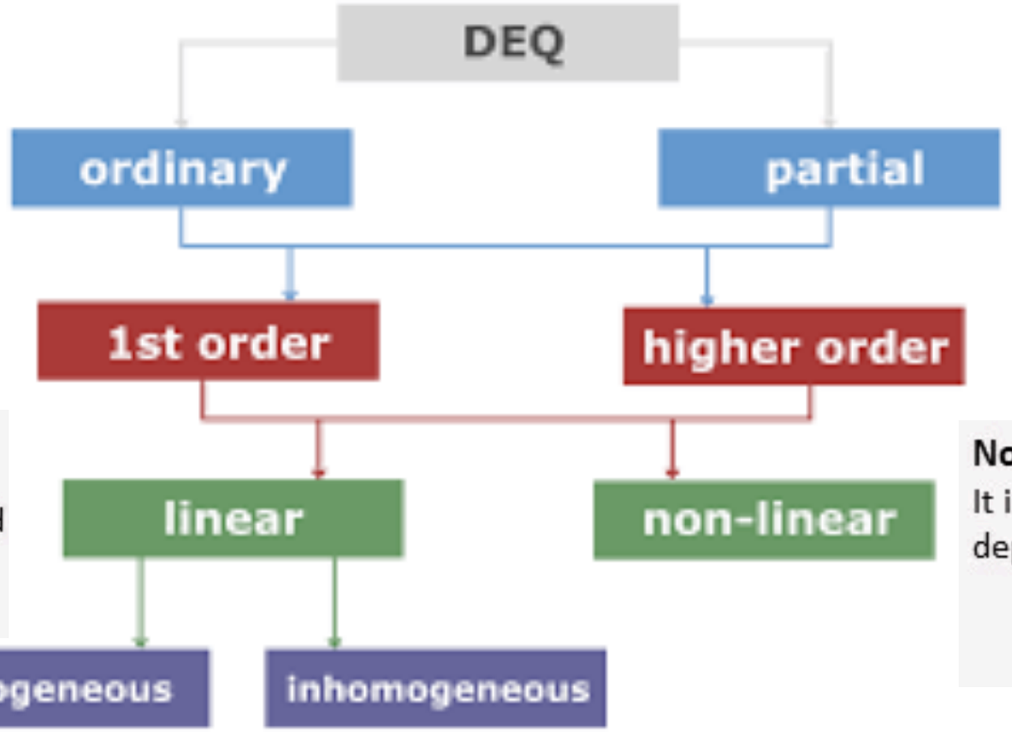
Overview

Classifications

Ordinary Differential Equation

It is a differential equation that involves one or more ordinary derivatives but without having partial derivatives.

$$m\frac{d^2x}{dt^2} = f(x)$$



Partial Differential Equation

Partial differential equation is a differential equation that involves partial derivatives. It has two or more independent variables.

$$\frac{\partial^2 u}{\partial x^2} + 4xy\frac{\partial^2 u}{\partial y^2} + u = 2\left(\frac{\partial^2 u}{\partial x^2}\right)^2 + 4\frac{\partial^3 u}{\partial x \partial y^2} = 10x$$

Linear Differential Equation

It is first degree with respect to the dependent variable(s) and its derivatives that can be expressed in the form

$$\frac{dy}{dx} + p(x)y = q(x)$$

Non-Linear Differential Equation

It is second degree or higher with respect to dependent variables and its derivatives.

$$\frac{d^2y}{dx^2} - \left(\frac{dy}{dx}\right)^2 + 12y = \cos x$$

Homogeneous Differential Equation

It is first order differential equation which can be in written as,

$$y'' + f(x)y' + g(x)y = 0$$

Non-homogeneous Differential Equation

It is a differential equation whose right-hand side is not equal to zero. A 2nd order non-homogeneous equation can be written in this form.

$$y'' + f(x)y' + g(x)y = r(x)$$

Initial & Boundary conditions:

Initial Value Problem

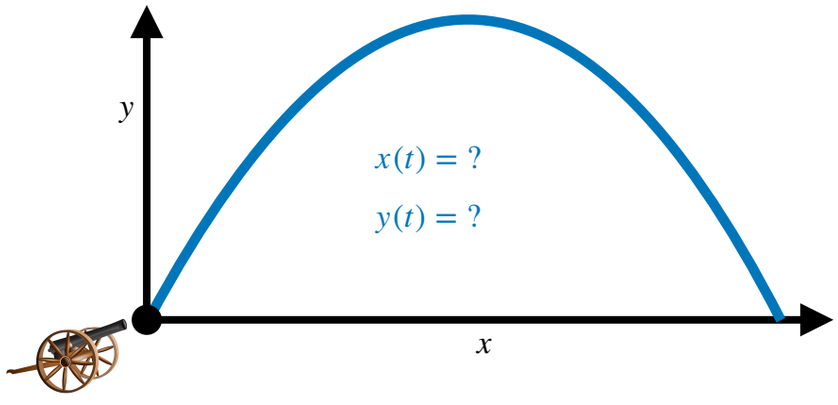
Initial Value

$y(t=0) = y_0$

$y'(t=0) = y_0'$

There is only one unique solution.

Note: Both y and y' are evaluated at the at the same time/point.



Boundary Value Problem

Boundary Value

$y(t=0) = y_0$

$y(t=c) = y_1$

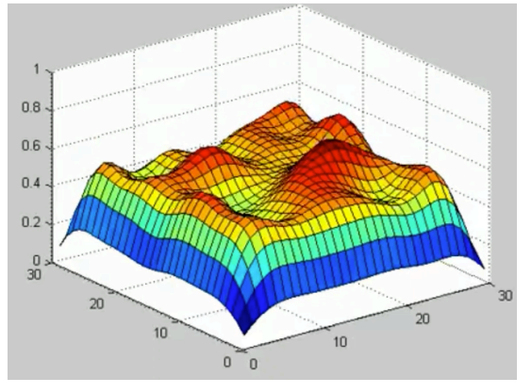
or

$y'(t=0) = y_0'$

$y'(t=c) = y_1'$

There are many possible solutions.

Note: They are evaluated at different point of time.

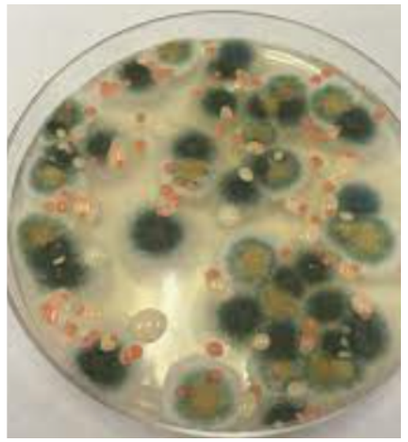


Example-1

Exponential growth-decay

Model:

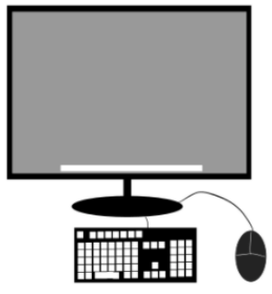
$$\frac{dx}{dt} = kx \qquad x(t) = ?$$



$x(t) =$ number of bateria cells

Solve:





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

$$\frac{dx}{x} = k\,dt$$

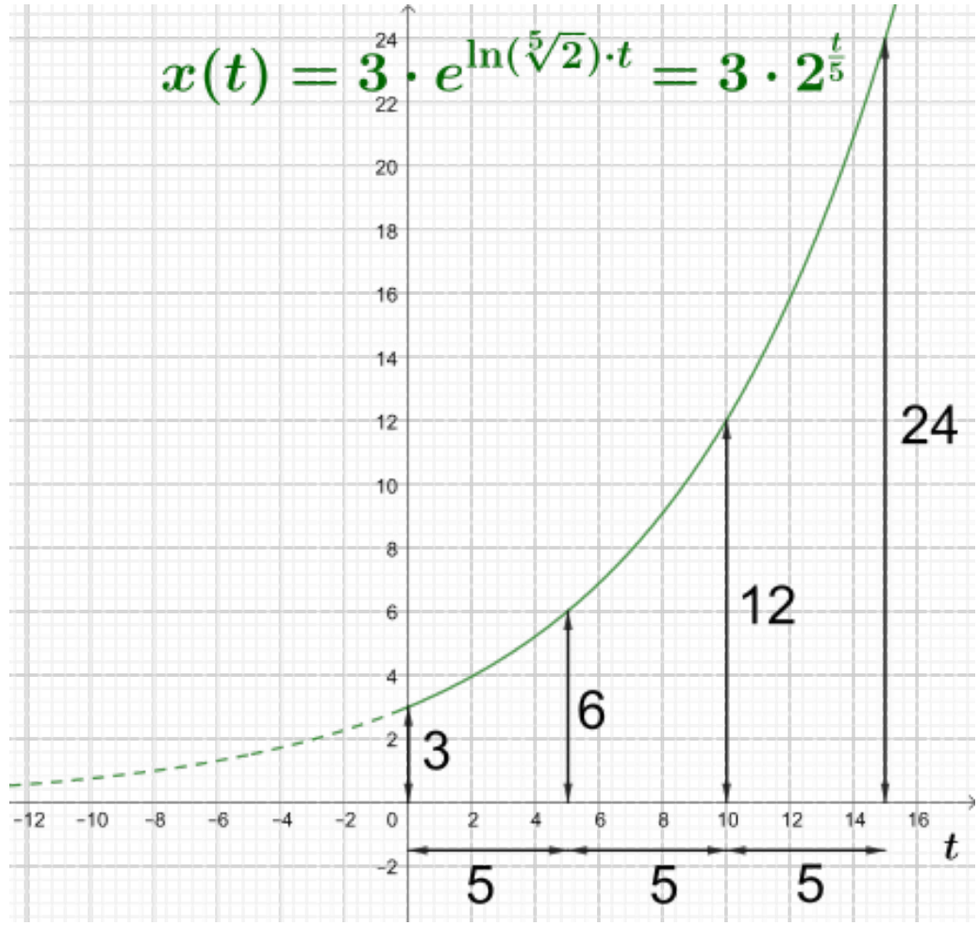
$$\int_{x_0}^{x(t)} \frac{dx}{x} = k\int_0^t dt$$

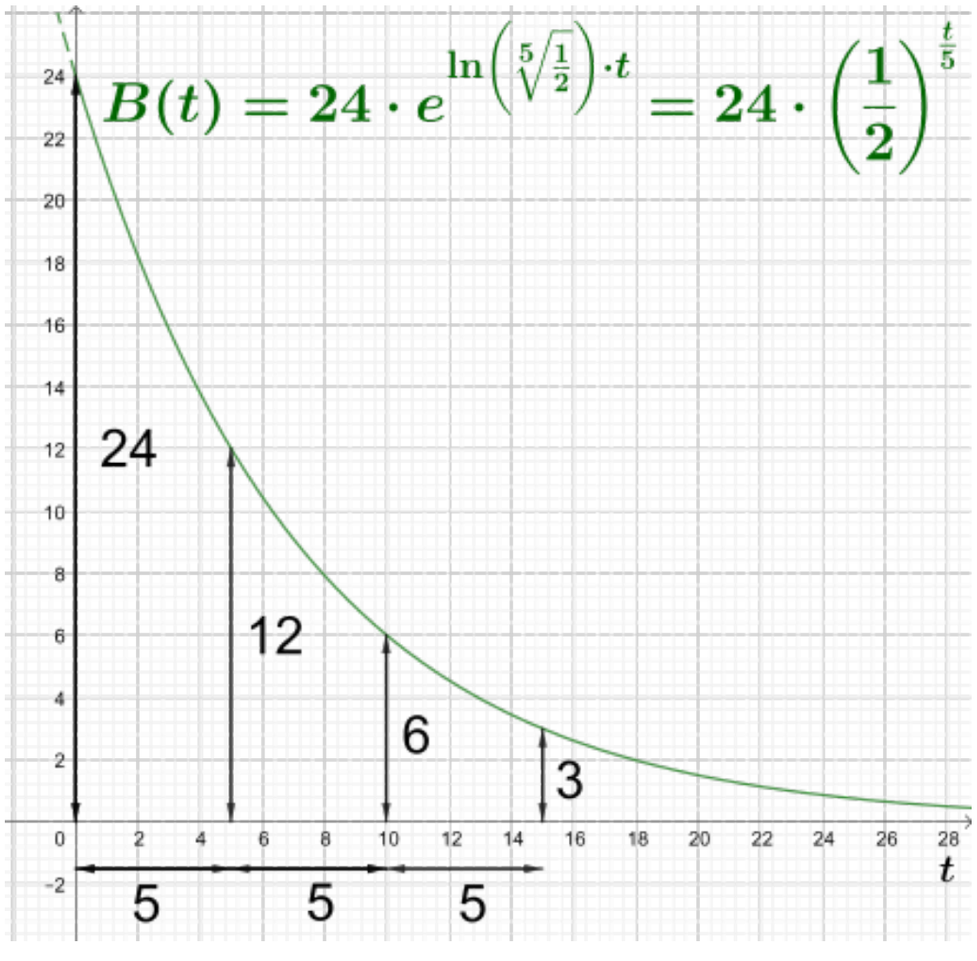
$$\ln\frac{x(t)}{x_0} = kt\,.$$

Solution: $x(t) = x_0 e^{kt} = x_0 e^{\frac{t}{\tau}}$

$k < 0$, then the quantity experiences exponential decay.

PREDICTIVE POWER





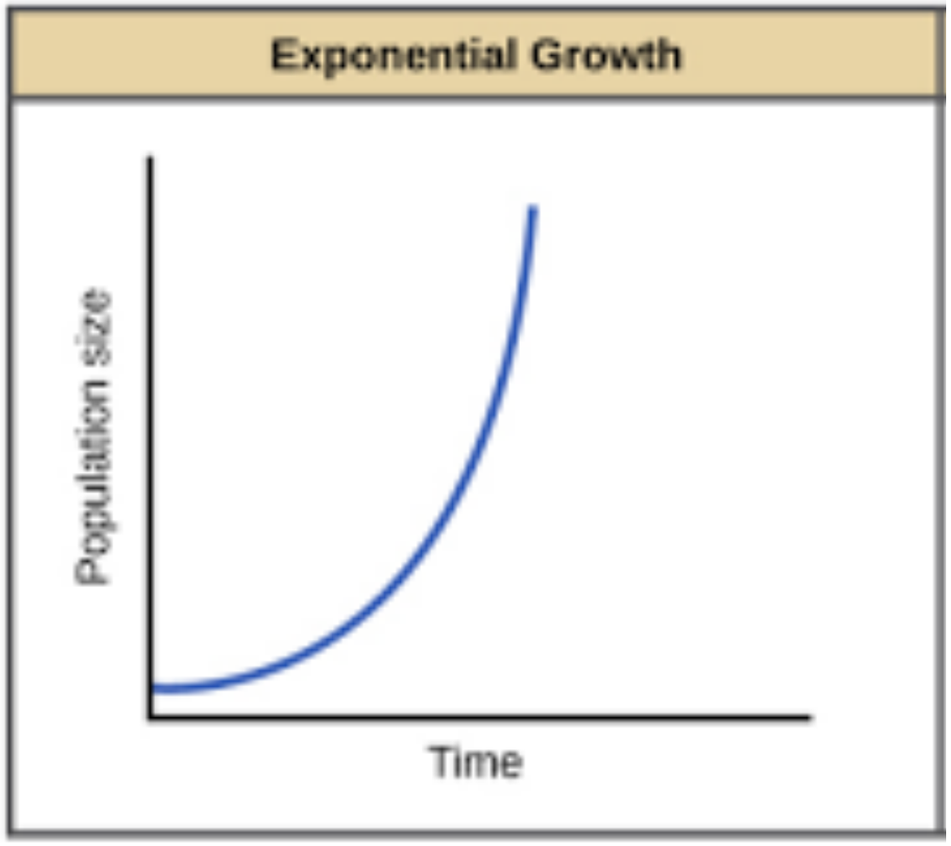
Example-2

Logistic growth

$$\frac{d}{dx}f(x) = f(x)\big(1 - f(x)\big)$$

$$f(x) = \frac{e^x}{e^x + 1} = \frac{1}{1 + e^{-x}}.$$

$$\frac{df(x)}{dx} = \frac{k}{a}f(x)\big(a - f(x)\big), \quad f(0) = a/(1 + e^{kr})$$

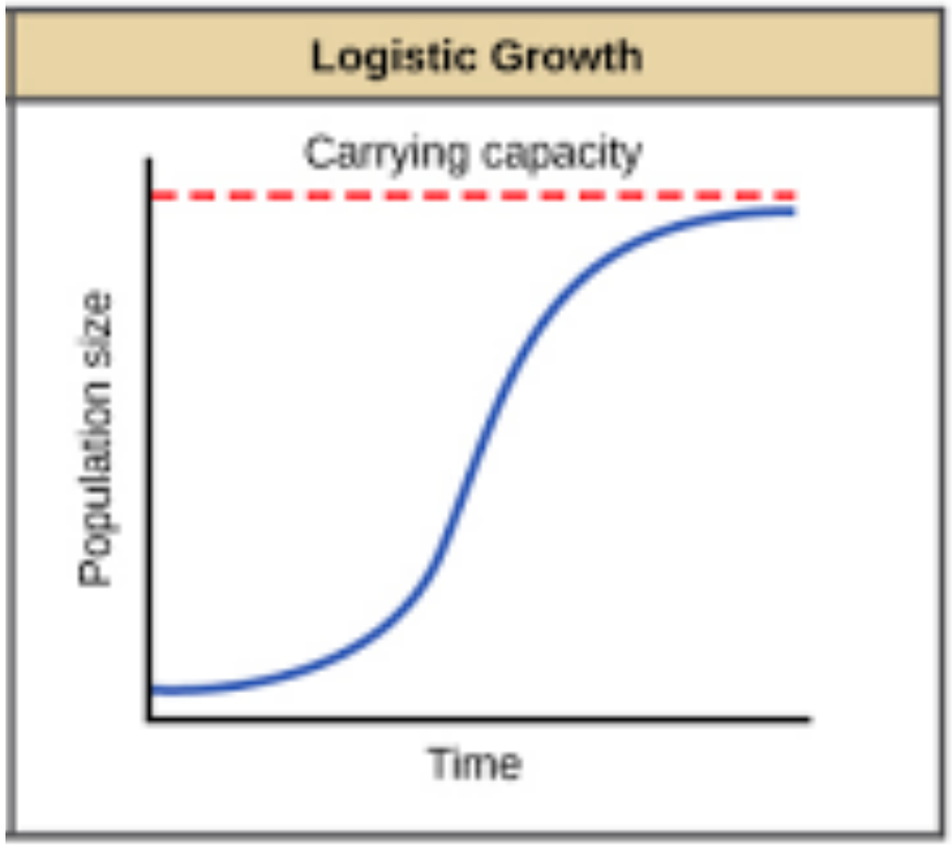


modeling population growth

$$\frac{dP}{dt} = rP\left(1 - \frac{P}{K}\right),$$

r defines the growth rate and K is the carrying capacity.

$$P(t) = \frac{KP_0e^{rt}}{K + P_0\,(e^{rt} - 1)} = \frac{K}{1 + \left(\frac{K - P_0}{P_0}\right)e^{-rt}},$$



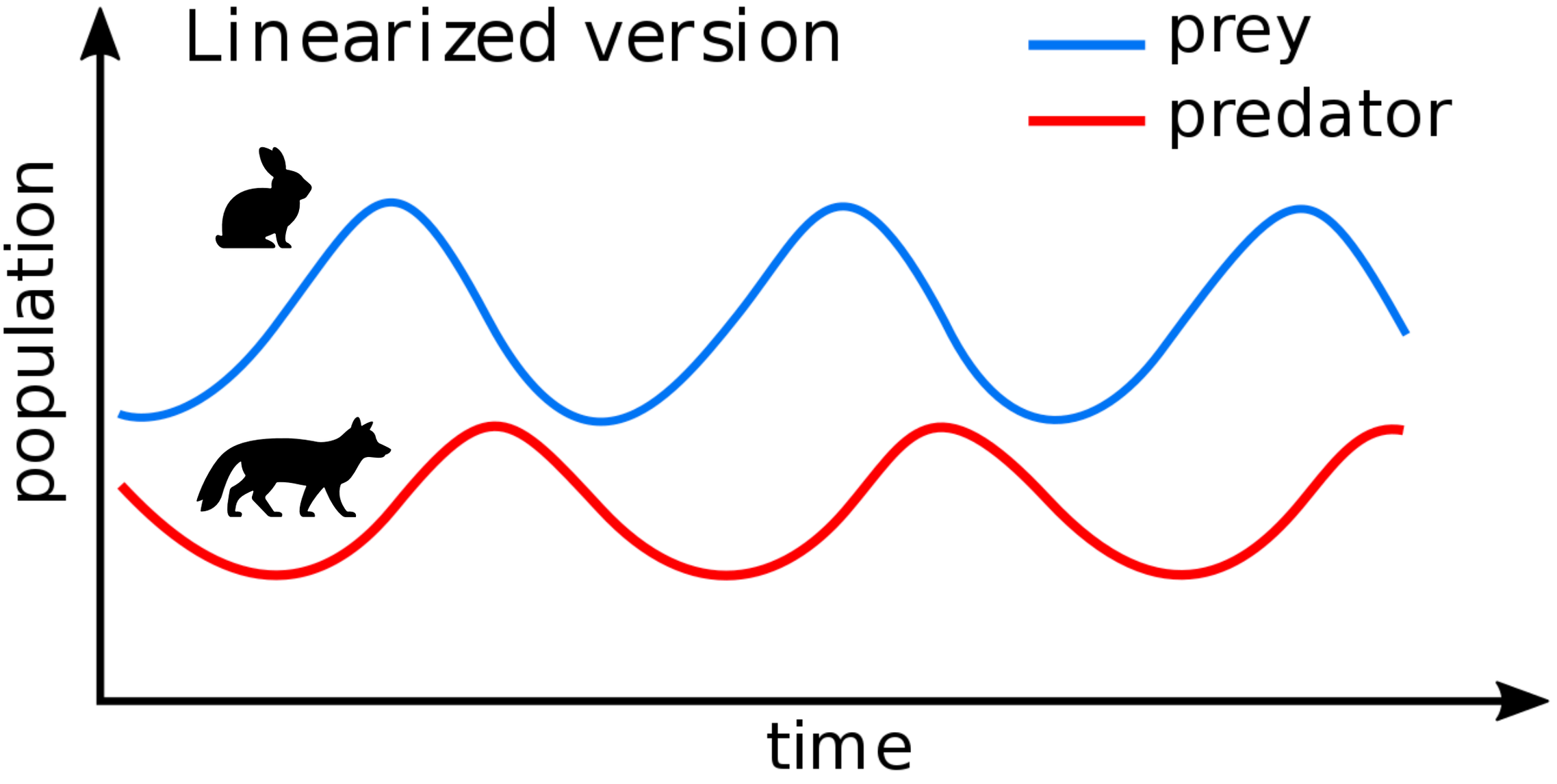
Good resource: http://faculty.sfasu.edu/judsontw/ode/html-20180819/systems01.html

Example-3

$$\frac{dx}{dt} = \alpha x - \beta xy,$$

$$\frac{dy}{dt} = \delta xy - \gamma y,$$

- x is the number of prey (for example, rabbits);
- y is the number of some predator (for example, foxes);
- $\frac{dy}{dt}$ and $\frac{dx}{dt}$ represent the instantaneous growth rates of the two populations;
- t represents time;
- $\alpha, \beta, \gamma, \delta$ are positive real parameters describing the interaction of the two species.



Example-4

Projectile motion

Model: System of ODEs

$$F_x = ma_x = m\frac{d^2x}{dt^2} = 0$$

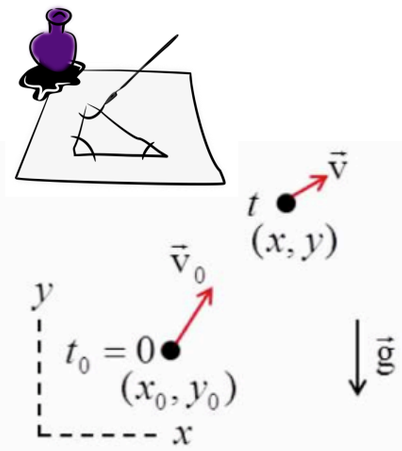
$$F_y = ma_y = m\frac{d^2y}{dt^2} = -mg$$

Initial conditions: $\mathbf{r}_0 = (x_0, y_0)$

$\mathbf{v}_0 = (v_0^x, v_0^y)$

solve → **integrate**

Analytic Solution



$$\int_{v_{x0}}^{v_x} dv_x = \int_0^t (0)dt \qquad \int_{v_{y0}}^{v_y} dv_y = \int_0^t g\, dt = g\int_0^t dt$$

$$v_x\Big|_{v_{x0}}^{v_x} = 0 \qquad v_y\Big|_{v_{y0}}^{v_y} = g\,t\Big|_0^t$$

$$v_x - v_{x0} = 0 \qquad v_y - v_{y0} = g\,(t-0)$$

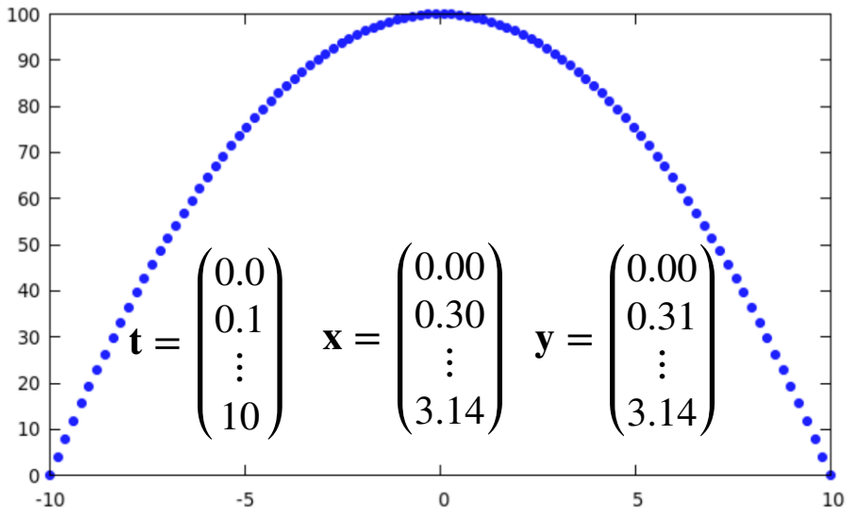
$$\boxed{v_x = v_{x0}} \qquad \boxed{v_y = v_{y0} + g\,t} \quad \text{if } g = -9.81 \text{ m/s}^2$$

$$v_y = v_{y0} - g\,t \quad \text{if } g = +9.81 \text{ m/s}^2$$

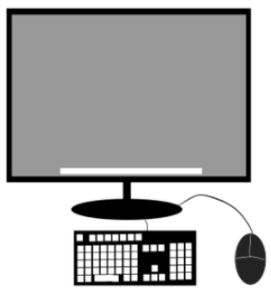
California State Polytechnic University, Pomona

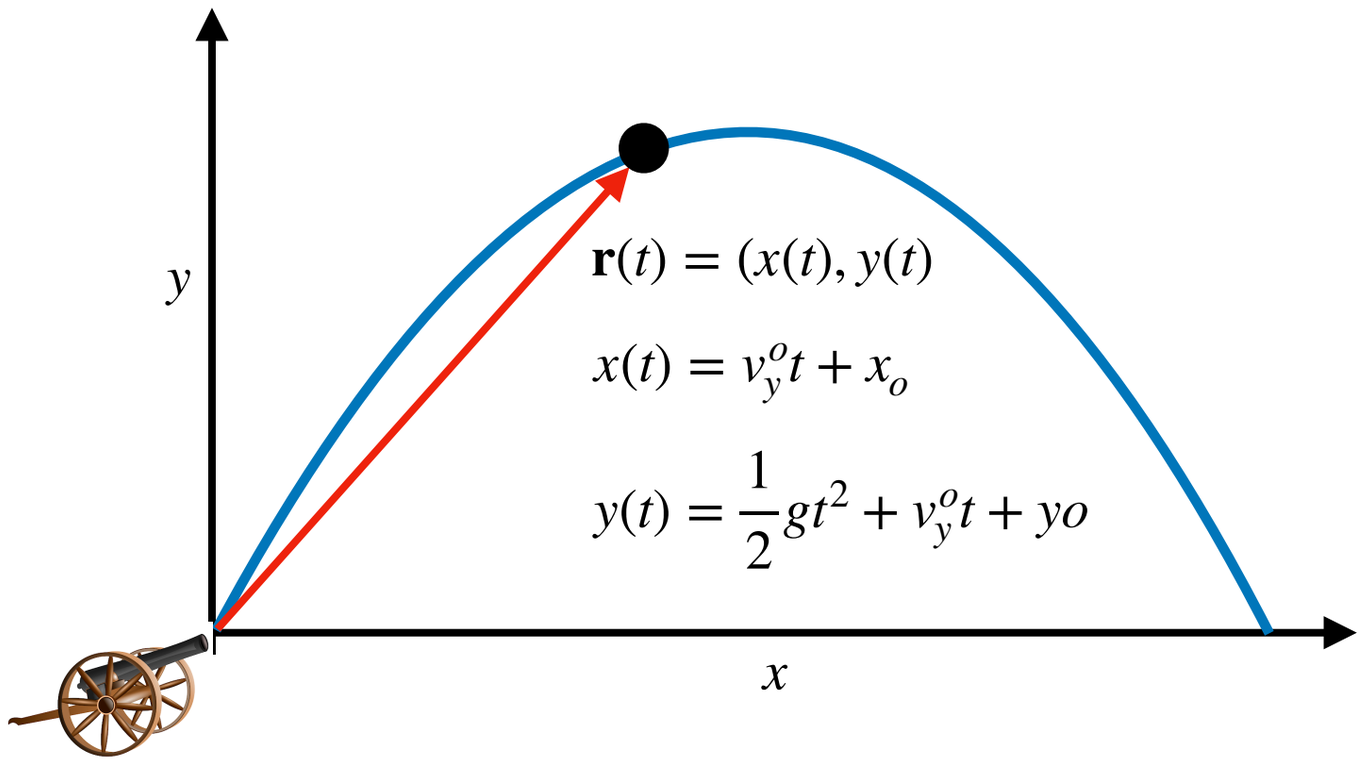
Numerical solution

e.g. Euler's method



$$\mathbf{t} = \begin{pmatrix} 0.0 \\ 0.1 \\ \vdots \\ 10 \end{pmatrix} \quad \mathbf{x} = \begin{pmatrix} 0.00 \\ 0.30 \\ \vdots \\ 3.14 \end{pmatrix} \quad \mathbf{y} = \begin{pmatrix} 0.00 \\ 0.31 \\ \vdots \\ 3.14 \end{pmatrix}$$



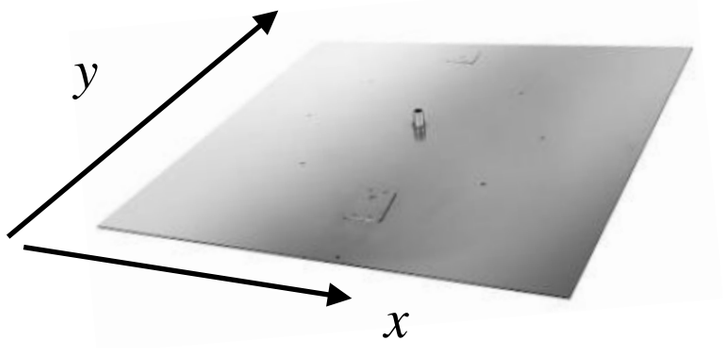


Example-5

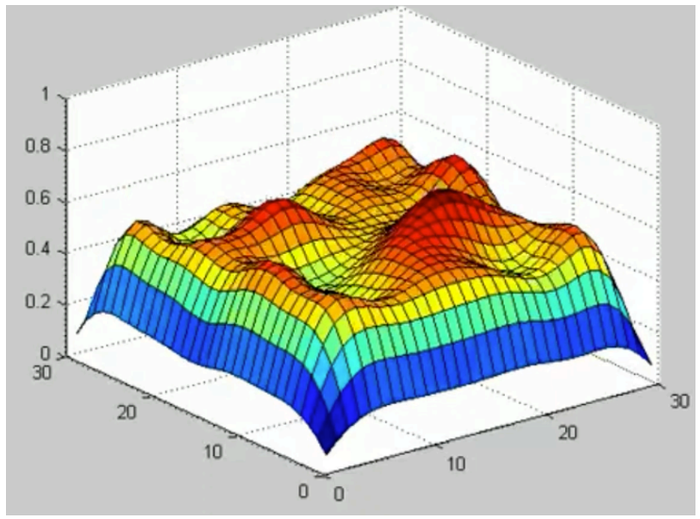
$$y = f(\mathbf{x}, t) = f(x_0, x_1, \ldots, x_N, t)$$

spacial temporal

Square sheet of metal



Initial temperature distribution $T = T(x, y)$



Predict future Temperature?

$$T = T(x, y, t) = ?$$

Solve heat equation

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$

PDE: partial differential equation

FINITE DIFFERENCED HEAT EQUATION

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\dot{q}}{k} = 0$$

$$\frac{T_{m+1,n} - 2T_{m,n} + T_{m-1,n}}{\Delta x^2} + \frac{T_{m,n+1} - 2T_{m,n} + T_{m,n-1}}{\Delta y^2} + \frac{\dot{q}}{k} = 0$$

if $\Delta x = \Delta y$

$$T_{m+1,n} + T_{m-1,n} + T_{m,n+1} + T_{m,n-1} + \frac{\dot{q}\Delta x^2}{k} - 4T_{m,n} = 0$$

