Fundamentals of Computational Biology – U2

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Lotka – Voltera model or prey – predator model

$$\frac{d(Prey)}{dx} = Rate\ of\ pruction\ - predation - death$$

$$\frac{d(Predator)}{dx} = Rate\ of\ pruction\ - death$$

$$or$$

$$\frac{d(Prey)}{dx} = f(prey) - f(predator) - f(prey)$$

$$\frac{d(Predator)}{dx} = f(predator) - f(predator)$$

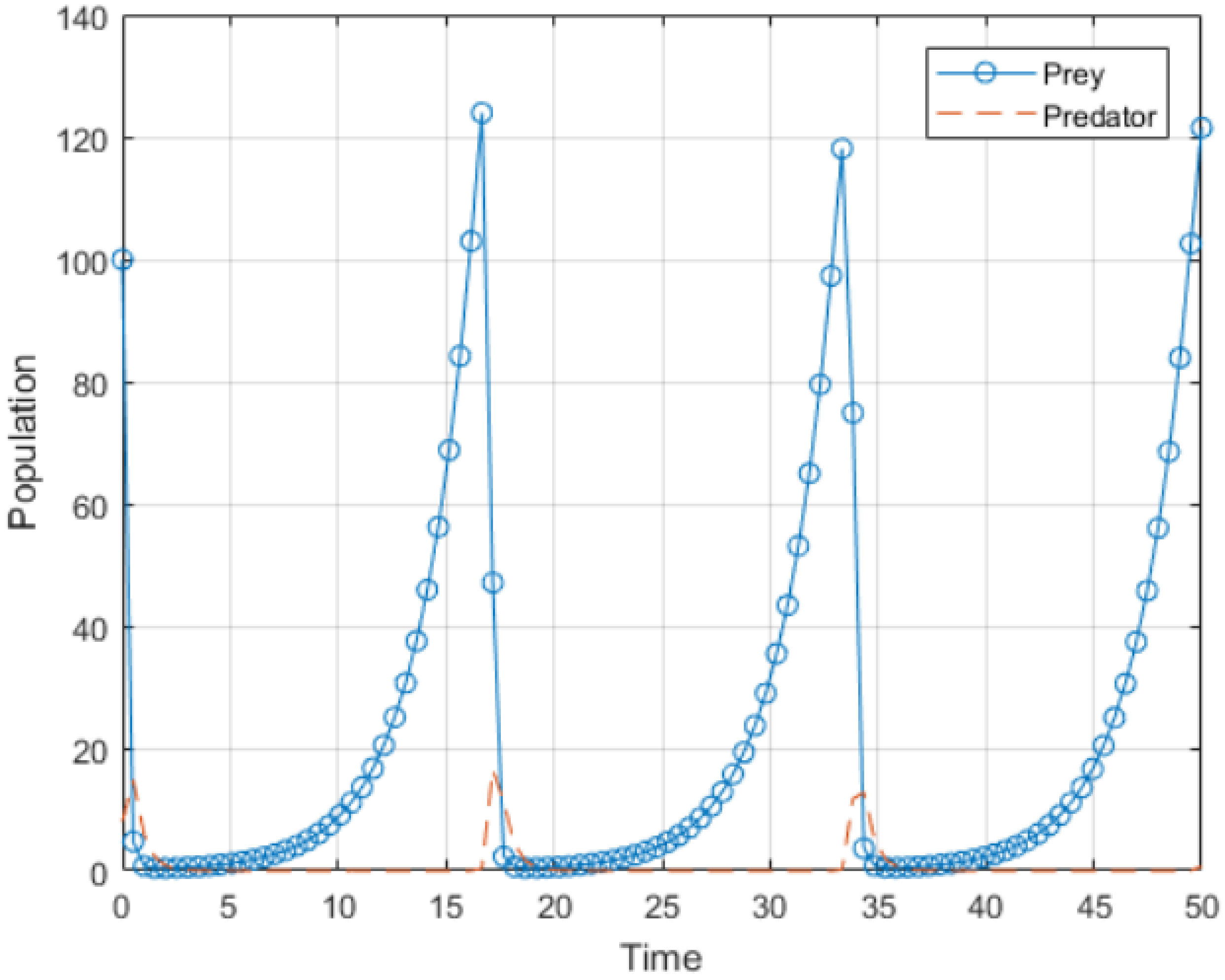
Mathematical model

$$\frac{d(prey)}{dx} = \frac{dR}{dt} = kR - aRW - k_{dr}R$$

$$\frac{d(predator)}{dx} = \frac{dW}{dt} = bRW - k_{dw}W$$

k = 0.08, *a* = 0.001, *kdr* = 0.02, *b* = 0.0002, kdw= = 0.0002

Solving LV model



Matlab codes

```
function dxdt = f2(t,x)
dxdt = [0;0];
alpha = 0.4; beta = 0.4; delta = 0.09; gamma = 2.0;
dxdt(1) = alpha*x(1) - beta*x(1)*x(2); %prey
dxdt(2) = delta*x(1)*x(2) - gamma*x(2); %predators


y0 = [100;8];
soln = ode45(@f2,[0 100],y0)


t = linspace(0,50,100);
y(:,1) = deval(soln,t,1); %Prey
y(:,2) = deval(soln,t,2); %Predator
%Predator-prey function


figure
plot(t,y(:,1),'-o',t,y(:,2),'--');
grid on;
legend('Prey','Predator');
xlabel('Time');
ylabel('Population');
```

Population dynamics:

- Probability recap:
- Probability of a coin toss?
- Probability of two coin toss? Two heads? At lease one head?
- Probability of one queen from a deck of cards?
- Two cards drawn randomly, what is the probability of getting card jack of diamond and other card as a king?

Population dynamics

- A population is a group of individuals of the same species living in the same general area.

- Density
  - Is the number of individuals per unit area or volume.
- Dispersion
  - Is the pattern of spacing among individuals within the boundaries of the population.

- Immigration and birth add individuals whereas death and emigration remove individuals.

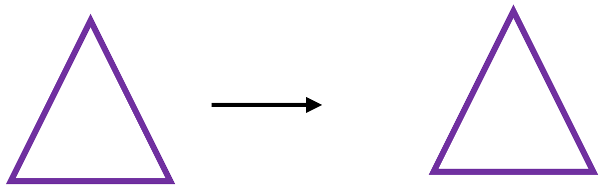
- Steady state population = $birth + immigration - death - emigration$

Population dynamics

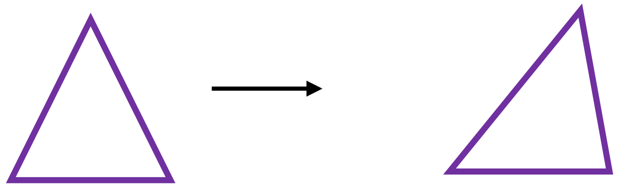
Different factors that can affect the effective population size?

- Birth rate?
- Death rate?
- Recourse availability?
- Competing species?
- Predators?
- Survival strategies?
- Migration if any?
- Robustness vs evolvability?

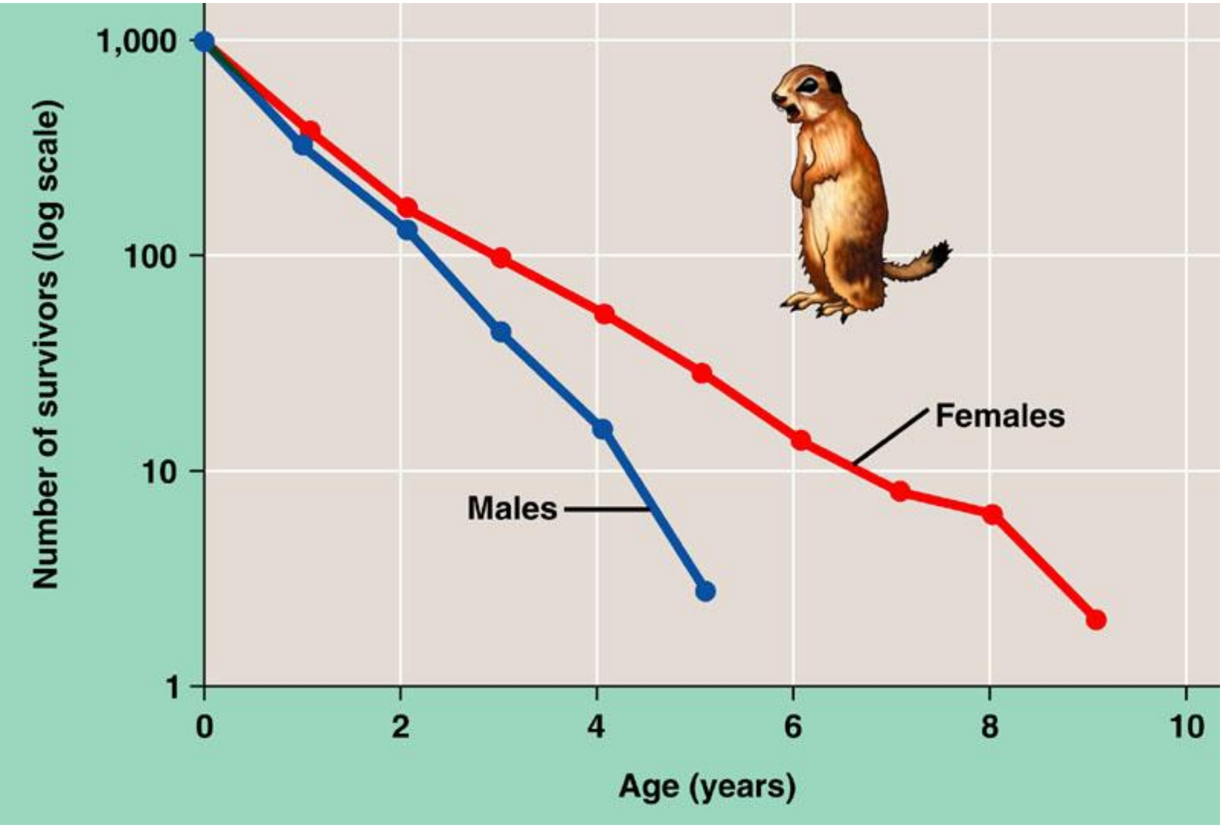
- Robustness?

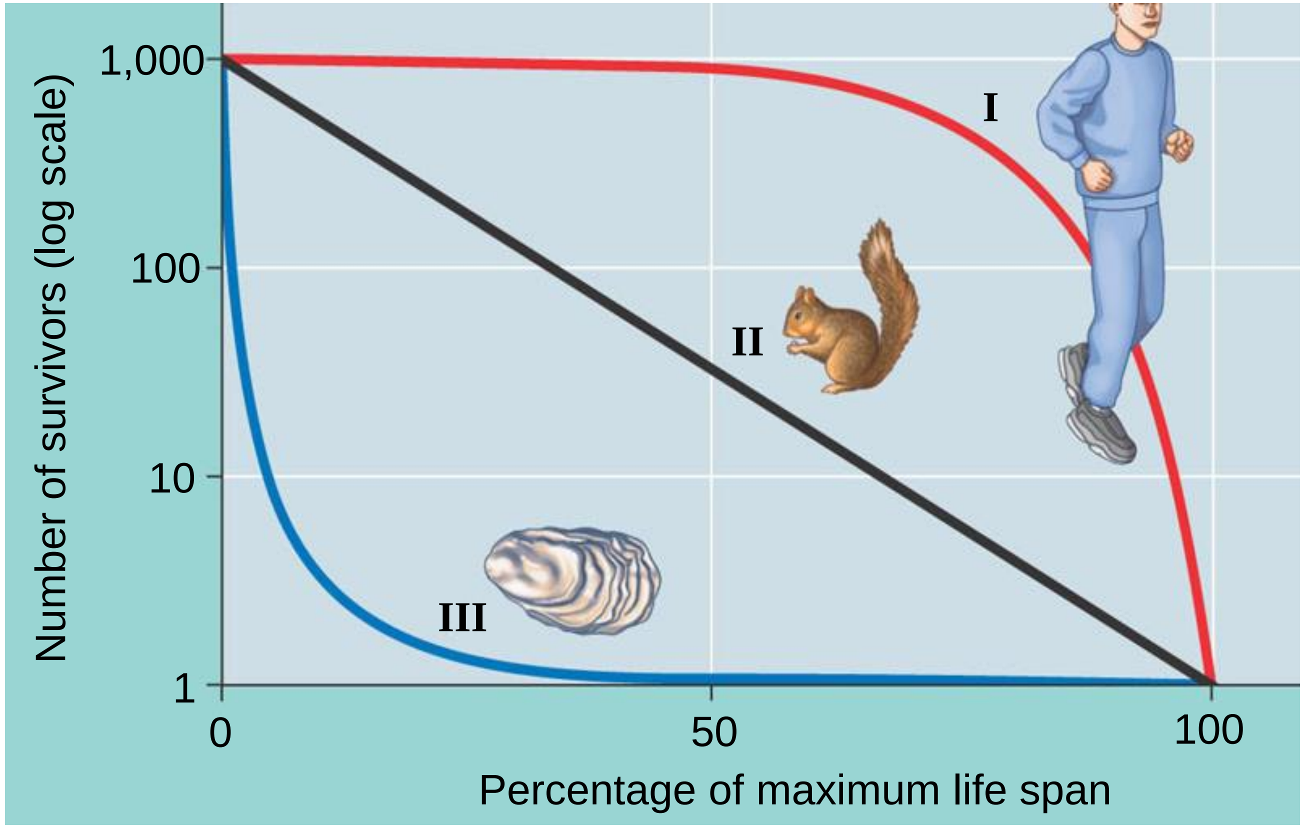


- Evolvability?

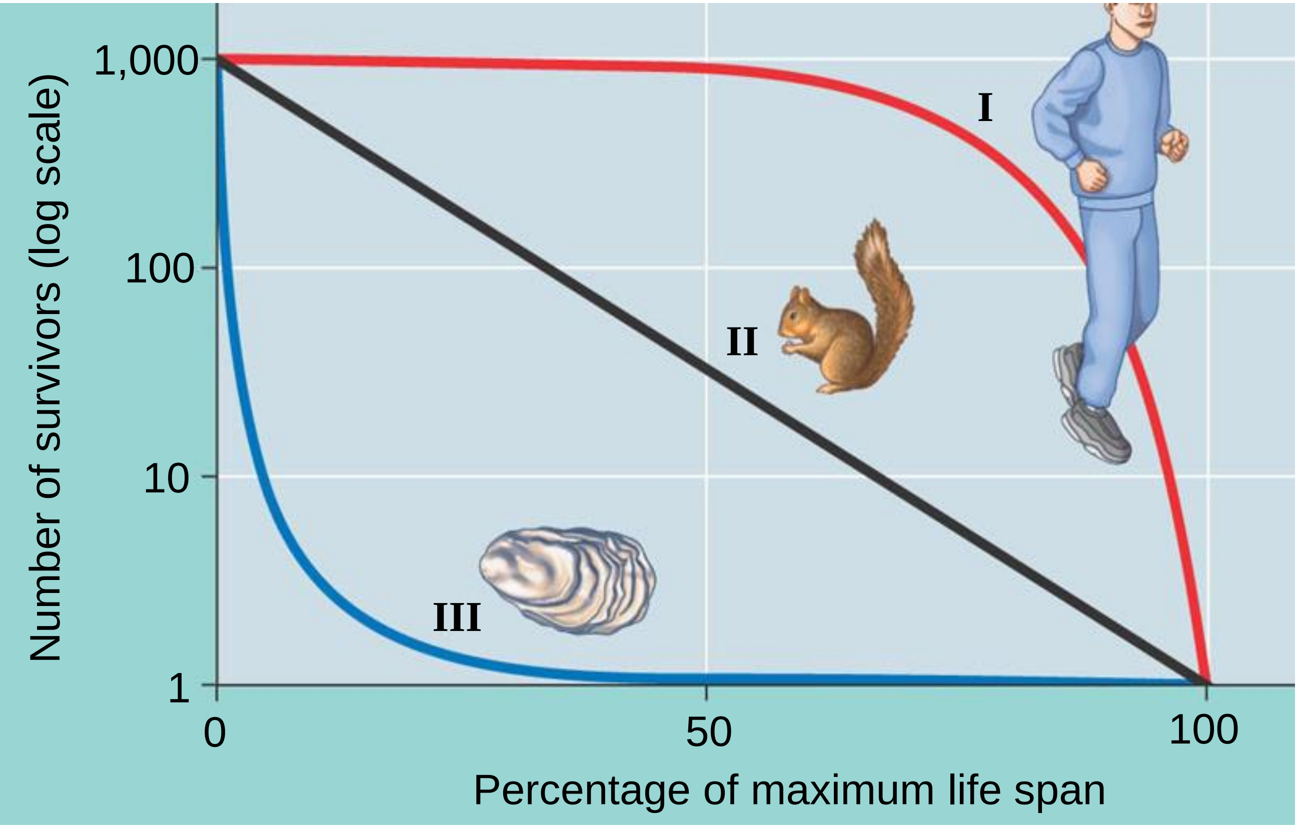


Survivors plot





Decay rates



$$\frac{dN}{dx} = -kN$$

The Logistic Growth Model

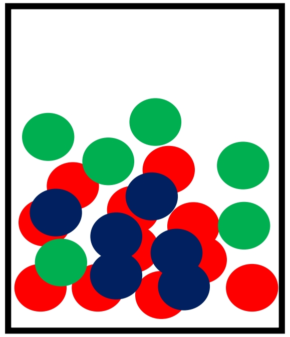
- Exponential growth cannot be sustained for long in any population.
- A more realistic population model limits growth by incorporating carrying capacity.
- Carrying capacity (*K*) is the maximum population size the environment can support

$$\frac{dN}{dt} = r_{max} N \frac{(K - N)}{K}$$

Survival models

Ball in a Jar Experiment.

10 R, 10 B, 10 G balls



→ Draw a ball randomly
Note down its colour.

→ put the ball back in Jar.
Add an extra same colour ball
Remove a ball randomly so that total numbers will be always constant.

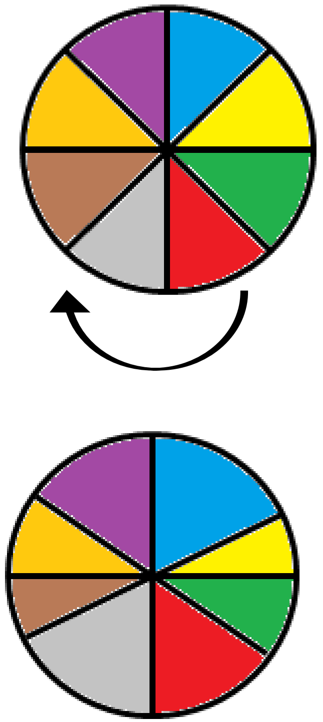
→ Repeat the experiment.

After n repetition, please predict the outcomes of this experiment.

This is a great coding problem, please try to solve it.

Survival models

Fly-wheel experiment

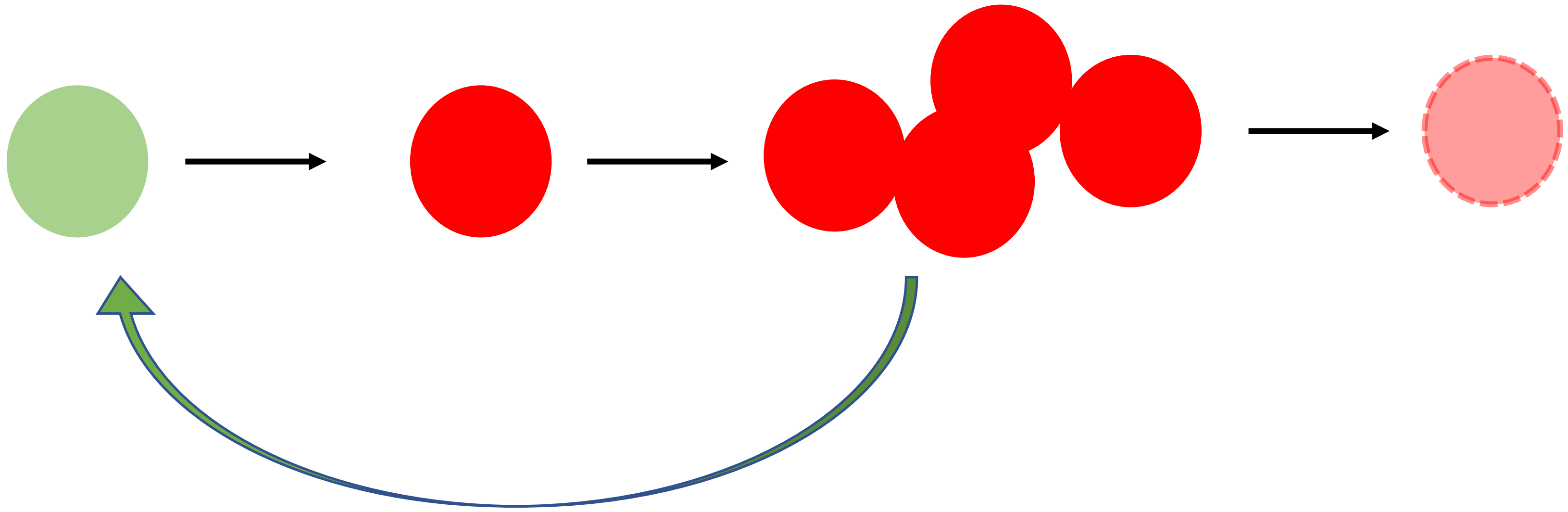


- Throw a dart in the rotating fly-wheel, select a section.
- Increase the area associated with selected section and randomly decrease same area from any of the section randomly.
- Repeat the experiment.

After n repetition, please predict the outcomes of this experiment.

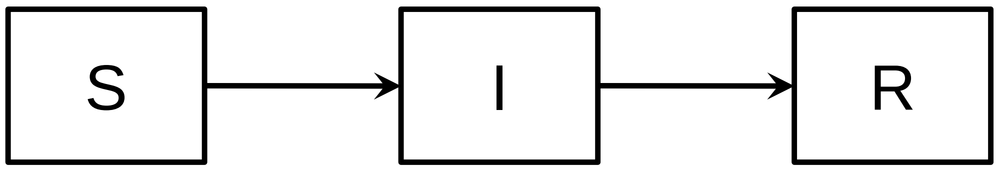
Try to code this guys.

Modelling infectious diseases



- A healthy individual becomes susceptible for infection.
- Once it catches infection, it further increase the number of healthy individuals to infected one.

SIR Model



S – Susceptible individuals

I – Infected individuals

R – Recovered individuals

- Large population
- Single initial case
- Rest of the population is fully susceptible

Examples:

- Influenza pandemics
- SARS
- Ebola

SIR Model

$S \rightarrow I \rightarrow R$

$$\frac{dS}{dt} = -\beta\frac{SI}{N}$$

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

$$\frac{dR}{dt} = \gamma I$$

$$N = S + I + R = constant$$

Where:

β is rate at which infection is spreading

γ is rate of recovery

N is total effective population

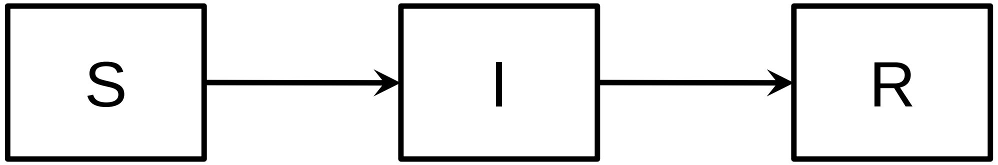
Initial conditions:

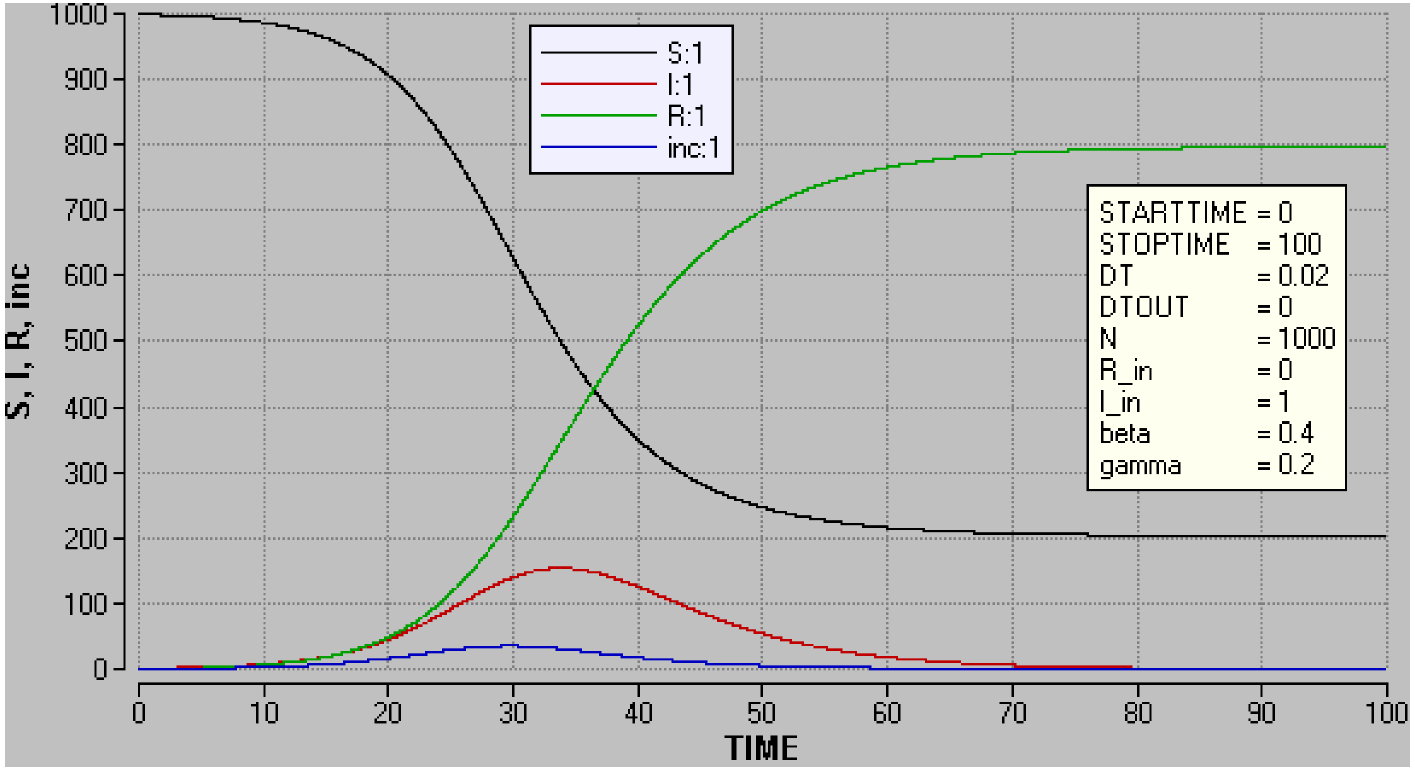
S(0)= S_{in}

I(o)= I_{in}

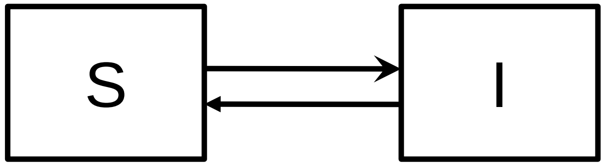
R(0)= R_{in}

SIR Model


S
I
R


S, I, R, inc
TIME
S:1
I:1
R:1
inc:1
STARTTIME = 0
STOPTIME = 100
DT = 0.02
DTOUT = 0
N = 1000
R_in = 0
I_in = 1
beta = 0.4
gamma = 0.2

SIS Model



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

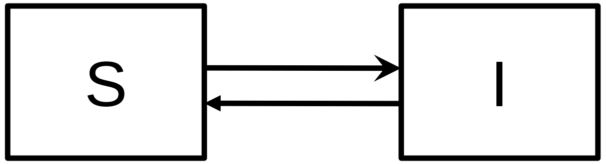
$$\frac{dI}{dt} = \beta \frac{SI}{N} - \gamma I$$

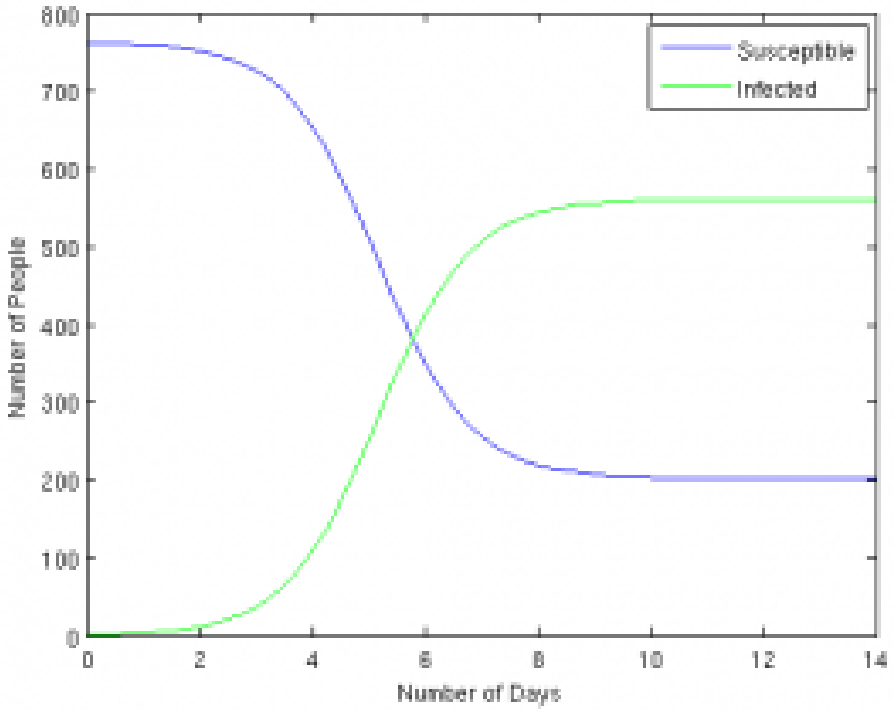
Examples:

- Chlamydia
- Human papilloma virus
- (Respiratory syncytial virus / influenza)

$$N = S + I = constant$$

SIS Model


S
I


Susceptible
Infected
Number of People
Number of Days
800
700
600
500
400
300
200
100
0
0
2
4
6
8
10
12
14

Threshold condition

- A large epidemic occurs if and only if

$$\beta > \gamma$$

- During the ’80s (HIV epidemic), biologists and epidemiologists stepped in, interpreting it as:

$$\beta / \gamma > 1$$

Basic reproduction number R_0

β = Average number of new cases generate by a single case, per unit of time, in a totally susceptible population

$\frac{1}{\gamma}$ = Average duration of the infectious period

$$\boxed{R_0 = \frac{\beta}{\gamma}}$$

- Called basic reproduction number
- Defined as the average number of new cases, generated by a single case, throughout the infectious period, in a totally susceptible population
- An epidemic occurs if and only if

$$R_0 > 1$$

R_0 for some infectious diseases

- Measles 12-18
- Mumps 4-7
- HIV/AIDS 2-5
- Influenza 2-3

Outbreak in a Cup: Set Up

- Set up the Initial Conditions:
  - 20 red beans
  - 1 white bean
- Without looking in the cup, a student from the group selects 2 beans from the cup.
- If both beans are the same color, simply return the beans.
- If one bean is red and the other white, remove the red bean and return 2 white beans to the cup.
- At each time step, record the event that occurs: either no change or a new infection.
- Repeat the process until told to stop.

Vaccination efficacy

Vaccine effectiveness: Reduced chance of disease in vaccinated group as compared to unvaccinated group.

80% efficacy means, 80% decrease in diseased condition among vaccinated group as compared to un-vaccinated population.

VE=(1-1/RR)x 100,
where RR is relative risk of developing disease among vaccinated group as compared to unvaccinated group.

VE=$\frac{ARU-ARV}{ARU}x100$

Where, ARU is attack rate of Unvaccinated people, ARV is attack rate of vaccinated people

Vaccination efficacy

- 24 infection reported to 12000 vaccinated individuals.
- 124 infection reported with unvaccinated 10000 individuals.
- Calculate the vaccine efficacy?

- RR= $\frac{(124/10000)}{(24/12000)} = 6.2$
- VE = (1-1/6.2)*100 = 83.9%

Or

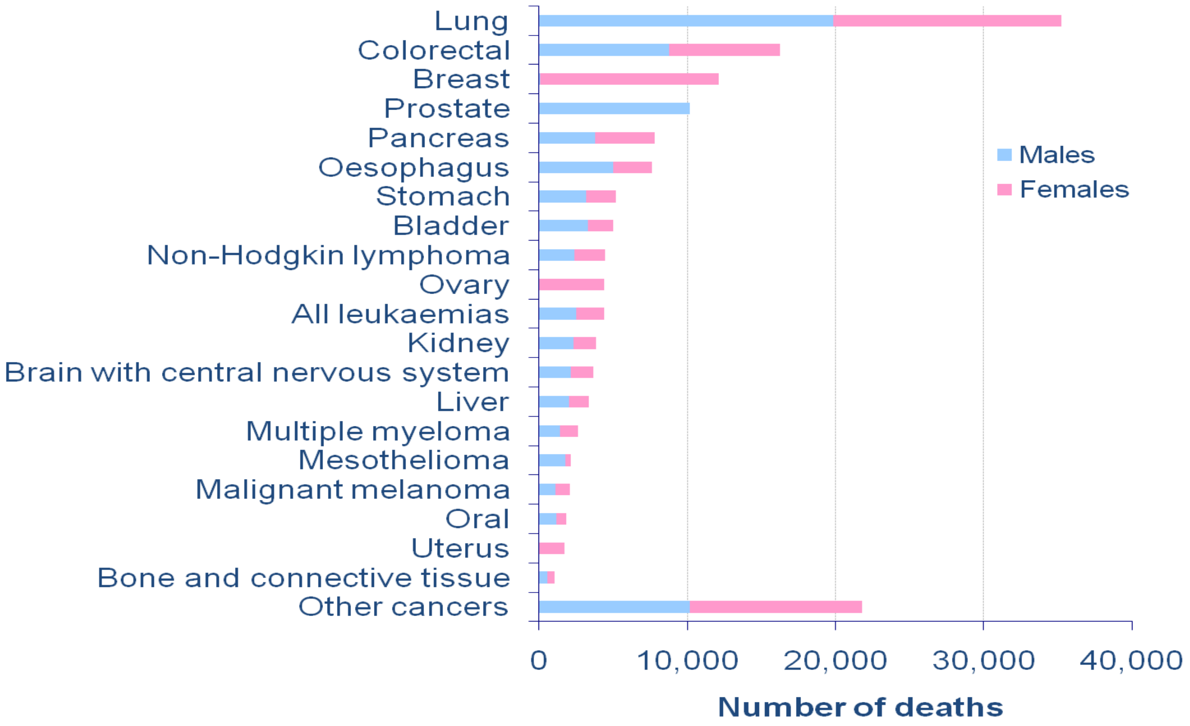
VE = $\frac{(124/10000)-(24/12000)}{(124/10000)} = 83.9\%$

Cancerous spread

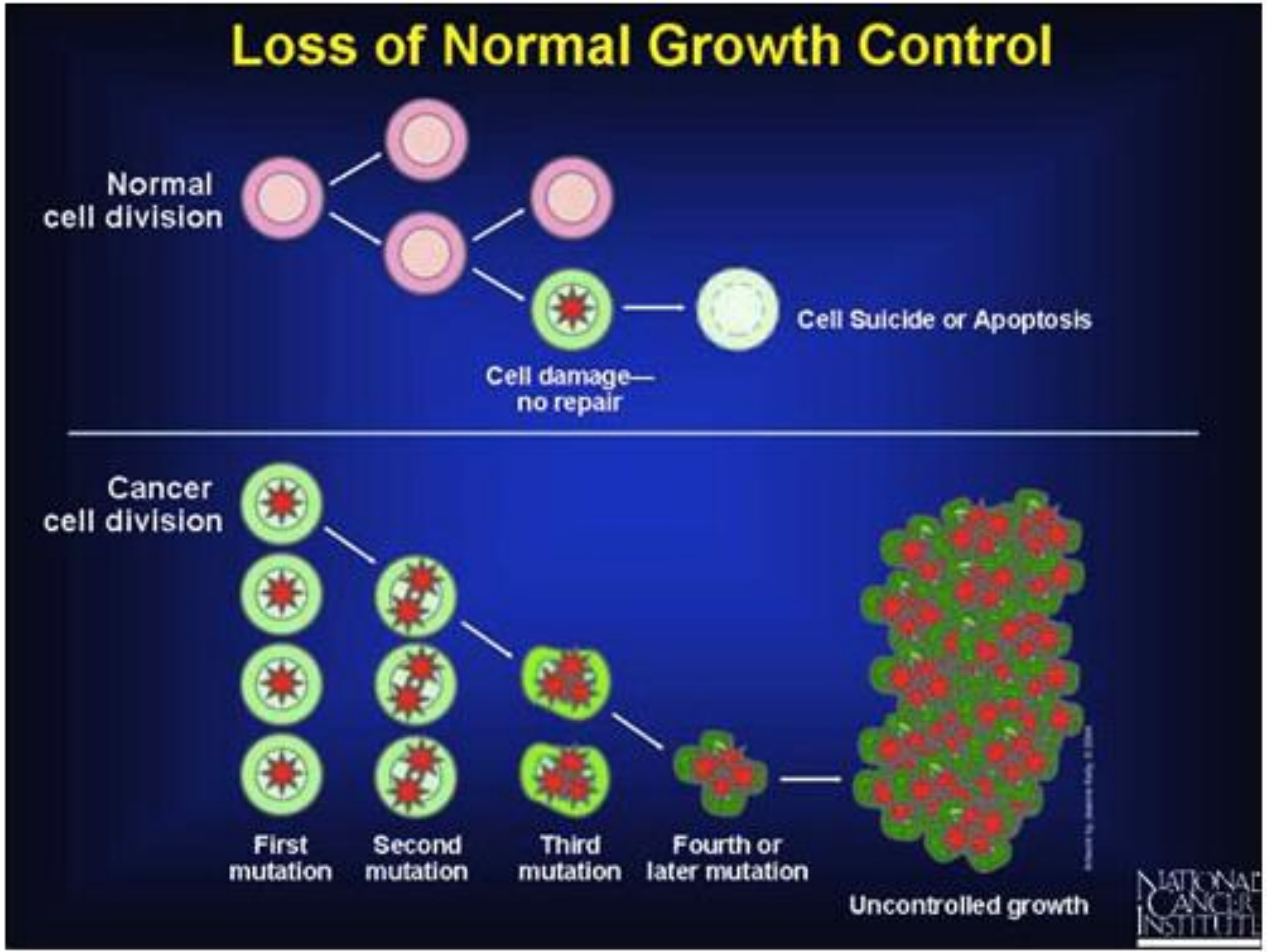
- What is a cancer?
  - a term used for diseases in which abnormal cells divide without control and are able to invade other tissues
  - Cancer cells spread to other parts of the body through the blood and lymph systems
  - More than 200 different types of cancer
  - All cancers derive from single cells that have acquired the characteristics of continually dividing in an unrestrained manner and invading surrounding tissues.
  - Cancer cells behave in this abnormal manner because of changes in the DNA sequence of key genes, which are known as cancer genes. Therefore all cancers are genetic diseases.

Cancerous spread

- One in three people in the Western world develop cancer and one in five die of the disease
- There are approximately 200 types of cancer, each with different causes, symptoms and treatments
- An individual's risk of developing cancer depends on many factors, including age, lifestyle and genetic make-up



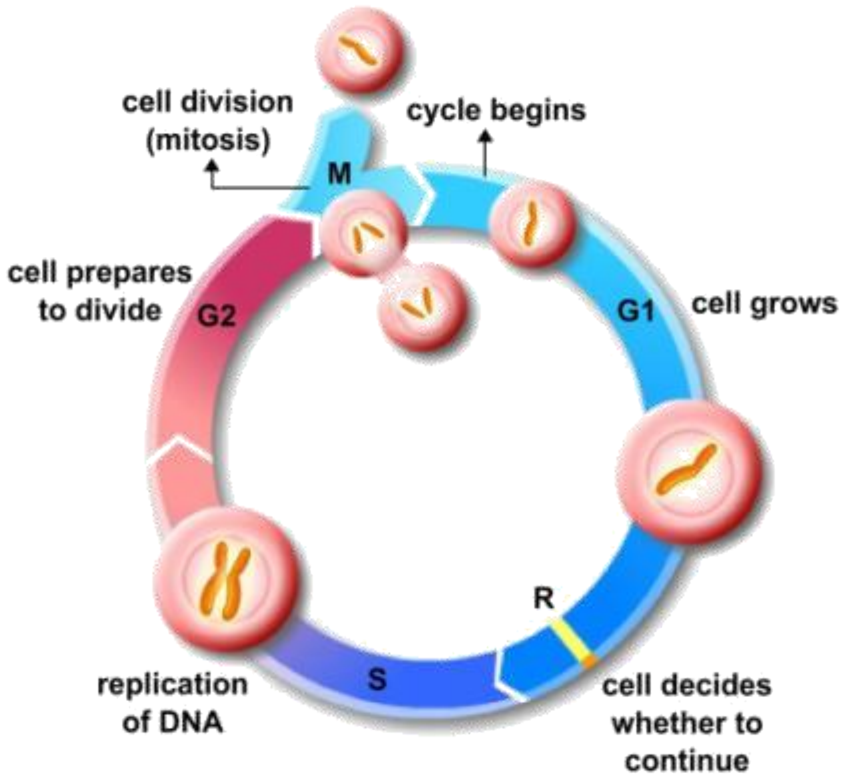
Cancerous spread



Main Categories

- **Carcinoma** - cancer that begins in the skin or in tissues that line or cover internal organs. There are a number of subtypes of carcinoma: adenocarcinoma, basal cell carcinoma, squamous cell carcinoma, transitional cell carcinoma.
- **Sarcoma** - cancer that begins in bone, cartilage, fat, muscle, blood vessels, or other connective or supportive tissue.
- **Leukemia** - cancer that starts in blood-forming tissue such as the bone marrow and causes large numbers of abnormal blood cells to be produced and enter the blood.
- **Lymphoma and myeloma** - cancers that begin in the cells of the immune system.
- **Central nervous system cancers** - cancers that begin in the tissues of the brain and spinal cord.

Cell cycle in cancer cells



Tumour suppressor genes (TSG) code for proteins that slow down cell growth. They can halt the cell growth cycle to stop unnecessary division or promote apoptosis (cell death) if the cell's DNA is damaged.