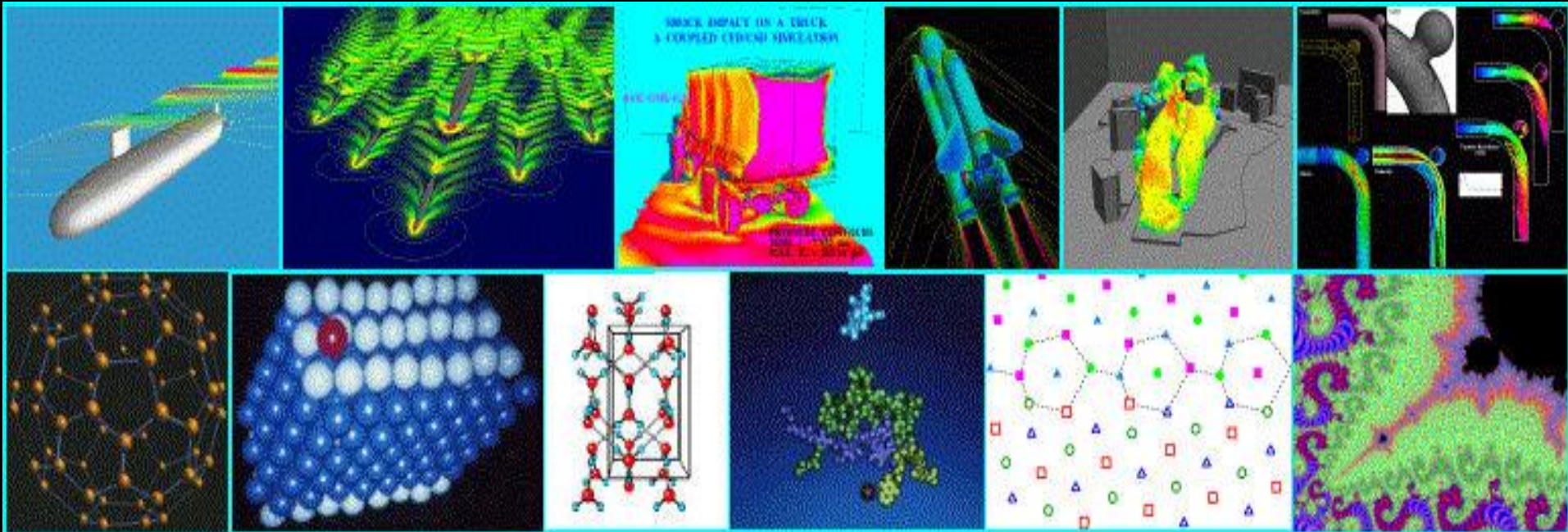


Computing for Scientists

Scientific Simulation (SS)

(Feb. 26, 2013 – April 02, 2013)



Jie Zhang

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CDS 130 - 003
Spring, 2013

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SS-1: Introduction

(Feb. 26, 2013)

Motivation

- Scientific simulation allows one to
 - (1) produce the quantitative details, and
 - (2) thus predict the behavior of a complex scientific system, e.g., physical systems, engineering systems, biological systems, environmental systems etc.
- It is a new way of scientific research, in addition to traditional experimental (including observations) and mathematical approaches.

Example

Merger of the Milky Way:

<http://video.google.com/videoplay?docid=3671579993993423979#>

The Milky Way and the Andromeda galaxy will likely fall together and merge within a few billion years. In this speculative simulation, the two galaxies flyby one another, exciting tidal tails and bridges and collide on a second pass finally merging after several convulsions. The last remnants of the smashed spirals show up as shells and ripples surrounding a newborn elliptical galaxy.

Example

Cellular Blood Flow:

<http://www.youtube.com/watch?v=o11NDvrZMNs&feature=related>

The RBCs are modeled as a membrane with hemoglobin inside with a viscosity of 6cP. Each RBC membrane is constructed of linear finite element triangular shells. These shell elements deform due to the fluid-structure interactions with the blood plasma and the hemoglobin.

Example

http://www.ncac.gwu.edu/research/setting_trends.html

Full-scale crash testing of several potential crash scenarios is cost-prohibitive and does not achieve comprehensive solutions. Instead, NCAC relies on simulating these scenarios on high-performance computers, which saves time and maximizes research dollars



Example: Equations

Many scientific simulations are based on so-called Navier-Stokes Equations (Note: do not worry about the math complexity)
http://www.cfd-online.com/Wiki/Navier-Stokes_equations

The instantaneous continuity equation (1), momentum equation (2) and energy equation (3) for a compressible fluid can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} [\rho u_j] = 0 \quad (1)$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} [\rho u_i u_j + p \delta_{ij} - \tau_{ji}] = 0, \quad i = 1, 2, 3 \quad (2)$$

$$\frac{\partial}{\partial t} (\rho e_0) + \frac{\partial}{\partial x_j} [\rho u_j e_0 + u_j p + q_j - u_i \tau_{ij}] = 0 \quad (3)$$

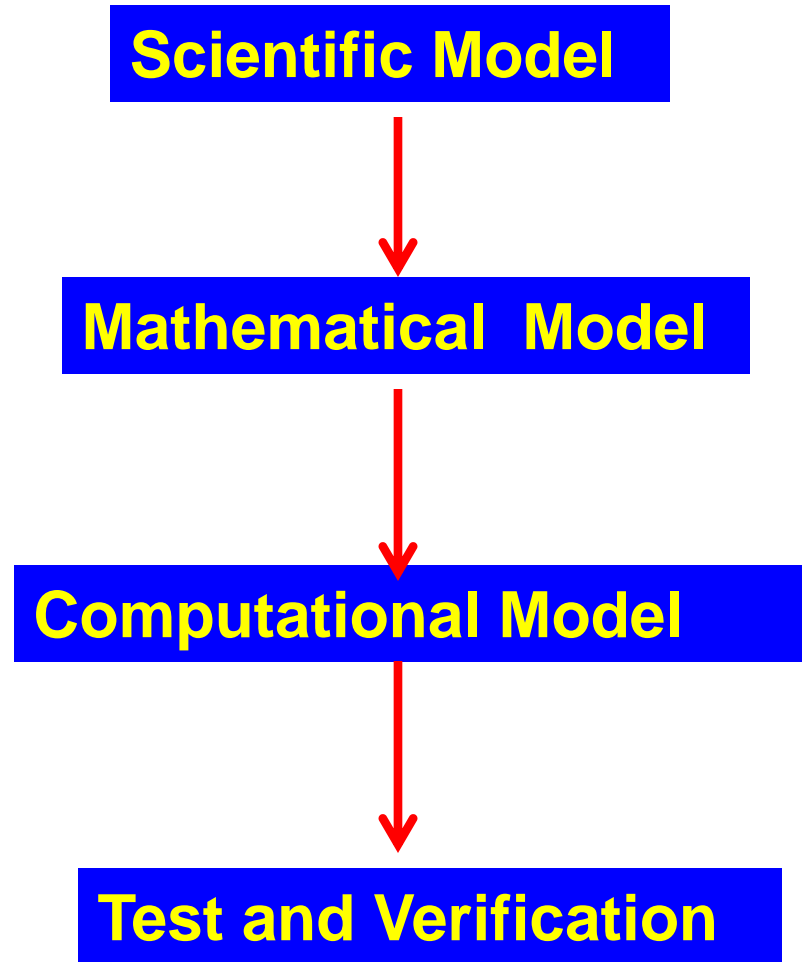
Navier-Stokes Equations: three differential equations

A Pipeline of Models

A common way that science gets done

1. Domain specialists (e.g., biologists) develop a conceptual representation of the system, so called **scientific model**
2. The domain specialists collaborate with mathematicians to develop a mathematical representation, or **mathematical model** that corresponds to the scientific model
3. The domain specialists and mathematicians work with computational scientists to implement the equations and explore the results using a computer, that is to develop a **computational model** of the mathematical model.
4. The computational methods need to be **tested**
5. Repeat steps 1 -> 2 -> 3 ->4 -> 1, gain better results.

Review: A Pipeline of Models



SS-2: Mathematical Models

(Feb. 26, 2013)

Objectives

1. Learn how to create a **mathematical model** based on the scientific question that you are asked to solve
 - Mathematic model is the mathematic representation of a given scientific question
 - **Scientific Model → Mathematical Model**
2. Mathematical model is necessary for subsequent computation, which solves the scientific problem
 - **Mathematical Model -> Computational Model**

Example 1

Scientific model:

Every year your bank account balance increases by 20%

Mathematical model:

$$B(\text{next-year}) = B(\text{this-year}) + 0.2 * B(\text{this-year}) \quad \% \text{okay}$$

$$B(i+1) = B(i) + 0.2 * B(i) \quad \% \text{ better mathematical}$$

Example 1 (continued)

Computational Model

```
>> B(i+1)=B(i)+0.2*B(i) % this is a good algorithm, but  
not good implementation
```

What is wrong with this?

B needs to be defined first for a computational model

```
>> B(1) = 1000 % assuming the balance of this year to  
be 1000, or any input number specified by the  
question
```

```
>> B(2)=B(1)+0.2*B(1)
```

Example 1 (continued)

Better Computational Model

Use FOR loop, but more constraints needed.

(1) The first year is \$1000

(2) The balance increases 20% every year

(3) Calculate the balance in the next 10 years.

```
>> B(1) = 1000
```

```
>> for i=[1:10]
```

```
    B(i+1)=B(i)+0.2*B(i)
```

```
end
```

What is B(11)?

Example 2

scientific model:

Every year your bank account balance increases by 20%.
Every year you pay a fee of \$100 to the bank

Mathematical model:

$$B(\text{next-year}) = B(\text{this-year}) + 0.2 * B(\text{this-year}) - 100$$

$$B(i+1) = B(i) + 0.2*B(i) - 100$$

Example 2 (continued)

Computational Model

More constrains needed.

To calculate the balance in the next year. The first year is \$1000

```
>> B(1) = 1000
```

```
>> B(2)=B(1)+0.2*B(1)-100
```

Example 2 (continued)

Better Computational Model

Use FOR loop.

```
>> B(1) = 1000  
  
>> for i=[1:10]  
    B(i+1)=B(i)+0.2*B(i)-100  
end
```

What is B(11)?

Example 3

Scientific Model

Every year your bank account balance doubles.

Question: What is the mathematical model?

Example 3 (continued)

Mathematic Model

Answer:

$$B(\text{next-year}) = 2 * B(\text{this-year})$$

Or

$$B(i+1) = 2 * B(i)$$

Example 3 (continued)

Computational Model

Question:

Assuming in the first year, the balance is \$1000.

Develop a computational model in Matlab to calculate the balance in the next 10 years?

What is the balance in the 11th year?

Example 3 (continued)

Answer:

```
>> clear %clear the existing variables
```

```
>> B(1)=1000
```

```
>> for i=[1:10]
    B(i+1)=B(i)*2
end
```

```
>> B(11)
```

```
Ans =
    1024000
```

Example 4

scientific model:

The death rate of the population in a country suffering from war is 3% per year and no babies are born

Question: What is the mathematical model?

Question: Develop a computational model to calculate the population in the next 10 years? What is population in the 11th year?
Assuming the initial population is 20 million.

Example 4 (continued)

Answer: (mathematic model)

$$P(\text{next-year}) = P(\text{this-year}) - 0.03 * P(\text{this-year})$$

Answer: (computational model)

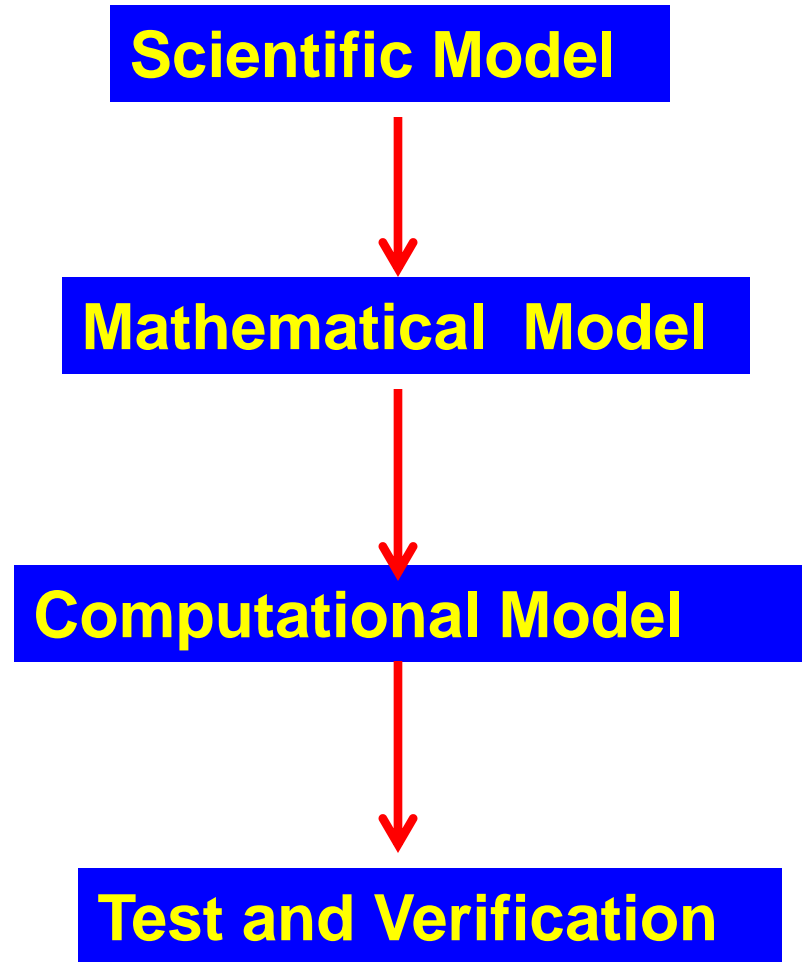
```
>> clear %clear the existing variables
>>P(1)=20000000 %20 million, also expressed by "2e7"
>>for i=[1:10]
    P(i+1)=P(i)-0.03*P(i)
end

>>P(11)
Ans =
    1.47e+07
```


**(February 26, 2013 Stops
Here)**

February 28, 2013

A Pipeline of Models



Review

scientific model:

The rabbit birth rate in an island is 10% per year and no rabbits die

Question: Write down the mathematical model of this question?

Review

Answer: (mathematic model)

$$R(\text{next-year}) = R(\text{this-year}) + 0.10 * R(\text{this-year})$$

OR

$$R(i+1) = R(i) + 0.10 * R(i)$$

Review

scientific model:

The rabbit birth rate in an island is 10% per year and no rabbits die

Question: Develop a computational model to calculate the rabbit population in the next 10 years? What is population in the 11th year?
Assuming the initial population is 100.

Review

Answer: (computational model)

```
>>clear
```

```
>>R(1)=100
```

```
>>for i=[1:10]
```

```
    R(i+1) = R(i) + 0.10 * R(i);
```

```
end
```

```
>>R(11)
```

```
ans =
```

```
    259.37
```

**Now consider a scientific model
with two inter-dependent
variables**

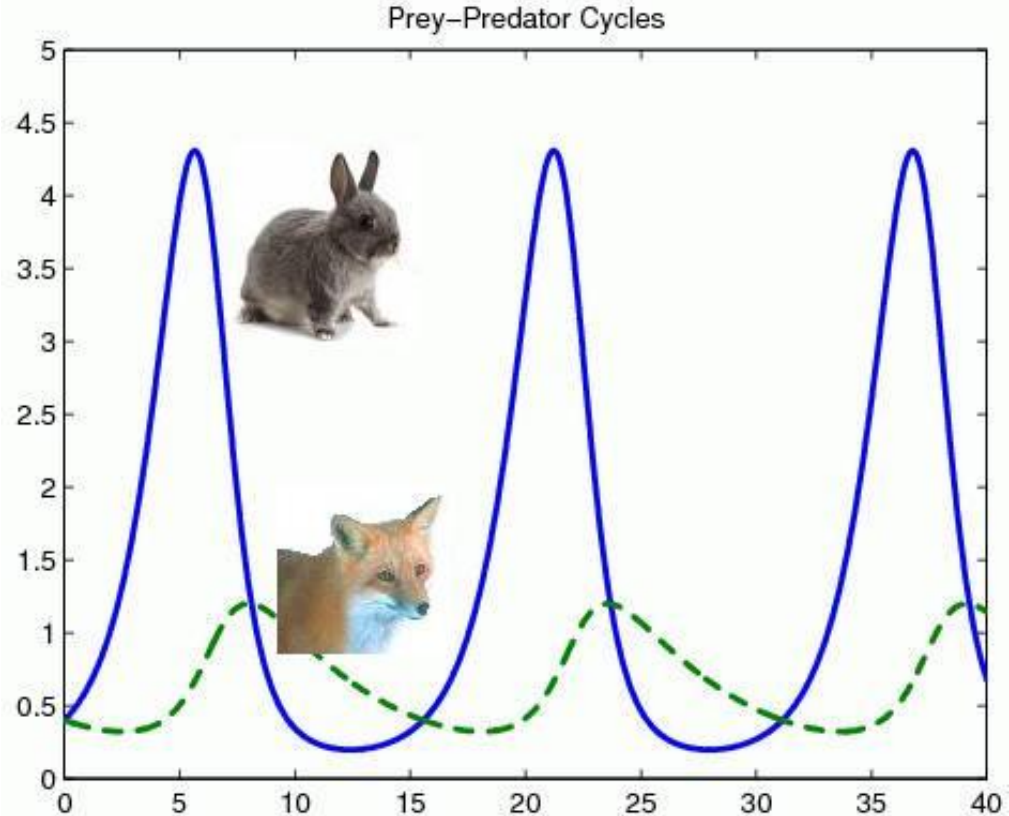
Predator – Prey Model



Consider a closed ecosystem, an island with only two species: foxes, the predator, and rabbits, the prey.

Imaging how the two populations change with time?

Predator – Prey Model



Periodical change of populations can happen

http://www.scholarpedia.org/article/Predator-prey_model

Predator – Prey Model



What if the predators are so greedy?

What if the preys are so easy to grow?

Predator – Prey Model

“Predator-prey models are arguably the building blocks of the bio- and ecosystems as biomasses are grown out of their resource masses. Species compete, evolve and disperse simply for the purpose of seeking resources to sustain their struggle for their very existence.

Depending on their specific settings of applications, they can take the forms of resource-consumer, plant-herbivore, parasite-host, tumor cells (virus)-immune system, susceptible-infectious interactions, etc.”

(http://www.scholarpedia.org/article/Predator-prey_model)

An online simulator:

<http://home.messiah.edu/~deroos/CSC171/PredPrey/PRED.htm>

Predator – Prey Model

scientific model for the rabbit:

The birth rate of rabbits is 50%. The death rate of rabbits is 0.02 times the number of rabbits multiplied by the number of foxes. Here, the value of 0.02 is also called the interaction constant.

Mathematical model:

$R(i)$: number of rabbits in year i

$F(i)$: number of foxes in year i

$$R(i+1) = R(i) + 0.50 * R(i) - 0.02 * R(i) * F(i)$$

Predator – Prey Model

Scientific model for the foxes:

The death rate of foxes is 10%. The birth rate of foxes is 0.001 times the number of foxes multiplied by the number of rabbits.

Mathematical model:

$$F(i+1) = F(i) - 0.1 * F(i) + 0.001 * F(i) * R(i)$$

Predator – Prey Model

The observations of this closed ecosystem

- Change in number of rabbits (prey) per year
 - increases in proportion to the number of rabbits (breeding like rabbits!) – **the birth rate of prey**
 - decreases in proportion to (the number of rabbits) x (number of foxes) **X the death rate of prey due to interaction with the predator (interaction constant 1)**
 - Does not depend on rabbits dying of natural death (negligible compared with the loss due to predator)
- Change in number of foxes (predator) per year
 - decreases in proportion to the number of foxes due to natural death – **the death rate of predator**
 - increases in proportion to (the number of rabbits) x (the number of foxes) **X the birth rate of predator depending on the food (prey) (interaction constant 2)**

Predator – Prey Model

scientific model:

- The birth rate of rabbits is 50%. The death rate of rabbits is 0.02 times the number of rabbits multiplied by the number of foxes.
- The death rate of foxes is 10%. The birth rate of foxes is 0.001 times the number of foxes multiplied by the number of foxes.
- The initial number of rabbits is 100, and that of foxes is 20
- Find out the number of rabbits and foxes in 40 years

Predator – Prey Model

Answer: (computational model)

```
>>clear
>>R(1)=100.0 %initial population of rabbits
>>F(1)=20.0 %initial population of foxs
>>BR_rabbit=0.5 %birth rate of rabbit
>>DR_rabbit_INT=0.02 %death date of rabbit (prey) due to interaction
>>DR_fox=0.1 %death rate of fox
>>BR_fox_INT= 0.001 % birth rate of fox (predator) due to interaction

>>for i=1:40
    R(i+1)=R(i)+BR_rabbit*R(i)-DR_rabbit_INT*R(i)*F(i)
    F(i+1)=F(i)-DR_fox*F(i)+BR_fox_INT*F(i)*R(i)
end

>>R %find the number of rabbits in 40 year
>>F %find the number of foxes in 40 years
```

Predator – Prey Model

Answer: (computational model) (continued)

```
>>figure(1);  
>>plot(R,'*') %make a plot showing rabbit evolution  
  
>>figure(2);  
>>plot(F,'-') %make a plot showing fox evolution
```

Predator – Prey Model

Practical problems with previous approach

1. It is not convenient to type multiple line programming codes in the command line. Any mistake means re-typing
2. To find the evolution, one needs to use a graphic plot to illustrate the evolution. The plot needs to be well annotated.

Sharpen your MATLAB skill

(1) How to make a simple plot

(2) How to write a program file

Feb. 28, 2013 Stopped Here

March 19, 2013

Review:

Predator – Prey Model

scientific model:

- The birth rate of rabbits is 50%. The death rate of rabbits is 0.02 times the number of rabbits multiplied by the number of foxes.
- The death rate of foxes is 10%. The birth rate of foxes is 0.001 times the number of foxes multiplied by the number of foxes.
- The initial number of rabbits is 100, and that of foxes is 20
- Find out the number of rabbits and foxes in 50 years

Review: program

Answer:

“prey_v1.m”

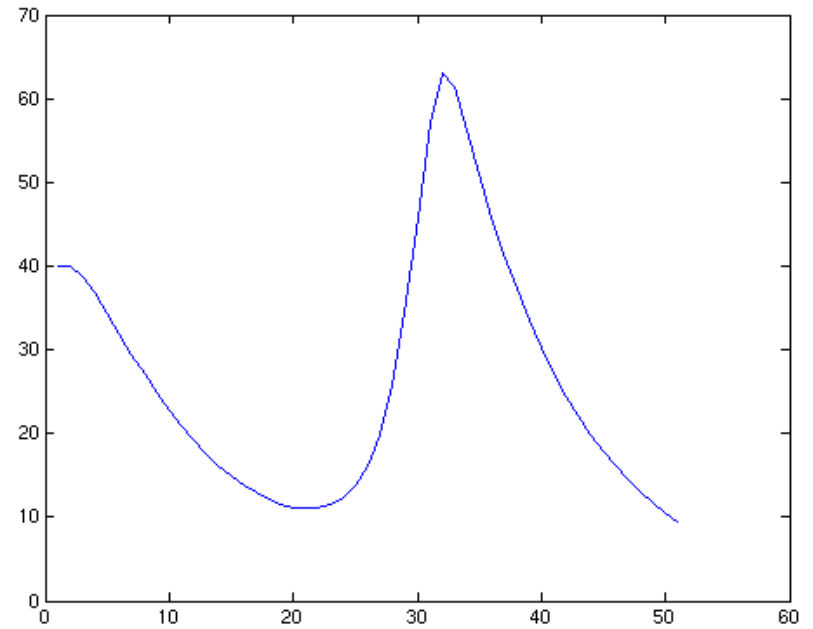
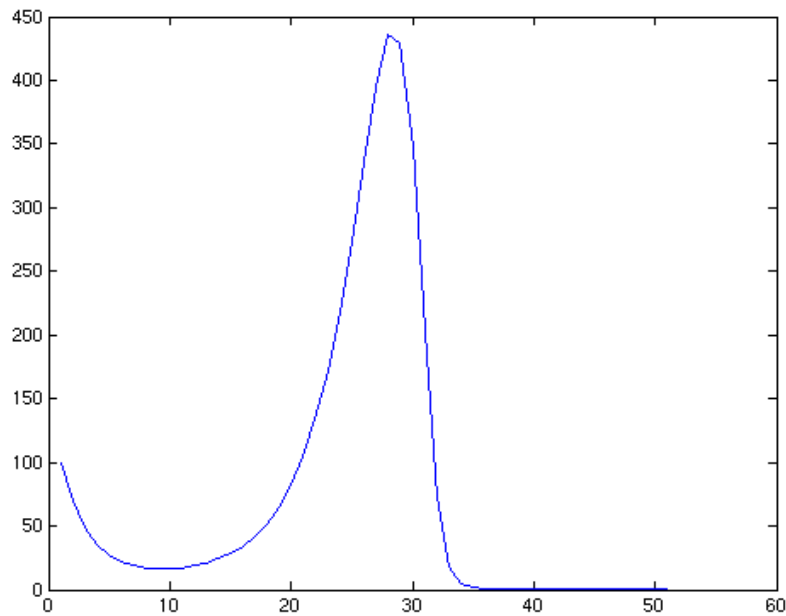
```
clear
R(1)=100.0 %initial population of rabbits
F(1)=40.0 %initial population of foxs
BR_rabbit=0.5 %birth rate of rabbit
DR_rabbit_INT=0.02 %death date of rabbit (prey) due to interaction
DR_fox=0.10 %death rate of fox
BR_fox_INT= 0.001 % birth rate of fox (predator) due to interaction

for i=1:50
    R(i+1)=R(i)+BR_rabbit*R(i)-DR_rabbit_INT*R(i)*F(i)
    F(i+1)=F(i)-DR_fox*F(i)+BR_fox_INT*F(i)*R(i)
end

hold off %clear the previous plot setting
figure(1) %make plot 1 for rabbit population evolution
plot(R)
figure(2) %make plot 2 in another window for fox fox population evolution
plot(F)
```

Review: program

Answer:
The output plots



Review: program

Advantages of the program files

- It is easy to make an update
- It is easy to find the results of new models

1. Run the evolution for the next 100 years
2. What if the rabbit birth rate is 30% (reduced from 50%)
3. What if the fox death rate is 20% (increased from 10%)
4. What if the rabbit death constant is 0.01 (reduced from 0.02)
5. What if the fox birth rate is 0.002 (increased from 0.001)

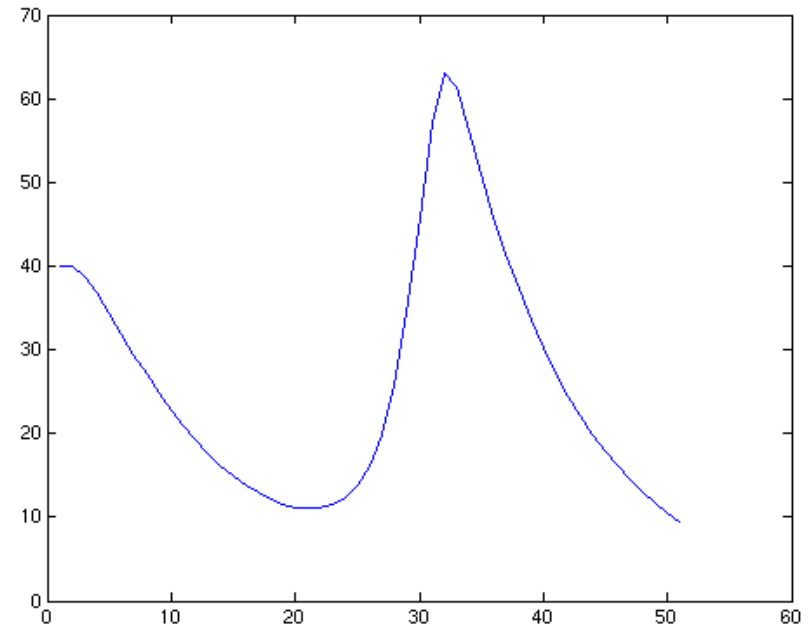
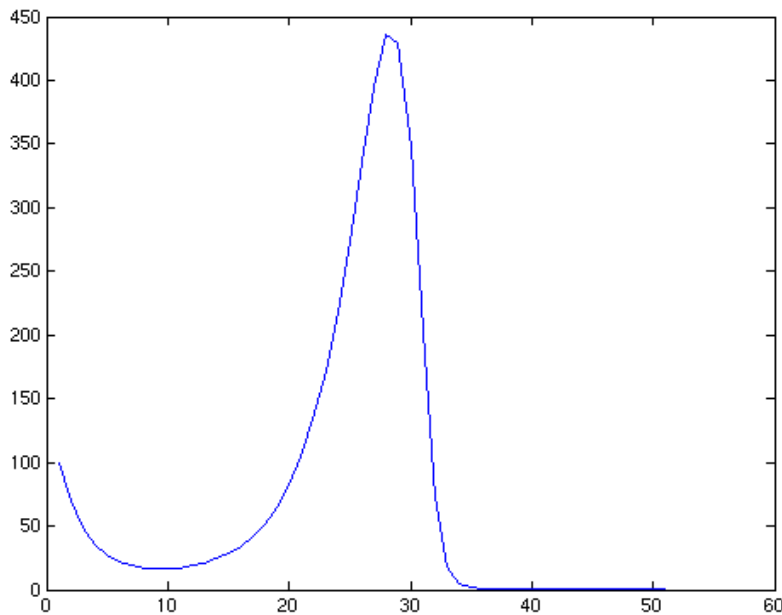
Matlab (advanced)

“plot” function

(March 19, 2013)

Predator-Prey Model

Answer:
The output plots



**The plots might be good enough for your own view,
but not fair to other readers**

“plot” function

Question: Continue to work on previous program “prey_v1.m”. Save it as “prey_v2.m”, and add the following functionalities.

- (1) Combine the two lines into the same plot window
- (2) Properly annotate the plot with title, axis labels
- (3) Properly annotate the two lines with different line properties, text labels and the legend

“plot” function

Answer:

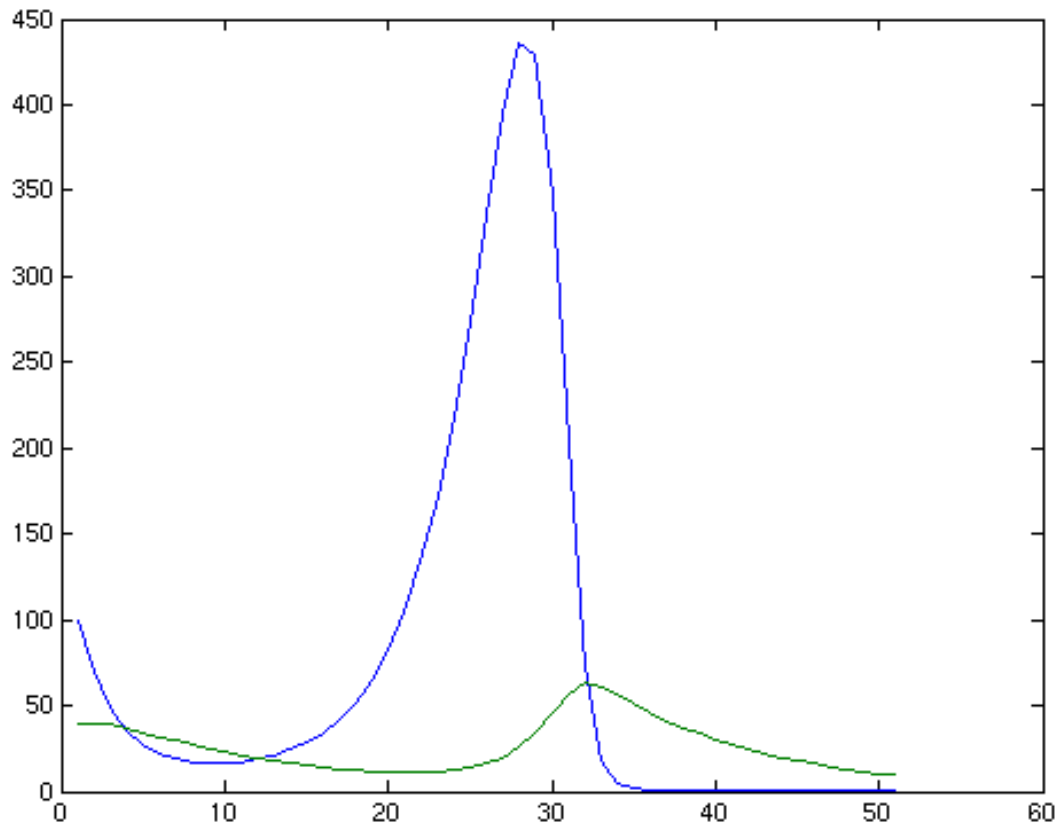
“prey_v2.m”

```
%  
%the calculation section, the same as in “prey_v1.m”  
%  
  
%---- plotting section ----%  
hold off      %clear the previous plot setting  
figure(1)    %make plot 1 for rabbit population evolution  
plot(R)  
hold all     %hold on all previous settings: plotting window, axis, styles  
plot(F)
```

“plot” function

Answer:

The output plots



Now, the two lines are plotted together.

The plot now needs to be properly labeled

“plot” function

Answer:

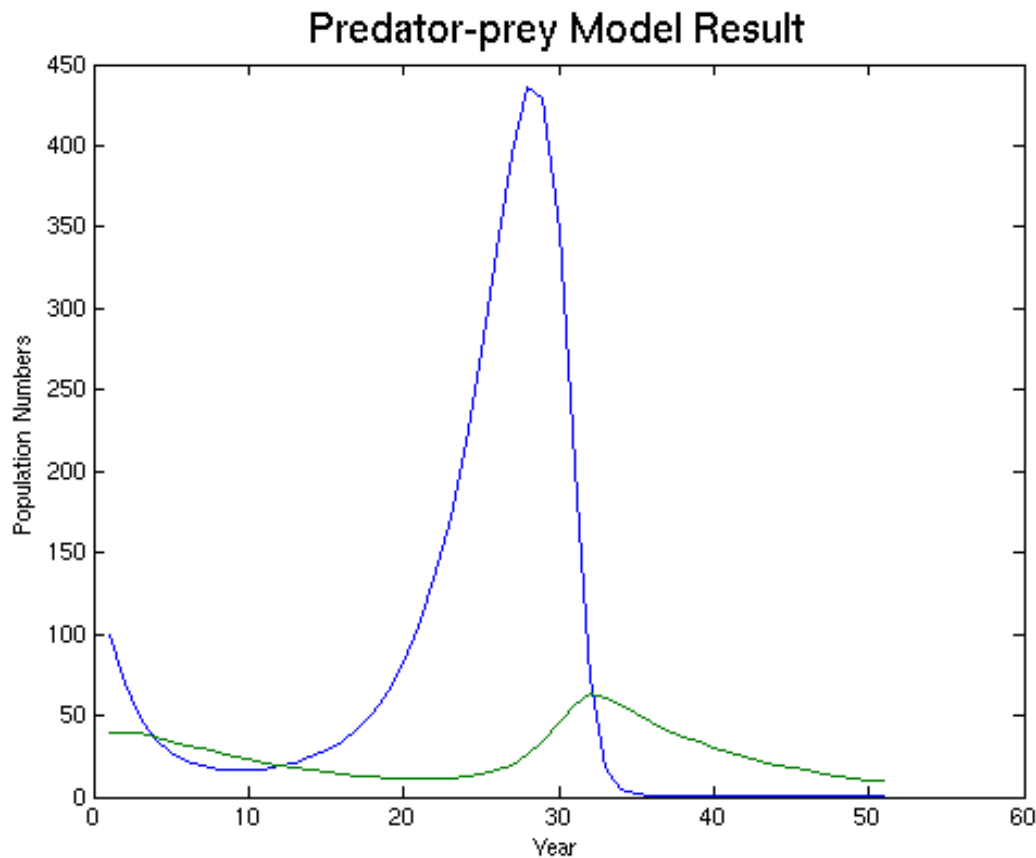
“prey_v2.m”

```
%  
%the calculation section, the same as in “prey_v2.m”  
%  
  
%---- plotting section ----%  
hold off      %clear the previous plot setting  
figure(1)    %make plot 1 for rabbit population evolution  
plot(R)  
hold all     %hold on all previous settings: plotting window, axis, styles  
plot(F)  
  
xlabel('Year') % X axis label  
ylabel('Population Numbers') % Y axis label  
title('Predator-prey Model Result',...  
      'FontSize',18)
```

“plot” function

Answer:

The output plots



Now, the plot is properly labeled.

Now, we can change the line styles, and add legends

“plot” function

Answer:

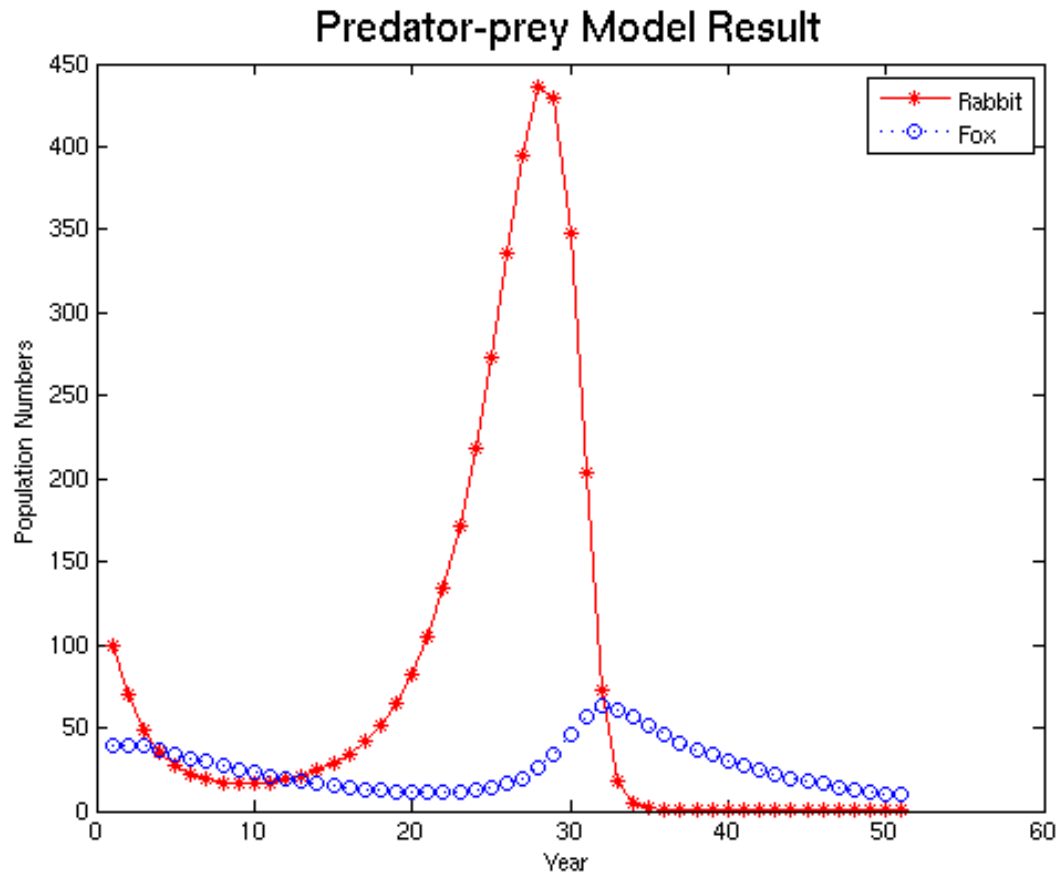
“prey_v2.m”

```
%  
%the calculation section, the same as in “prey_v2.m”  
%  
  
%---- plotting section ----%  
hold off      %clear the previous plot setting  
figure(1)     %make plot 1 for rabbit population evolution  
plot(R,'-*r)  % line specification: solid line, marker *, red color  
hold all      %hold on all previous settings: plotting window, axis, styles  
plot(F,':ob') % line specification: dotted line, marker circle, blue color  
legend('Rabbit','Fox') %legend  
  
xlabel('Year') % X axis label  
ylabel('Population Numbers') % Y axis label  
title('Predator-prey Model Result',...  
      'FontSize',18)
```

“plot” function

Answer:

The output plots



Now, good legend, and line styles.

“plot” function – Line Specification

The String Syntax. For example

```
>>plot(x, y, '-*r')
```

The three symbols ‘- * r’ are for line style (solid line), data marker (asterisk), and line color (red), respectively.

Specify Line Style

'-'	Solid line (default)
'--'	Dashed line
'.'	Dotted line
'-.'	Dash-dot line
'none'	No line

“plot” function – Line Specification

Marker Specifiers

'+' Plus sign

'o' Circle

'*' Asterisk

'.' Point

'x' Cross

'square' or 's'

Square

'diamond' or 'd'

Diamond

'^' Upward-pointing triangle

'v' Downward-pointing triangle

'>' Right-pointing triangle

'<' Left-pointing triangle

'pentagram' or 'p'

Five-pointed star (pentagram)

'hexagram' or 'h'

Six-pointed star (hexagram)

'none' No marker (default)

“plot” function – Line Specification

Color Specifiers

r Red
g Green
b Blue
c Cyan
m Magenta
y Yellow
k Black
w White

“plot” function

Watch the video:

<http://www.mathworks.com/products/featured/videos/?video=Interactively-Creating-Plots>

“plot” function

Find more information about “plot” or any other build-in functions, you can type-in the function name in the search window, which results in the display of the full document.

“plot” function

Exercise: The question below is written in algorithm style. You need to implement the algorithm in Matlab, save the file and output the figure. The figure needs to be properly labeled. The two lines need to be properly annotated. The lines should have a legend,

x=[-pi, +pi]

y1=sin(x)

y2=cos(x)

plot(x,y1)

plot(x,y2)

“plot” function

Answer:

“sin.m”

```
clear    %clear the variable

%----model calculation section---
x=[-pi:pi/10:pi]  %create twenty data points
y1=sin(x)        %
y2=cos(x)

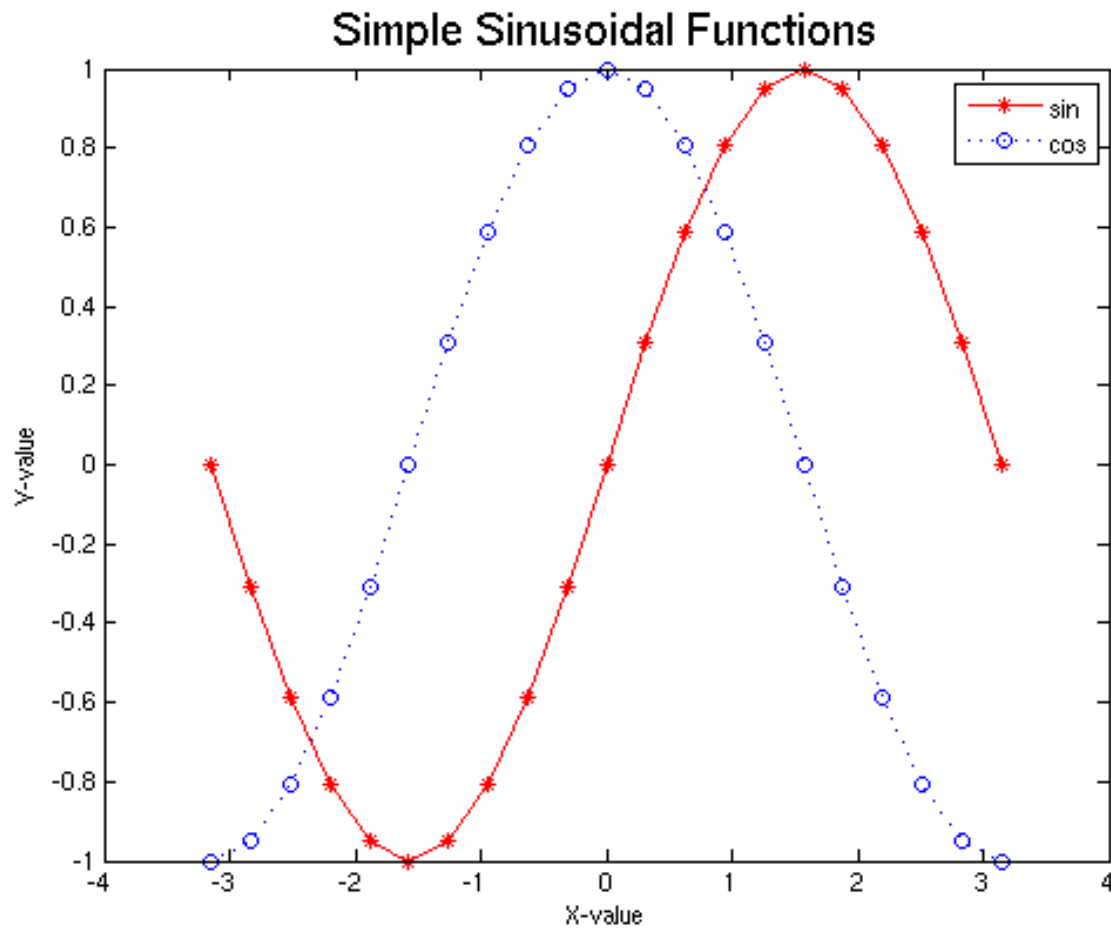
%---- plotting section ---%
hold off %clear the previous plot setting
figure(1) %make plot in figure 1
plot(x,y1,'-*r') %line specification: solid line, marker *, red color
hold all %hold on all previous settings: plotting window, axis, styles
plot(x,y2,':ob') %line specification: dotted line, marker circle, blue
legend('sin','cos')

xlabel('X-value') % X axis label
ylabel('Y-value') % Y axis label
title('Simple Sinusoidal Functions',...
      'FontSize',18)
```

“plot” function

Answer:

The output plot



**March 19, 2013 Stopped
Here**

March 21, 2013

Review: “plot” function

Watch the video:

<http://www.mathworks.com/videos/interactive-plot-creation-with-the-plot-tools-68989.htm>

Review: “plot” function

Exercise: The question below is written in algorithm style. You need to implement the algorithm in Matlab, save the file and output the figure. The figure needs to be properly labeled. The line needs to be properly annotated. The line should have a legend.

$$y = x^2$$

Where x is in the range between 0 and 5

Use “plot”, “xlabel”, “ylabel”, “title”, “legend”

SS-3 Computational Models

SS-3.1 – Basics

SS-3.2 – Differentiation

SS-3.3 -- Integration

SS-3.1 Basics

I have so far treated a computational model as of programming and implementation, and have shown many examples. Now, let me formally introduce several basic concepts essential to any computational model

Objectives: introduce the concept of

1. Algorithm

2. Iteration

3. Initial Condition

4. Interval and Sub-interval

Algorithm

In mathematics and computer science, an algorithm is an effective method expressed as a finite set of well-defined instructions for implementing a function.

Computational Model =

(1) Algorithm (general, universal)

+

(2) Programming (depending on languages you use)

Algorithm

- Algorithm is a generic program instruction.
- It is also called **pseudo-code**, not specific implementation
- It can then be implemented in any program language, e.g., Matlab, Python, C, C++, Java, Fortran, IDL et al

Algorithm

Question:

Construct an algorithm of finding the largest number in an array?

Algorithm

```
Array A(N) %input an array of N elements  
val_max = 0 % initialize parameter max
```

```
Begin Iteration N Times
```

```
    IF val_max < A(i)
```

```
        THEN val_max = A(i)
```

```
    ELSE do-nothing
```

```
End Iteration
```

Algorithm

Question:

Construct an algorithm of finding the largest number in an array? You need to program it using MATLAB

Programming (mymax.m)

```
clear
A=[1,4,8,3,2,5]   %provide a sample array

val_max=0;
for i=[1:6]
    if val_max < A(i)
        val_max = A(i);
        display('New max value is found')
    else
        display('DO NOTHING')
    end
end

val_max
```

Algorithm

**A more generic programming (mymax2.m):
Define a function “mymax2”, take an array
as input, and the result as output**

```
function val_max=mymax2(A)

val_max=0;
n=numel(A) %find the number of elements in an array
for i=[1:n]
    if val_max < A(i)
        val_max = A(i);
        display('New max value is found')
    else
        display('DO NOTHING')
    end
end

return
```

Algorithm

How to use the self-defined function: simply call the name

```
>>A = [1,2,3,4,3,2,1]    %input array
```

```
>>mymax2(A)    %find the maximum value of array A
```

```
>>M=mymax2(A)    % return the maximum value to M
```

```
>>B=[1, 2, 3, 4, 5, 6, 1]
```

```
>>mymax2(B)
```

Iteration

$$X(i+1) = X(i) + \text{“Function of } X(i)\text{”}$$

- Iteration is the most fundamental method in computational models that represents a dynamic scientific system.
 - For example, the time change or evolution of a system (population, money in the bank etc)
- Used for solving differential equations
 - e.g., knowing the rate of change of the population
- Used for solving integration equations
 - e.g., total area enclosed by a Gaussian function

$$y = e^{-x^2}$$

Iteration

```
>for i=[1:N]
>X(i+1) = X(i) + “FUNCTION of X(i)”;
>end
```

- The output of current iteration is used as the input of the next iteration

i: the sequence number of the iteration, representing the **independent variable**, usually the “**time**”, e.g., year in population growth

N: total number of iterations

X: the **dependent variable**, an unknown function, but the model seeks to find

FUNCTION(X(i)): the known function representing the knowledge or model of the system

Initial Condition

The result of a real model depends on the initial condition

A specific scientific model:

Every year your bank account balance increases by 10%.

Assuming in the first year, the balance is \$1000.

What is the balance in the 10th year?

Question: what is the initial condition?

Initial Condition

Answer: In the first year, the balance is \$1000.

**March 21, 2013 Stopped
Here**

March 26, 2013

Review

SS 3.1 Computational Model: Basics

1. Algorithm
2. Iteration
3. Initial Condition
4. Interval and Sub-interval

Interval and Sub-Interval

The result of a computational model depends on the interval and sub-interval.

A specific scientific model:

Every year your bank account balance increases by 12%.

Assuming in the first year, the balance is \$1000.

What is the balance in the 10th year?

Question: what is the interval of the model?

What is the sub-interval of the model?

Interval and Sub-Interval

Answer: The interval is from year 1 to year 10.
The sub-interval is every one year.

Question: what happens if the sub-interval changes? Will this change the result?

Interval and Sub-Interval

Specific scientific models:

Model 1:

Every year your bank account balance increases by 12%.
Assuming in the first year, the balance is \$1000.
What is the balance in the 10th year?

Model 2:

Every month your bank account increases by 1%
Assuming in the first month of the first year, the balance is
\$1000.
What is the balance at the end month of the 10th year?

What are the commons and differences of the two models?

Interval and Sub-Interval

Answer:

The two models share the same scientific knowledge or algorithm: increasing by 12% on a yearly base, or “equivalently” by 1% on a monthly base

The two models have the “same” interval: 10 years or 120 months

The **difference** is that the two models have different sub-intervals: every year versus every month

Interval and Sub-Interval

Question: implement the following models in a single program

Model 1:

Every year your bank account balance increases by 12%.

Assuming in the first year, the balance is \$1000.

What is the balance in the 10th year?

Model 2:

Every month your bank account increases by 1%

Assuming in the first month of the first year, the balance is \$1000.

What is the balance at the end month of 10th year?

Write a program code to implement the two models, and make a plot to show the results?

Interval and Sub-Interval

```
clear      %clear existing variables
BM1(1)=1000; %model 1 initial condition
BM2(1)=1000; %model 2 initial condition
```

“bank_interval.m”

```
for i=[2:10]
    BM1(i)=BM1(i-1)+0.12*BM1(i-1);
end
```

```
for i=[2:120]
    BM2(i)=BM2(i-1)+0.01*BM2(i-1);
end
```

```
clf      % clear existing figure drawings
x2=[1:120];
plot(x2,BM2,'-*b')
```

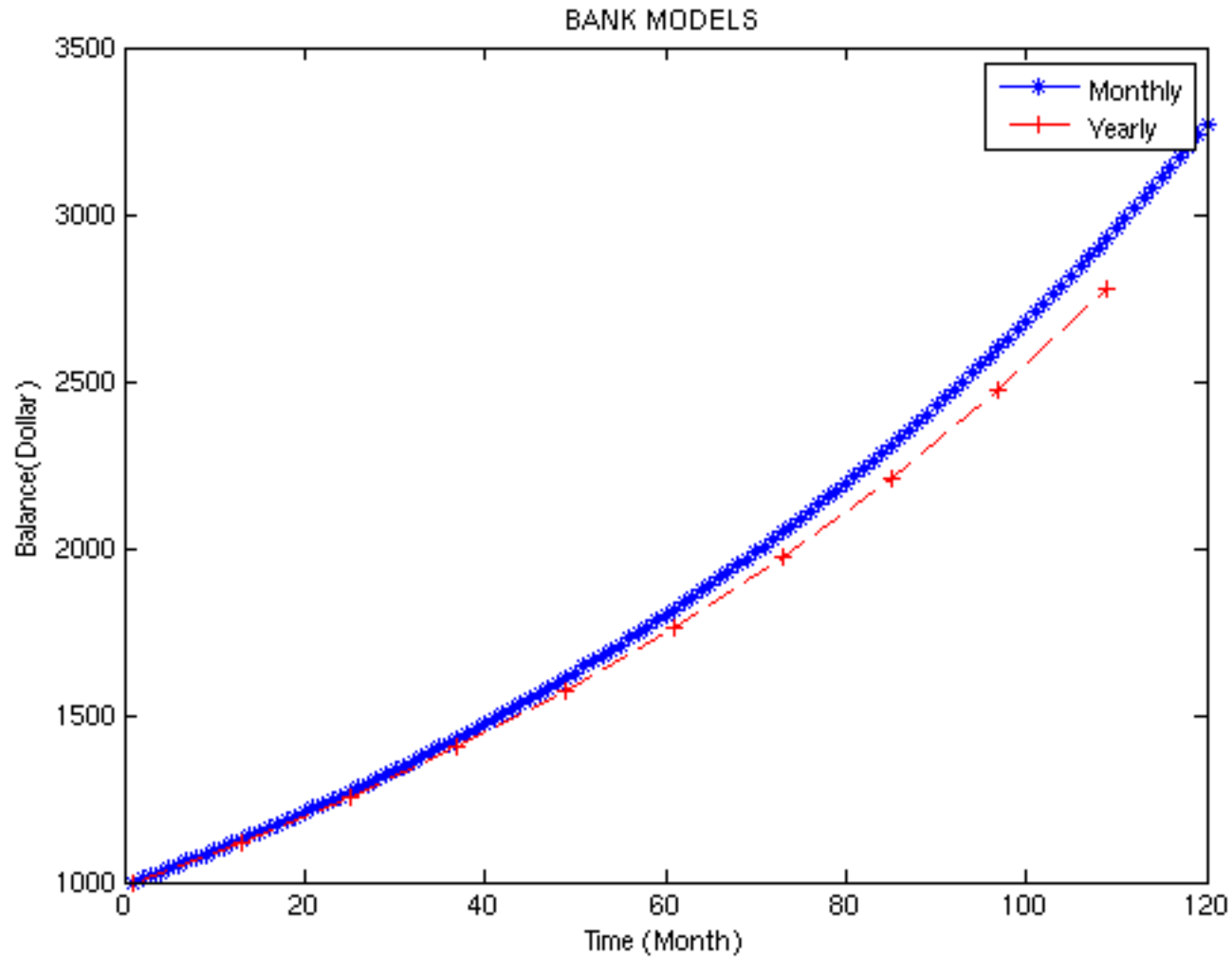
```
xlabel('Time (Month)')
ylabel('Balance(Dollar)')
title('BANK MODELS')
```

```
hold all
```

```
x1=[0:9]*12+1
plot(x1,BM1,'--+r')
```

```
legend('Monthly','Yearly')
```

Interval and Sub-Interval



Interval and Sub-Interval

Yearly	Model	Monthly	Model
$i=1$ (Beginning of year 1)	\$1000	$i=1$ (Beginning of Month 1)	\$1000
$i=2$ (Beginning of year 2) (Beginning of month 13)	\$1120	$i=13$ $i=1+12*(2-1)$ (Beginning of month 13)	\$1127
$i=5$ (Beginning of year 5) (Beginning of month = $1 + 12*4 = 49$)	\$1574	$i=49$ $i=1+12*(5-1)$ (beginning of month 49)	\$1612
$i=10$ (Beginning of year 10) (Beginning of month = $1+12*9=109$)	\$2773	$i=109$ $i=1+12*(10-1)$ (beginning of month 109)	\$2929

Interval and Sub-interval

- In numerical simulation, one has to specify the calculation **interval** and **sub-interval**
- **Interval** is the domain of the calculation
- **Sub-interval** is the step-size in each iteration of the numerical calculation
 - We have assumed that the sub-interval is every one year in many examples. But this is for convenience only, it can be every one month, or even every day

The Effects of Sub-interval

- A smaller sub-interval requires more steps of calculation
- But, a smaller sub-interval provides more detailed evolution
- Furthermore, a smaller sub-interval provides a more **accurate** result
 - This conclusion will be further illustrated in the context of differentiation and integration

SS-3.2: Differential Equations

(March 26, 2013)

Differential Equations

- It is an equation to describe **the rate of change** of one parameter (or several parameters) in a scientific system
- The rate of change could be in time (t)
- The rate of change could also be in position, along x in one dimension, along (x, y) in two dimensions, and along (x, y, z) in three dimensions

Mathematic Notation

The rate of change of parameter P with time t is defined by a function $f(P)$. The differential equation notation shall be

$$\frac{\Delta P}{\Delta t} = f(P), \quad \text{or formally}$$

$$\frac{dP}{dt} = f(P) \quad \text{as } \Delta t \text{ becomes infinitely small}$$

ΔP : difference of parameter P , or change of P

dp : differential change (infinitely small change) of P

Δt : difference of time t , or change of t ; the **subinterval**

dt : differential change (infinitely small change) of t

Thus, $\Delta P / \Delta t$ is the rate of change

$f(P)$: a known function, i.e., the knowledge of the system

Example 1

Scientific model:

Your bank account balance has an interest rate of 12% compounded yearly. What is the differential equation?

$$\frac{\Delta P}{\Delta t} = 0.12 * P$$

In this case, the parameter P stands for the bank balance, and

$$\frac{\Delta P}{\Delta t} = f(P)$$

$$f(P) = 0.12 \times P$$

Example 1

Now, use a computational model to solve the differential question?

The differential equation can be easily converted into the familiar mathematical model. They are equivalent.

$$\frac{\Delta P}{\Delta t} = 0.12 * P$$

Differential Equation

$$\frac{\Delta P}{\Delta t} = \frac{P(i+1) - P(i)}{t(i+1) - t(i)} = \frac{P(i+1) - P(i)}{1} = 0.12 * P(i)$$

$$P(i+1) = P(i) + 0.12 * P(i)$$

The familiar mathematic model

Differential Equations

$$\frac{\Delta P}{\Delta t} = f(P)$$

The subinterval “ Δt ” is a finite value in computational models, e.g., one year, one month, one day.

However, in **calculus**, “ Δt ” is infinitely small. The mathematical notation is slightly different

$$\frac{dP}{dt} = f(P)$$

dt: the infinitesimally small time interval
dt = Δt , as $\Delta t \rightarrow 0$

Example 2

Scientific model:

The human population grows at an annual rate of 2%.

- (1) What is the differential equation?
- (2) Convert the differential equation to a mathematic model
- (3) Write a computational model to calculate the population from year 2010 to year 2030, assuming the population in 2010 is 6.0 billion?
- (4) What are the populations in year 2020 and 2030?

Example 2

Answer:

(1) What is the differential equation?

$$\frac{\Delta P}{\Delta t} = 0.02 * P$$

(2) Convert the differential equation to a mathematic model

$$\frac{\Delta P}{\Delta t} = 0.02 * P$$

$$\frac{\Delta P}{\Delta t} = \frac{P(i+1) - P(i)}{t(i+1) - t(i)} = \frac{P(i+1) - P(i)}{1} = 0.02 * P(i)$$

$$P(i+1) = P(i) + 0.02 * P(i)$$

Example 2

Answer:

(3) Write a computational model to calculate the population from year 2010 to year 2030, assuming the population in 2010 is 6.0 billion?

```
P(1)=6.0;  
for i=[1:29]  
    P(i+1)=P(i)+0.02*P(i);  
end  
P(20)  
P(30)
```

(4) What are the populations in year 2020 and 2030?
8.74 in 2020, and 10.66 in 2030

**March 26, 2013 Stopped
Here**

March 28, 2013

Review: Differential Equation

- **Differential equation** defines **the rate of change**.
 - If you know the rate of change of one parameter, you should be able to calculate that parameter
 - e.g., velocity (the rate of change of distance) -> distance
 - e.g., acceleration (the rate of change of velocity->velocity)
 - e.g., interest rate (the rate of change of balance) -> balance

$$\frac{\Delta P}{\Delta t} = f(P)$$

**Differential Equation
in Computation**

$$\frac{dP}{dt} = f(P)$$

**Differential Equation
in Calculus:
dt = Δt, as Δt → 0**

Example 3

A scientific law is often expressed in differential equations, for a good reason.

Newton's Law of Cooling:

$$\frac{dT}{dt} = -q * (T - T_a)$$

T : temperature of object

T_a : ambient temperature

t : time

q : cooling coefficient

The cooling rate of an object is proportional to the temperature difference between the object and the ambient temperature

Example 3

Question:

An iron bar is heated to 1000°C . Assume the cooling coefficient is 0.2 per minute, and the ambient temperature is 30°C .

- (1) Convert the differential equation to a mathematic model?
- (2) Write a MATLAB program to calculate the bar temperature in one hour? Save the program as “cooling.m”
- (3) Also make a plot of the temperature curve?
- (4) What are the bar temperatures in 5th, 10th, 30th, and 60th minutes? How many minutes are needed for the bar temperature reducing to half?

Example 3

Answer:

(1) Convert the differential equation to a mathematic model?

$$\frac{dT}{dt} = -q^* (T - T_a)$$

$$\frac{dT}{dt} = \frac{\Delta T}{\Delta t} = \frac{T(i+1) - T(i)}{(i+1) - (i)} = T(i+1) - T(i)$$

Thus

$$T(i+1) - T(i) = -q^* (T(i) - T_a)$$

or

$$T(i+1) = T(i) - q^* (T(i) - T_a)$$

“cooling.m”

```
function [T] = cooling ()
clear
T(1)=1000 % initial temperature
Ta=30    % ambient temperature
q = 0.2  % cooling coefficient

N=60    % interval 60 minutes

for i=[1:N-1]
    T(i+1)=T(i)-q*(T(i)-Ta);
end

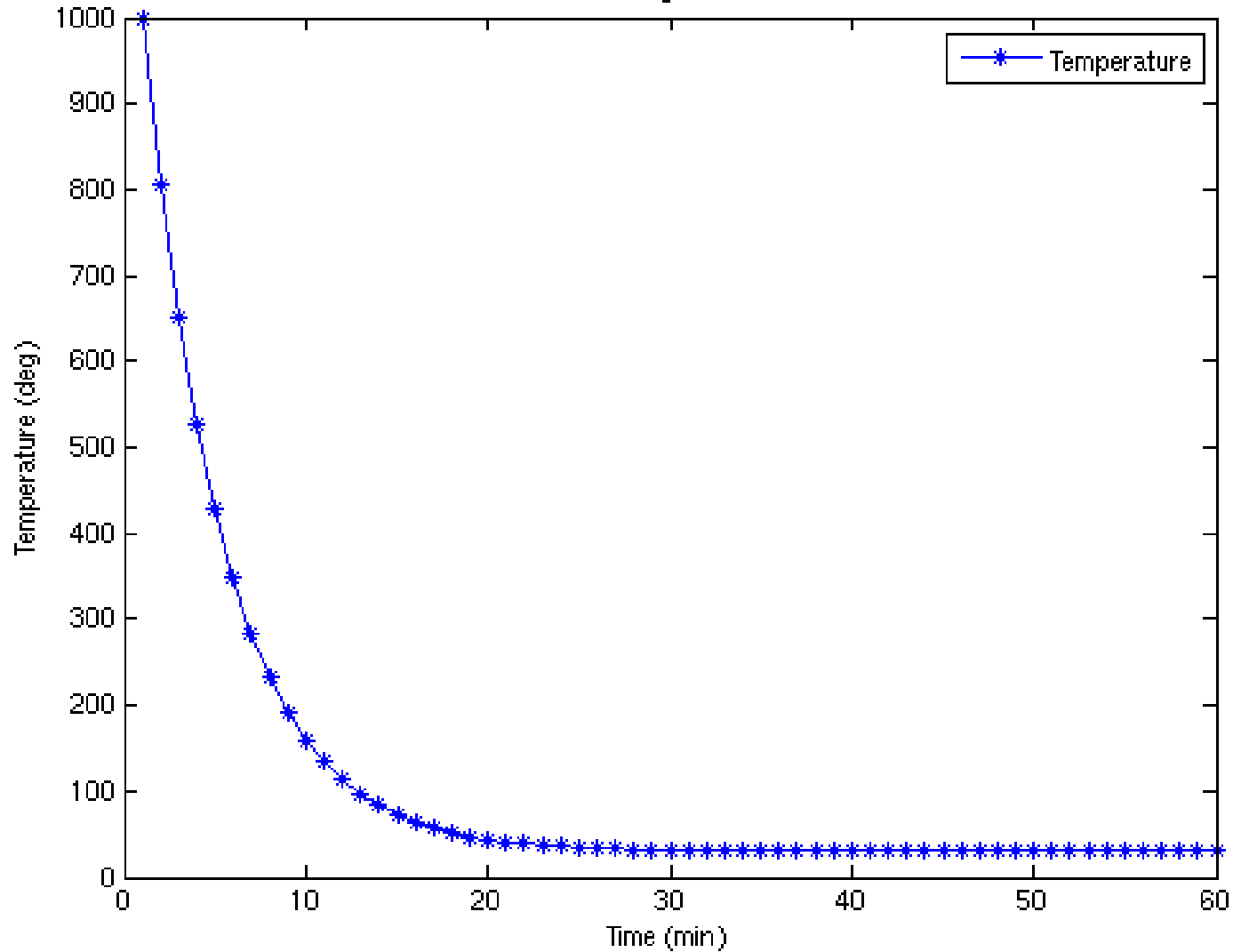
plot(T,'-b')
xlabel('Time (min)')
ylabel('Temperature (deg)')
title('cooling curve','FontSize',18)
legend('Temperature')

sprintf('Temperature in 5th minute = %f',T(5))
    %create a string to be displayed
sprintf('Temperature in 10th minute = %f',T(10))
sprintf('Temperature in 30th minute = %f',T(30))
sprintf('Temperature in 60th minute = %f',T(60))

end
```

Example 3

cooling curve



Example 3

Answer:

(4) What are the bar temperatures in 5th, 10th, 30th, and 60th minutes? Roughly how many minutes are needed for the bar temperature reduces to half?

Temperature in 5th minute = 427.312000

Temperature in 10th minute = 160.191196

Temperature in 30th minute = 31.501002

Temperature in 60th minute = 30.001858

In about four minutes, the temperature is reduced to half.

SS-3.3 – Integration

SS: Scientific Simulation (Section)

SS-3: Computational Model (Chapter 3)

SS-3.3. Integration (Sub-section)

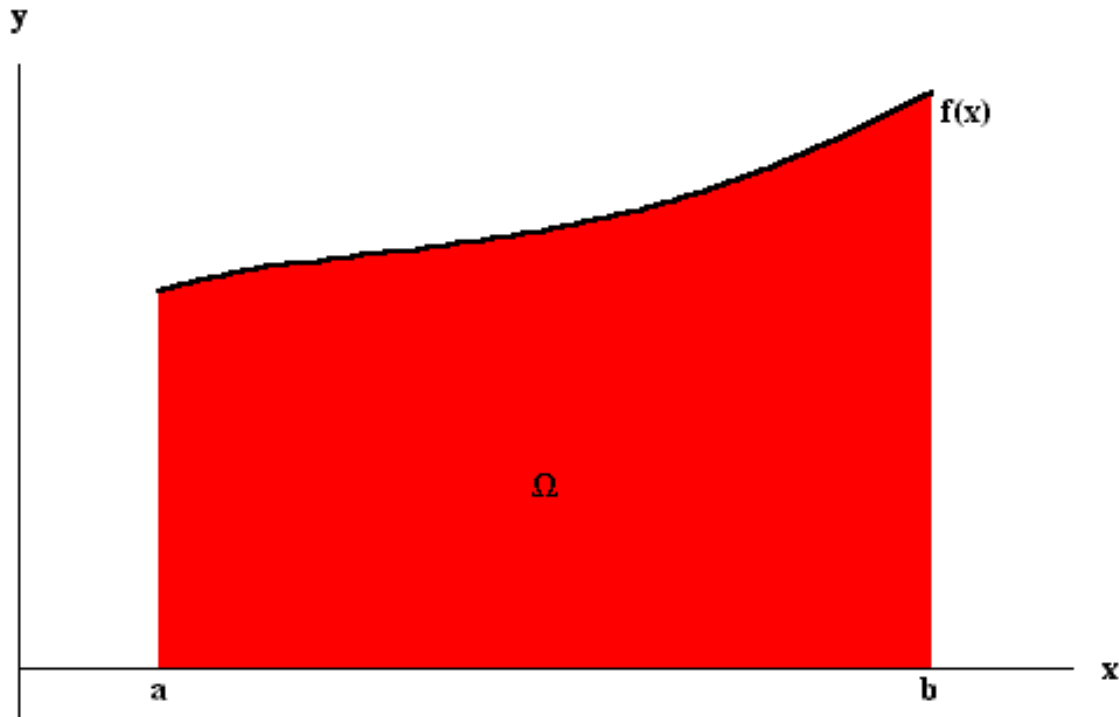
(March 28, 2013)

Integration

- **Integration is to find the sum of a function.**
 - It is related to differentiation. It is just exactly the opposite operation of a differentiation. Both integration and differentiation address the same scientific question
 - e.g., known the velocity, find the distance
 - One good analogy is of the relation between **division (differentiation) and multiplication (integration)**

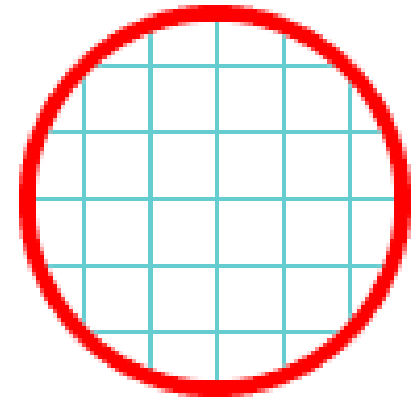
Integration

Integration can be defined as the total area enclosed by the function between the integration interval



Primitive Integration

- Primitive integration method has long been used by ancient mathematicians
- A good example is to find the area size of a circle, that leads to the discovery of π
 - The **piece-wise approach**
 - Count the small tiles with known size
 - The smaller the tile, the more accurate the circular area, thus the π
 - In other words, the smaller the sub-interval, the more the accuracy
 - For example. One circle has a radius of 1 meter. If filling the circle with 10 cm tiles, how many tiles will fit in?
 - The answer is ~ 314 , thus the π

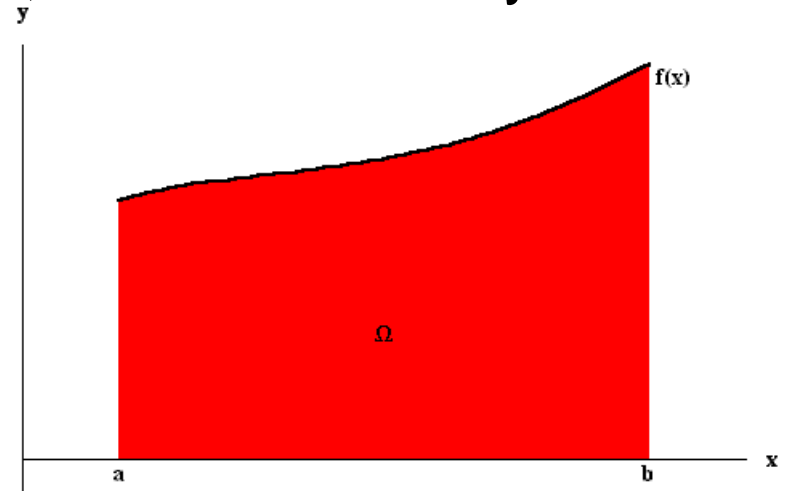


$$S = \pi r^2$$

Integration in Calculus

$$F = \int_a^b f(x) dx$$

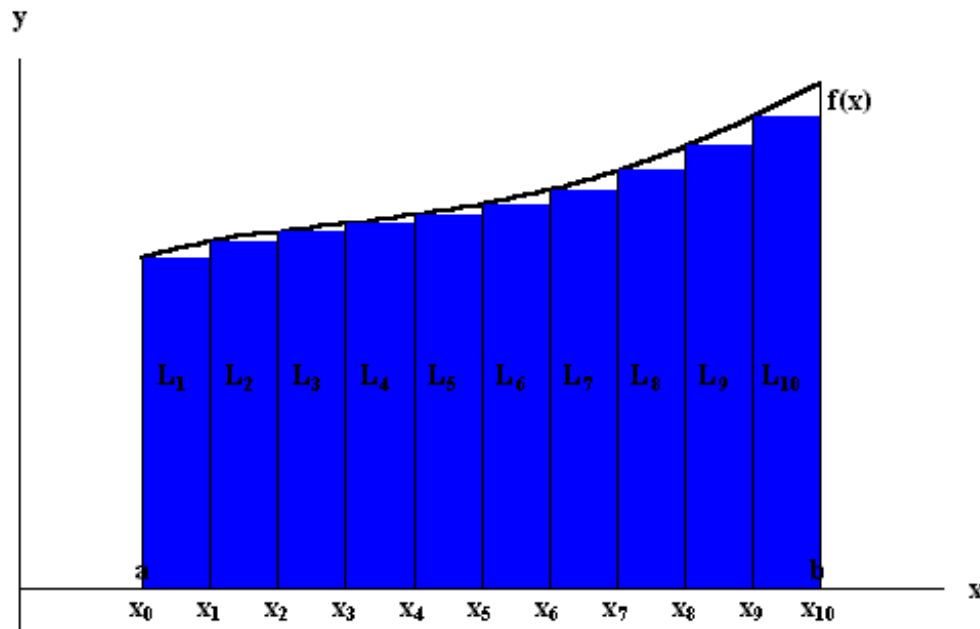
- $f(x)$: the given function
- F : integration
- $[a, b]$: the **interval** of the integration
 - a : lower limit, b : upper limit
- dx : the **sub-interval** of integration, which is infinitely small in calculus



Integration in Computation

Piece-wise Approach

The total area is approximated by the sum of the sizes of the rectangles ($L_1+L_2+L_3+\dots$). The size of each rectangle can be easily calculated over each sub-interval: $L_i = f(x_i) * \Delta x$, where Δx is a finite interval



Integration in Calculus to Integration in Computation

$$F = \int_a^b f(x) dx$$

$$dx \rightarrow \Delta x$$

$$f(x) \rightarrow f(x_i)$$

$$F = f(x_1) \cdot \Delta x + f(x_2) \cdot \Delta x + \dots + f(x_N) \cdot \Delta x = \sum_{i=1}^N f(x_i) \cdot \Delta x$$

N : number of rectangles , or number of iterations

Δx : sub - interval = $(b - a)/N$

$$x_i = x_1 + (i - 1) \cdot \Delta x$$

\Rightarrow

$$F(i + 1) = F(i) + f(x_i) \cdot \Delta x \quad \Rightarrow \quad F(N) \text{ is the result}$$

Example 1: $f(x)=x$

Question: integrate the function $f(x)=x$ from the interval $x=0$ to $x=5$.

$$f(x) = x$$

$$F = \int_0^5 x dx$$

- (1) Find the mathematical model of this integration question?
- (2) Take the number of sub-interval as 5, use your pencil to calculate the integration?
- (3) Implement a computational model. Write a MATLAB program to do the calculation. Find the values when the numbers of sub-interval are 10, 100, 1000, 10000 ,respectively

It is equivalent to find the area of a triangle with the base size of 5 and the height of 5.

The area value is expected to be 12.5

Example 1: $f(x)=x$

Answer:

(1) Find the mathematical model of this integration question?

$$F = \int_a^b f(x)dx$$

$$dx \rightarrow \Delta x$$

$$f(x) \rightarrow f(x_i)$$

$$F = f(x_1) \cdot \Delta x + f(x_2) \cdot \Delta x + \dots f(x_N) \cdot \Delta x$$

N : number of rectangles , or number of iterations

$$\Delta x : \text{sub - interval} = (b - a)/N$$

Algorithm for the computational model : the usage of iteration

$$x_1 = a$$

$$F(1) = f(x_1) \cdot \Delta x$$

$$x_i = x_{i-1} + \Delta x$$

$$F(i + 1) = F(i) + f(x_i) \cdot \Delta x \quad \text{until find } F(N)$$

Example 1: $f(x)=x$

Answer: Take the number of sub-interval as 5, use your pencil to calculate the integration?

$$\Delta x = (b - a) / N = (5.0 - 0) / 5 = 1.0$$

$$x(1) = a = 0;$$

$$x(2) = x(1) + \Delta x = 1.0$$

$$x(3) = x(2) + \Delta x = 2.0$$

$$x(4) = x(3) + \Delta x = 3.0$$

$$x(5) = x(4) + \Delta x = 4.0$$

$$F = x(1) \cdot \Delta x + x(2) \cdot \Delta x + x(3) \cdot \Delta x + x(4) \cdot \Delta x + x(5) \cdot \Delta x$$

$$F = (0 + 1.0 + 2.0 + 3.0 + 4.0) * 1.0 = 10.0$$

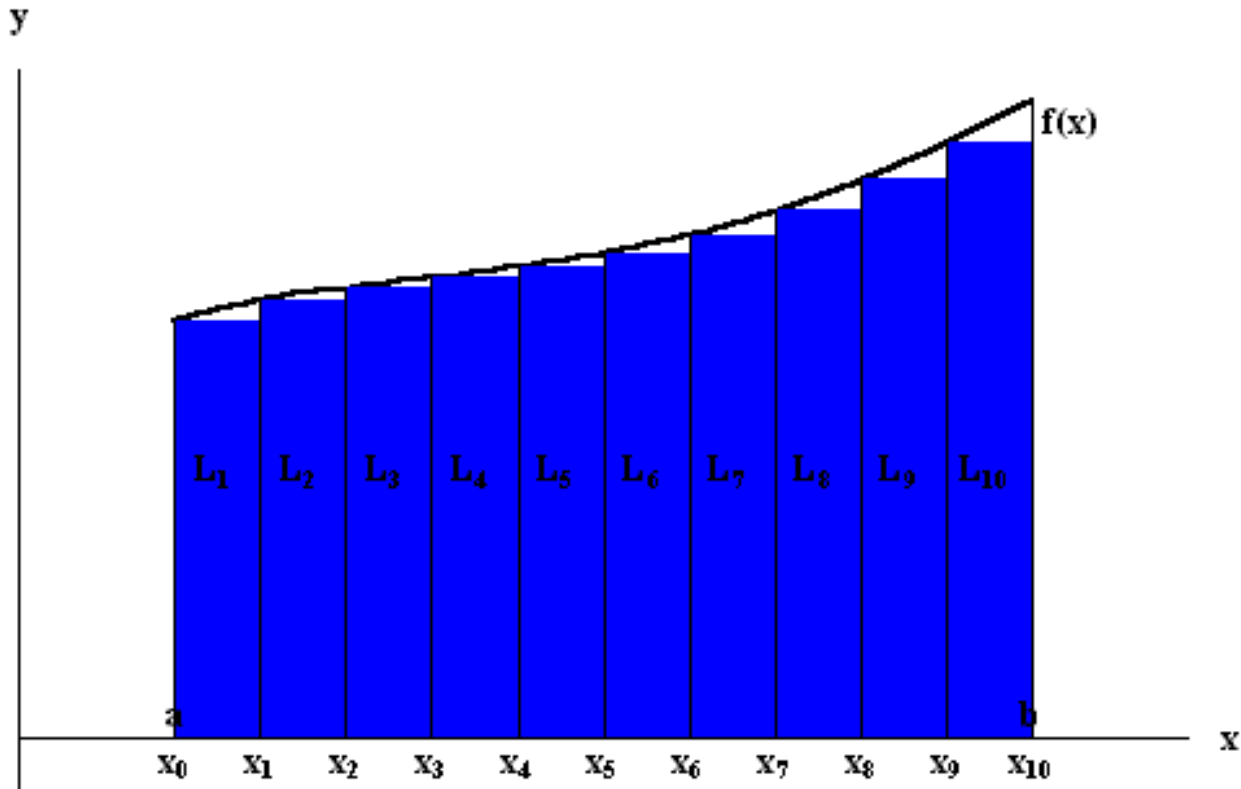
The approximate value (10.0) is smaller than the true value (12.5). Why?

**March 28, 2013 Stopped
Here**

April 02, 2013

Review: Integration

The total area is approximated by the sum of the sizes of the rectangles ($L_1+L_2+L_3+\dots$). The size of each rectangle can be easily calculated over each sub-interval: $L_i = f(x_i) * \Delta x$, where Δx is a finite interval



Review: Integration

$$F = \int_a^b f(x)dx$$

$$dx \rightarrow \Delta x$$

$$f(x) \rightarrow f(x_i)$$

$$F = f(x_1) \cdot \Delta x + f(x_2) \cdot \Delta x + \dots + f(x_N) \cdot \Delta x = \sum_{i=1}^N f(x_i) \cdot \Delta x$$

N : number of rectangles , or number of iterations

Δx : sub - interval = $(b - a)/N$

$$x_i = x_1 + (i - 1) \cdot \Delta x$$

\Rightarrow

$$F(i + 1) = F(i) + f(x_i) \cdot \Delta x \quad \Rightarrow \quad F(N) \text{ is the result}$$

Example 1: $f(x)=x$

“area1.m”

```
N=10; %number of rectangles, or iteration  
a=0; % lower limit  
b=5.0; % upper limit  
del_x=(b-a)/N; %the sub-interval
```

```
x(1)=a; % a=0  
F(1)=x(1)*del_x;
```

```
for i=[2:N]  
    x(i)=x(i-1)+del_x;  
    F(i)=F(i-1)+x(i)*del_x;  
end
```

```
F(N)
```

**F=11.25, getting closer to
the true value**

Example 1: $f(x)=x$

Using 10 rectangles: $N=10$, sub-interval $\Delta x=0.5$

$$F=11.2500$$

Using 100 rectangles: $N=100$, sub-interval $\Delta x=0.05$

$$F=12.3750$$

Using 1000 rectangles: $N=5000$, sub-interval $\Delta x=0.005$

$$F=12.4875$$

Using 10000 rectangles: $N=10000$, sub-interval $\Delta x=0.0005$

$$F=12.4988$$

Therefore, the smaller the sub-interval, the better the accuracy

Example 1: $f(x)=x$

“area1_input.m” %take input: number of interval

```
function A = area1_input(N)
a=0; % lower limit
b=5.0; % upper limit
del_x=(b-a)/N; %the sub-interval
```

```
x(1)=a; % a=0
F(1)=x(1)*del_x;
```

```
for i=[2:N]
    x(i)=x(i-1)+del_x;
    F(i)=F(i-1)+x(i)*del_x;
end
```

```
A = F(N);
```

```
return
end
```

>% call the function

>area1_input(10)

>area1_input(100)

>area1_input(1000)

>area1_input(10000)

Example 2: $f(x)=x^2$

Question: integrate the function $f(x)=x^2$ from the interval $x=0$ to $x=5$.

$$f(x) = x^2$$

$$F = \int_0^5 x^2 dx$$

- (1) Take the number of sub-interval as 5, use your pencil to calculate the integration?
- (2) Implement the computational model. Write a MATLAB program to do the calculation. Find the values when the numbers of sub-interval are 10, 100, 1000, 10000 ,respectively

Example 2: $f(x)=x^2$

Using 5 rectangles: $N=5$,

$$\Delta x = (b - a) / N = (5.0 - 0) / 5 = 1.0$$

$$x(1) = a = 0;$$

$$x(2) = x(1) + \Delta x = 1$$

$$x(3) = x(2) + \Delta x = 2$$

$$x(4) = x(3) + \Delta x = 3$$

$$x(5) = x(4) + \Delta x = 4$$

$$F = (x(1))^2 \cdot \Delta x + (x(2))^2 \cdot \Delta x + (x(3))^2 \cdot \Delta x + (x(4))^2 \cdot \Delta x + (x(5))^2 \cdot \Delta x$$

$$F = (0 + 1 + 4 + 9 + 16) \cdot 1 = 30$$

This approximate value is smaller than the true value (true value = 41.6666)

Example 2: $f(x)=x^2$

“area2.m” %take input: number of interval

```
function A = area2(N)
a=0; % lower limit
b=5.0; % upper limit
del_x=(b-a)/N; %the sub-interval
```

```
x(1)=a; % a=0
F(1)=x(1)^2*del_x;
```

```
for i=[2:N]
    x(i)=x(i-1)+del_x;
    F(i)=F(i-1)+x(i)^2*del_x;
```

```
end
```

```
A = F(N);
```

```
return
```

```
end
```

```
>% call the function
```

```
>area2(10) % 35.6250
```

```
>area2(100) %41.0437
```

```
>area2(1000) %41.6042
```

```
>area2(10000) %41.6604
```

SS-4: Scientific Method

(April 02, 2013)

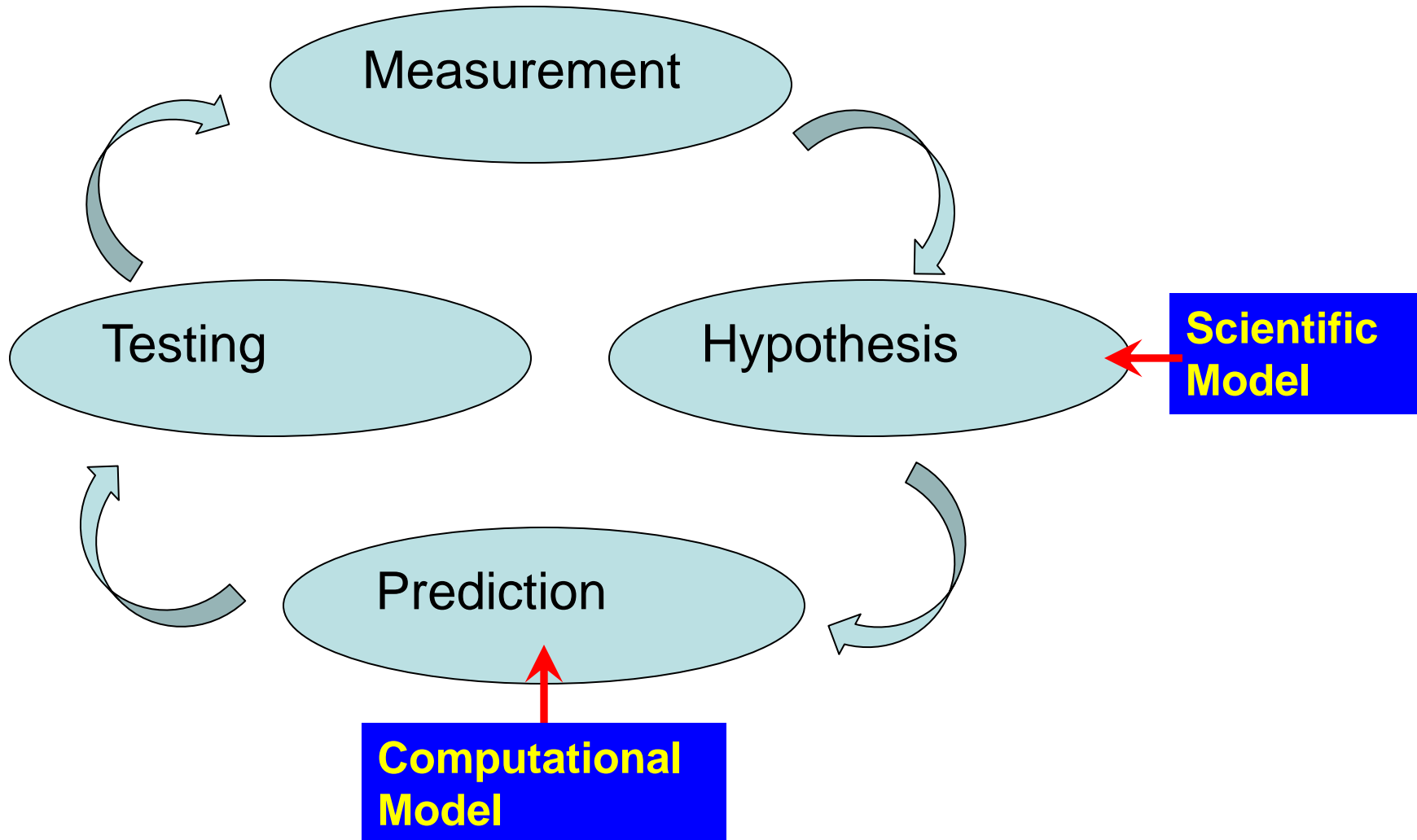
Scientific Method

- Four essential elements of a scientific method:

1. Measurement (or observation)
2. Hypothesis
3. Prediction
4. Testing

- It is an iterative process until the prediction is consistent with the measurement
- The hypothesis becomes a theory.

Scientific Method



The End

(April 02, 2013)