Lecture 4

Lecture 1-3

In Computational analysis of physical problems we represent functions like $f(x)$ as discrete points on a grid.

Why we do?

We can use these discrete values to quickly give numerical approximations to the derivative and the integral.

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x-h)}{2h}.$$

more accurate because it's centered about the value of *x* where we want the derivative to be evaluated.

Lecture 1-3

Looked at how to calculate 1st derivative using MATLAB with some examples.

Assignment: how to calculate a second derivative.

how to choose the step size *h*.

How to use linear extrapolation to find the derivatives at the endpoints.

Plot the difference between the approximate and exact.

Differential eqn.

- A **differential equation** is an equation that contains one or more derivatives.
- **initial condition** is the value of the dependent variable when the independent variable is zero.
- A **solution** to a differential equation is a function that satisfies the equation and initial condition(s).

Next is → Difference eqn.

Difference Equation

Example: Growth or Decay

We consider time advancing in small, incremental steps. For time, t, and length of a time step, Δt, the **previous time** is $t - \Delta t$.

<u>System dynamics tool → population example</u>

(rate of change of population (growth)→ dP/dt = rP; r is the growth rate)

Difference eqn: where *population*(t) is the population at time t and *population*($t - \Delta t$) is the population at time $t - \Delta t$:

population(t) = *population*($t - \Delta t$) + (*growth*) * Δt

growth* = *growth_rate* * *population

Difference eqn.

(new population) = (old population) + (change in population)

or

$$population(t) = population(t - \Delta t) + \Delta\, population$$

where **Δpopulation** is a notation for the **change in population**.

We approximate the change in the population over one time step, $\Delta\, population$ or $(growth) * \Delta t$, as the finite difference of the population at one time step and at the previous time step, $population(t) - population(t - \Delta t)$.

Difference eqn.

finite difference equation, indicates that the population at one time step is the population at the previous time step plus the change in population over that time interval:

$$population(t) = population(t - \Delta t) + \Delta population$$

we have an approximation of the derivative dP/dt as follows:

growth* = delta *population*/ delta *t

Radioactive decay

Numerically solved the problem of Radioactive decay: If there are N atoms of an unstable element with an exponential decay rate of "r or gamma" then the DE of how N decreases in time is (note: decay rate and mean lifetime (tau) are different)

$$\frac{dN}{dt} = -\gamma N$$

which is just a single first order differential equation whose solution is

$$N(t) = N(0)e^{-\gamma t} \ .$$

the instantaneous rate of change of *N* with respect to *t*, $N'(t) = dN/dt$, is the instantaneous rate of decay.

Algorithm (pseudocode) for simulation of radioactive decay

initialize *simulationLength*
initialize *number_atoms*
initialize *decay-Rate (or mean lifetime)*
initialize length of time step Δt
Num_of_Iterations ← *simulationLength* / Δt

for *i* going from 1 through *num_of_iterations*
do the following:
decay ← *decay-Rate* * *number_atoms*
number_atoms ← *number_atoms* (+/-) *decay* * Δt
$t \leftarrow i * \Delta t$

display *t*, *decay*, and *number_atoms*

Imp considerations

- Output looks reasonable?
- Agree with exact results if available?
- Code gives the same result for different time steps.

- What errors?
- Characteristic time scale?