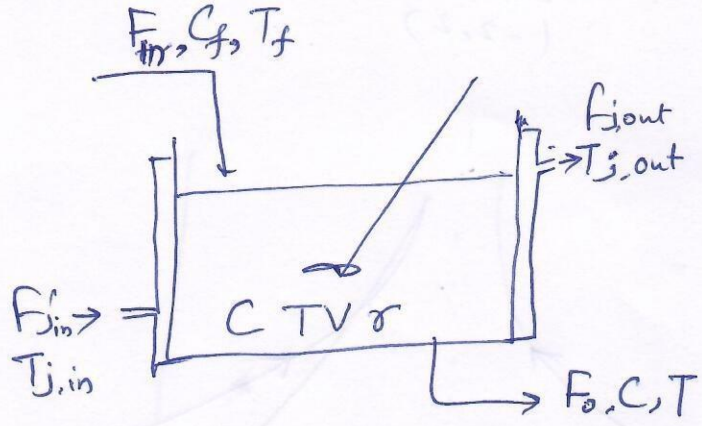
Week 6

Application : Reactor stability analysis $\quad A \rightarrow B$

$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r \qquad \text{(Component balance)}$$

$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho C_p}\right) r - \frac{UA}{V\rho C_p}(T - T_j) \qquad \text{(Energy balance)}$$



Concentrations & Temp. in the reactor = ?

complete mixing

CSTR.

Uniform mixing.

1^{st} order

Irreversible.

$r = KC_A$

$$\frac{dh}{dt} = \frac{1}{A}(q_1 - q_2)$$

$$\frac{dV\rho}{dt} = F_{in}\rho_{in} - F_{out}\rho$$

$$\frac{dVC}{dt} = F_{in}C_f - F_{out}C - rV$$

$$F_{in} = F_{out} = F \; ; \; \frac{dV}{dt} = 0$$

let ρ = constt.

~~$\frac{dV}{dt}$ ... F_{in} F_{out}~~ (1)

B.

from <u>Component balance & Energy balance</u>

Dynamical ~~[illegible]~~ variable $[C \ T]'$

2nd order system
Non-linear system

at steady state

$$\frac{dc}{dt} = 0$$

$$\frac{F}{V}(C_f - C_s) - r = 0$$

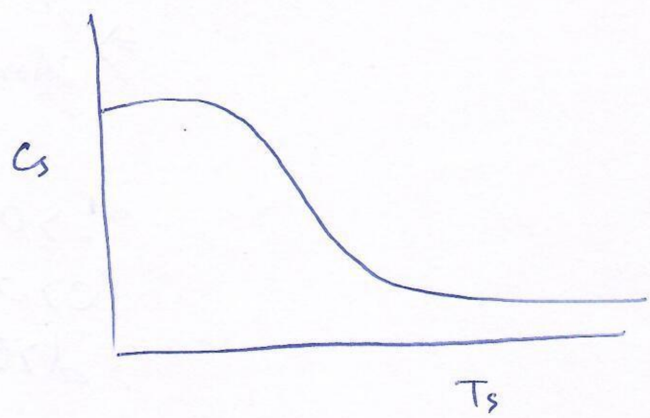
$$\frac{F}{V}(C_f - C_s) - k_0 e^{-E/RT_s} C_s = 0 \Rightarrow \frac{F}{V}C_f - \frac{F}{V}C_s - k_0 e^{-E/RT_s} C_s = 0$$

$$\boxed{C_s = \frac{\frac{F}{V}C_f}{\frac{F}{V} + k_0 e^{-E/RT_s}}}$$

let $\frac{F C_f}{V} = a$; $\frac{F}{V} = b$

$\frac{-E}{R} = c$

$$C_s = \frac{a}{b + k_0 e^{c/T_s}}$$



Also,

$$\frac{dT}{dt} = 0$$

$$\frac{F}{V}T_f - \frac{F}{V}T_s + \left(\frac{-\Delta H}{\rho C_p}\right) k_o e^{-E/RT_s} \left(\frac{\frac{F}{V}C_f}{\frac{F}{V} + k_o e^{-E/RT_s}}\right) - \frac{UA}{V\rho C_p} \cdot T_s$$

$$+ \frac{UA}{V\rho C_p} T_j = 0$$

$$\underbrace{\left(\frac{F}{V} + \frac{UA}{V\rho C_p}\right)T_s - \left(\frac{FT_f}{V} + \frac{UAT_j}{V\rho C_p}\right)} = \frac{\left(\frac{-\Delta H}{\rho C_p}\right) k_o e^{\frac{-E}{RT_s}} \left(\frac{FC_f}{V}\right)}{\left(\frac{F}{V}\right) + k_o e^{-E/RT_s}}$$

let

$$\frac{F}{V} + \frac{UA}{V\rho C_p} = p$$

$$\frac{FT_f}{V} + \frac{UAT_j}{V\rho C_p} = q$$

$$LHS = pT_s - q \Rightarrow \text{linear}$$

$$\frac{-\Delta H k_o FC_f}{V\rho C_p} = a$$

$$\frac{E}{R} = b \; ; \; \frac{F}{V} = c ;$$

$$k_o = d$$

$$RHS = \frac{a e^{-\frac{b}{T_s}}}{c + d e^{-b/T_s}}$$

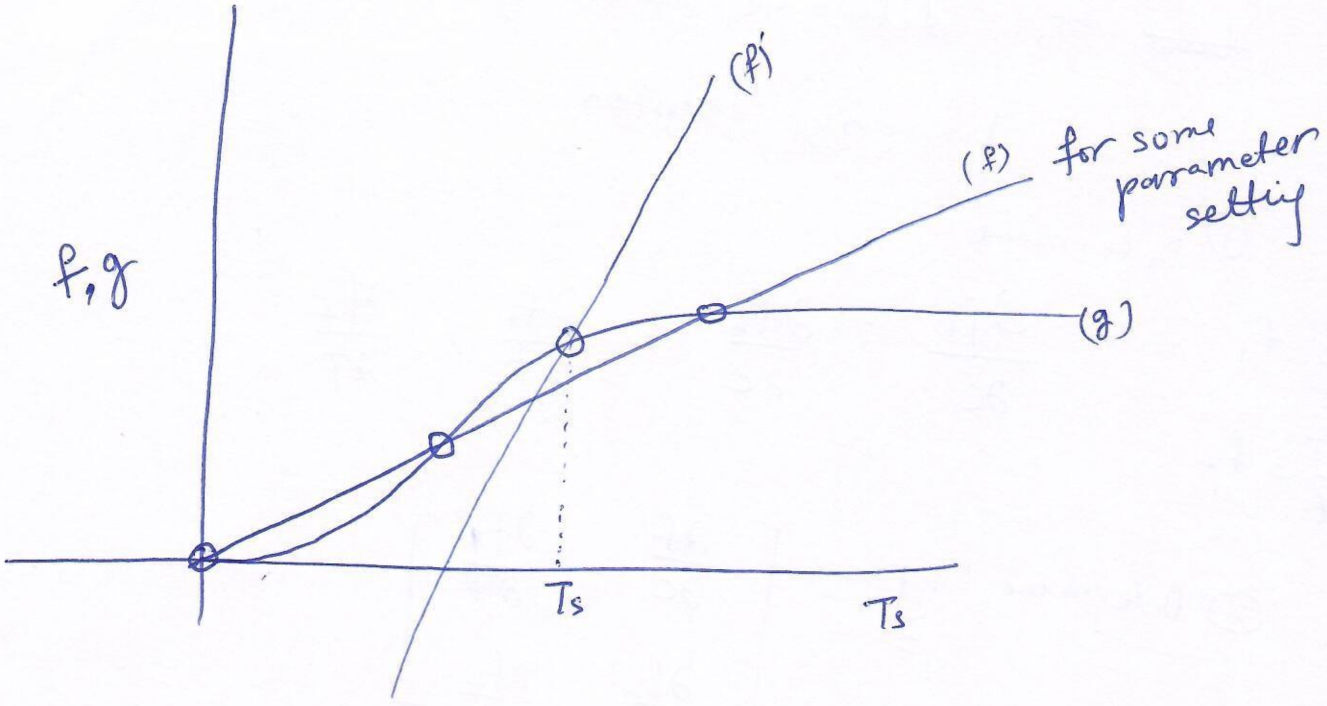
$\Rightarrow$ Non-linear

$b > 0$

$c > 0$

$d > 0$

a may be positive or negative depending on exothermic or endothermic

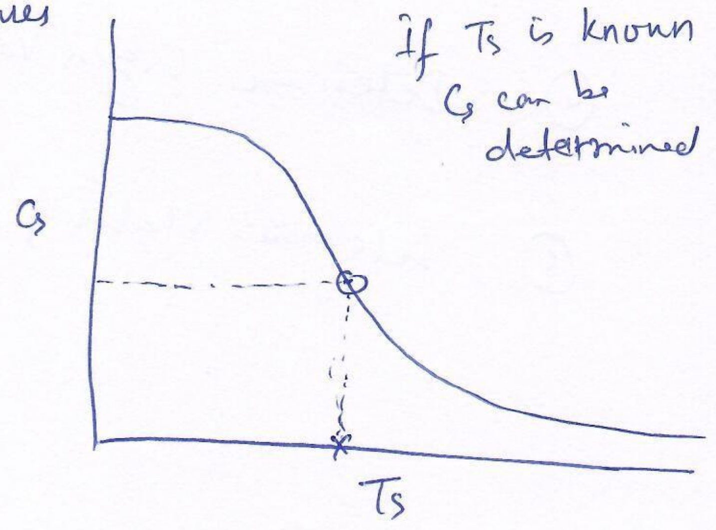


Intersection of LHS & RHS should give steady state
(f) (g)

⇒ 3 steady state temperatures

⇓

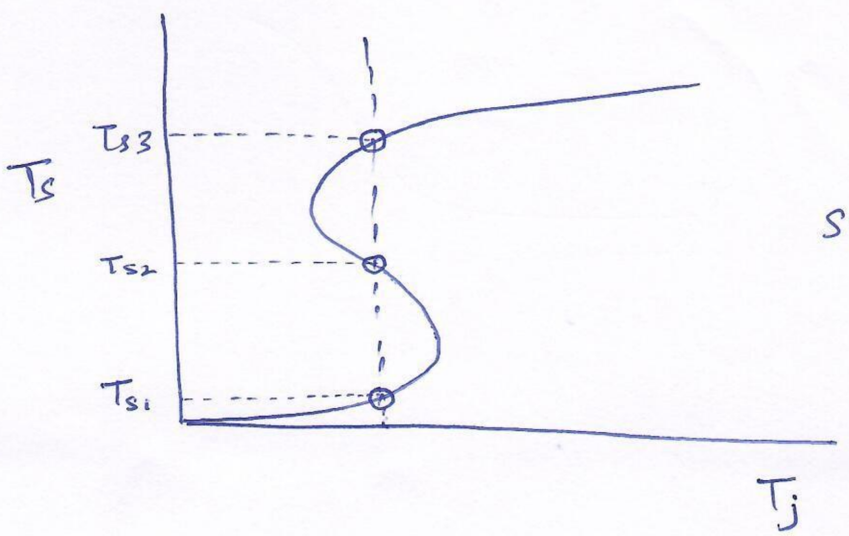
WHAT IS THE STABILITY OF THESE SOLUTIONS ?



if T_s is known C_s can be determined

We can draw T_s vs T_j

DIY



STABILITY ??

~~this~~ To determine stability —

linearize system

① Determine

$\frac{dC}{dt} = f_1$ $\qquad \frac{\partial f_1}{\partial C}$; $\frac{\partial f_2}{\partial C}$; $\frac{\partial f_1}{\partial T}$; $\frac{\partial f_2}{\partial T}$

$\frac{dT}{dt} = f_2$

② Determine $\underline{\underline{J}} = \begin{bmatrix} \frac{\partial f_1}{\partial C} & \frac{\partial f_1}{\partial T} \\ \frac{\partial f_2}{\partial C} & \frac{\partial f_2}{\partial T} \end{bmatrix}$

③ Determine $\underline{\underline{J}}$ at steady states. (T_{S1}, T_{S2}, T_{S3})

④. Determine Eigen Values.

⑤ Determine stability based on Eigen Values.

Example 2 - Analysis of infectious disease dynamics

Population changes w.r.t time
↳ Dynamical system

Kermack - Mckendrick (SIR) model (1927)

Assumptions :-

1. Total population is constant
2. Population is divided into 3 compartment

$S \rightarrow$ Susceptibles (can catch disease)

I.- Infectives (can transmit)

R- Removed. [Recovered, deaths, etc.]

3. Recovery confers immunity to the individual
4. Incubation period is zero
5. population is well-mixed

Mathematically

Gain in infective class $\propto$ no. of infectives & susceptibles

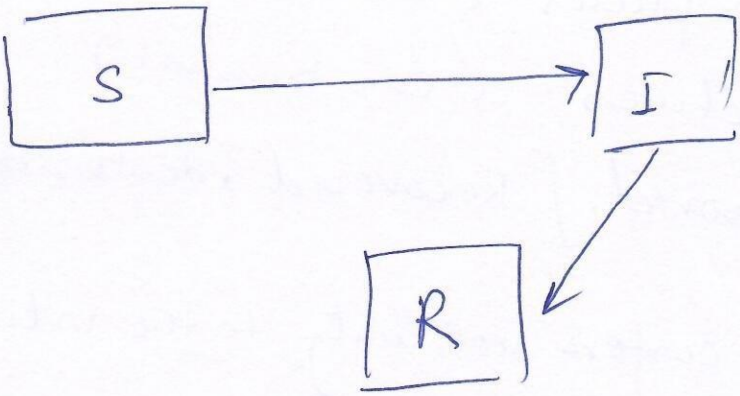
$$\frac{dI}{dt} = r S I \qquad r = \text{constt.}$$

rate of removal of infectives $\propto$ no. of infectives

$$\frac{dI}{dt} = -aI \qquad a \to \text{parameter constt.}$$

Combining

$$\frac{dI}{dt} = rSI - aI$$



$$S \to \boxed{I} \to R$$
$$rSI - aI$$

$$\frac{dS}{dt} = -rSI$$

$$\frac{dR}{dt} = aI$$

Initial conditions

$S(0) = S_0$

$I(0) = I_0$

$R(0) = 0$

$r > 0$ infection rate

$a > 0$ removal rate

Q. Given r, a, S_0 and the initial number of infectives I_0, whether the infection will spread or not ?

Q. If it spread, How will it develop with time ?

Q When will it start to decline ?

Q. When do you declare the spread of an infection disease an epidemic ?

Dynamical Variables $= [S \ I \ R]'$

Order $= 3$

Non-linear

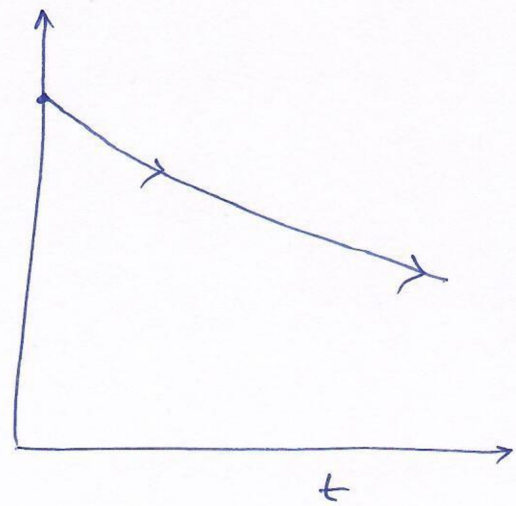
Autonomous system

$$\left.\frac{dS}{dt}\right|_{t=0} = -r S_0 I_0$$

$r > 0$; $S_0 > 0$

$I_0 > 0$

$$\left.\frac{dS}{dt}\right|_{t=0} < 0$$



$$\left.\frac{dI}{dt}\right|_{t=0} = rS_0I_0 - aI_0$$

$$= (rS_0 - a)\, I_0$$

Increase in infection

$$\begin{cases} (rS_0 - a) > 0 \Rightarrow \left.\frac{dI}{dt}\right|_{t=0} > 0 \\ (rS_0 - a) < 0 \Rightarrow \left.\frac{dI}{dt}\right|_{t=0} < 0 \end{cases}$$

$$rS_0 - a > 0$$

$$\frac{rS_0}{a} > 1$$

$R_0 = \frac{rS_0}{a} \Rightarrow$ Reproduction number

$\downarrow$

number of secondary infections produced by one primary infection in a wholly susceptible population.

If $R_0 > 1$

$\hookrightarrow$ pandemic.

$R_t = \frac{rS(t)}{a} \Rightarrow$ Replacement no.

$\downarrow$

no of persons getting contaminated by the disease on coming in contact with an infectious person during their course of infectiousness

$$\frac{dS}{dt} = -\gamma S I \qquad \frac{dR}{dt} = aI$$

$$I = \left(\frac{-1}{\gamma}\right)\frac{1}{S}\frac{dS}{dt} \qquad \frac{dR}{dt} = \left(\frac{-a}{\gamma}\right)\frac{d}{dt}\ln(S)$$

$$I = \left(\frac{-1}{\gamma}\right)\frac{d}{dt}(\ln S) \qquad R = \left(\frac{-a}{\gamma}\right)(\ln S)$$

We know $S + R + I = N$ (total population)

$$\frac{dS}{dt} + \frac{dR}{dt} + \frac{dI}{dt} = 0$$

$$\frac{d}{dt}(S + R + I) = 0$$

$$S + \left(\frac{-a}{\gamma}\right)\ln S + \left(\frac{-1}{\gamma}\right)\frac{d}{dt}(\ln S) = N$$

let $\ln S = x$

$S = e^x$

$$e^x - \frac{1}{\gamma}\frac{dx}{dt} - \frac{a}{\gamma}x = N$$

Solve for x

$$\frac{dx}{dt} = f(x)$$

then determine

S
R $\longrightarrow$ Mathematically complex
I

<u>Alternate Approach is required</u>

$$\frac{dS}{dt} = -\gamma S I$$

$$\frac{dI}{dt} = \gamma S I - a I$$

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

$$\frac{dI}{dS} = \frac{\gamma S I - a I}{-\gamma S I}$$

$$\frac{dI}{dS} = -1 + \left(\frac{a}{\gamma}\right)\frac{1}{S}$$ ← Variation of no. of infectives as function of variation in no. of Susceptibles

$$dI = \left[-1 + \frac{a}{\gamma}\frac{1}{S}\right] dS$$

$$I = -S + \frac{a}{\gamma}(\ln S) + C$$

$S_0 + I_0 = N$

but

$S + I < N$

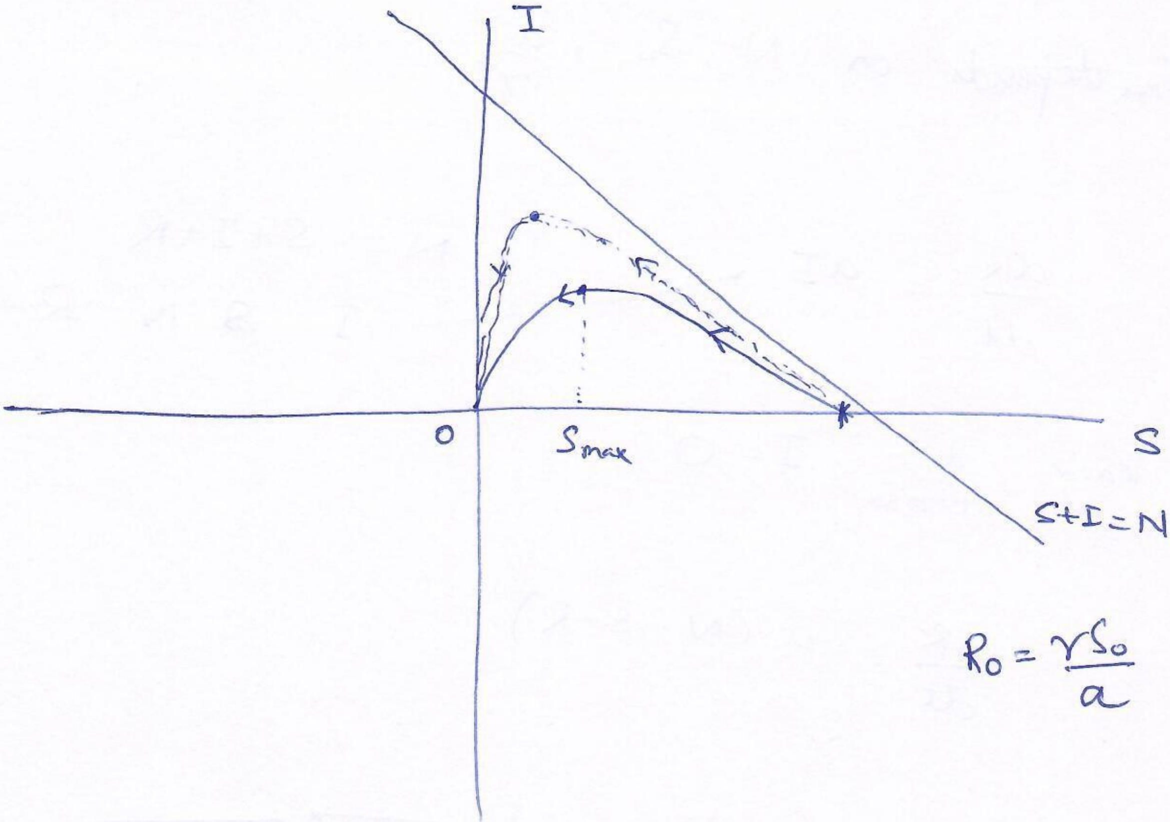
$$I_0 = -S_0 + \frac{a}{\gamma}\ln S_0 + C$$

$$C = I_0 + S_0 + \left(\frac{-a}{\gamma}\right)\ln S_0$$

$$C = N + \left(\frac{-a}{\gamma}\right)\ln S_0$$

$$I = -S + \frac{a}{\gamma}\ln S + N + \left(\frac{-a}{\gamma}\right)\ln S_0$$

$$I = -S + C_1 \ln S + N + C_2$$



$$R_0 = \frac{\gamma S_0}{a}$$

at the peak $\frac{dI}{dt} = 0$

$$\gamma S I - a I = 0$$

$$(\gamma S - a) I = 0$$

$$\gamma S - a = 0$$

At ~~...~~ $S_{max} = \frac{a}{\gamma}$ we get peak

$$I = -S + \left(\frac{a}{\gamma}\right) \ln S + N + \left(-\frac{a}{\gamma}\right) \ln S_0$$

for maxima

$$I_{max} = \left(-\frac{a}{\gamma}\right) + \left(\frac{a}{\gamma}\right) \ln\left(\frac{a}{\gamma}\right) + N + \left(-\frac{a}{\gamma}\right) \ln(S_0)$$

$$I_{max} = \frac{a}{\gamma}\left(-1 + \ln\left(\frac{a}{\gamma S_0}\right)\right) + N$$

I_{max} depends on N, S_0, $\frac{a}{\gamma}$

$$\frac{dR}{dt} = aI \qquad N = S+I+R$$

$$I = N - R - S$$

We know $\lim_{t\to\infty} I = 0$

$$\frac{dR}{dt} = a(N-S-R)$$

Use Euler Method : Numerical Method

$$S_{n+1} = S_n + (\Delta t)(-\gamma S_n I_n)$$

$$I_{n+1} = I_n + (\Delta t)(\gamma S_n I_n - aI_n)$$

$$R_{n+1} = R_n + \Delta t\,(aI_n)$$

S_0, I_0, R_0, γ, a, Δt

$$S_1 = S_0 + \Delta t\,(-\gamma S_0 I_0)$$

$$S_2 = S_1 + \Delta t\,(-\gamma S_1 I_1)$$

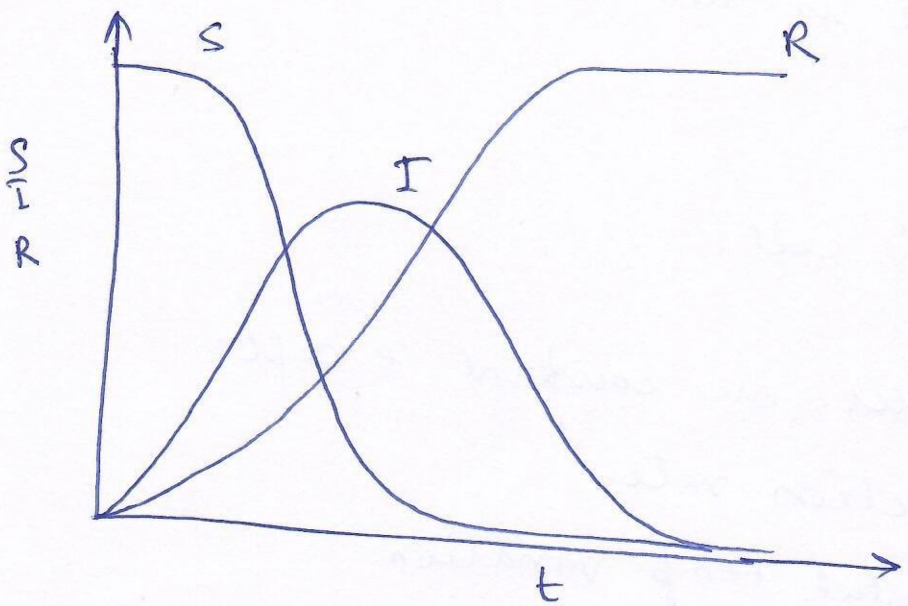
$\vdots$

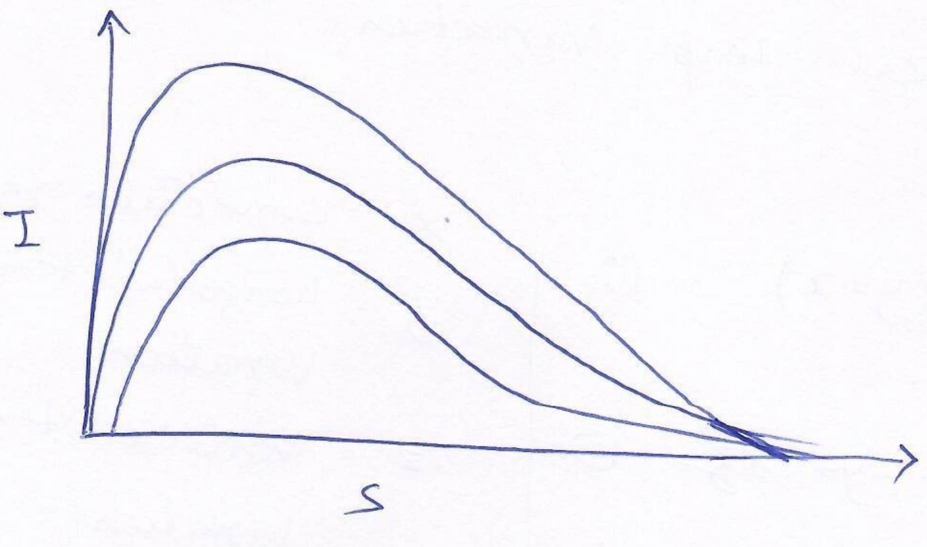
In discrete t-domain (time domain)

$$S_{t+1} = S_t - r S_t I_t$$

$$I_{t+1} = I_t + r S_t I_t - a I_t$$

$$R_{t+1} = R_t + a I_t$$





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Example 3. Atmosphere dynamics using Lorenz equation

Assumption

1. Consider earth's atmosphere to consist of a single fluid particle.
2. The particle is heated from below & cooled from outside
3. 2-D fluid cell
4. all variables are constant except
   - convection rate
   - horizontal temp. variation
   - vertical temp. Variation

$$f_1 = \frac{dx}{dt} = \sigma(y-x) \quad \text{--- (1)}$$

$$f_2 = \frac{dy}{dt} = rx - y - xz \quad \text{--- (2)}$$

$$f_3 = \frac{dz}{dt} = xy - bz \quad \text{--- (3)}$$

x = convection rate

y = horizontal temp. variation

z = vertical temp. variation.

σ = prandtl no.

r = rayleigh no.

b = system size

$\sigma, r, b > 0$

$\sigma > b + 1$

Dyn. variable = $[x \ y \ z]'$

order = 3

Non-linear,

Autonomous.

equilibrium solution

$$f_1 = f_2 = f_3 = 0$$

$$\sigma(y-x) = 0$$

$$x_e = y_e \quad \text{—— (4)}$$

$$rx - y - xz = 0$$

$$rx_e - x_e - x_e z_e = 0$$

$$\left.\begin{array}{l} x_e = 0 \ ; \ \cancel{z_e =} \\ y_e = 0 \\ z_e = 0 \end{array}\right] \text{—— (5)} \qquad \text{equilibrium s.1}$$

$$z_e = r - 1$$

$$x_e^2 = b(r-1)$$

$$x_e = y_e = \pm\sqrt{b(r-1)}$$

$$\begin{bmatrix} x_e \\ y_e \\ z_e \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sqrt{b(r-1)} \\ \sqrt{b(r-1)} \\ r-1 \end{bmatrix}, \begin{bmatrix} -\sqrt{b(r-1)} \\ -\sqrt{b(r-1)} \\ r-1 \end{bmatrix}$$

if $r < 1$; imaginary solution.

To make realistic solutions, lets say

for $r < 1$; $[0;0;0]$ is a solution

if $r = 1$; $[0;0;0]$ is solution

if $r \geq 1$ $[0;0;0]$

$$\begin{bmatrix} \sqrt{b(r-1)} \\ \sqrt{b(r-1)} \\ (r-1) \end{bmatrix} ; \begin{bmatrix} -\sqrt{b(r-1)} \\ -\sqrt{b(r-1)} \\ (r-1) \end{bmatrix}$$

so system has bifurcation at $r = 1$

f_1, f_2, f_3 are complex to solve by hand so

lets linearize

$$\frac{\partial f_1}{\partial x} = -\sigma ; \quad \frac{\partial f_1}{\partial y} = \sigma ; \quad \frac{\partial f_1}{\partial z} = 0$$

$$\frac{\partial f_2}{\partial x} = r-z ; \quad \frac{\partial f_2}{\partial y} = -1 ; \quad \frac{\partial f_2}{\partial z} = -x$$

$$\frac{\partial f_3}{\partial x} = y ; \quad \frac{\partial f_3}{\partial y} = x ; \quad \frac{\partial f_3}{\partial z} = -b$$

$$\underline{\underline{J}} = \begin{bmatrix} -\sigma & \sigma & 0 \\ r-z & -1 & -x \\ y & x & -b \end{bmatrix}$$

at equilibrium solutions.

$$\underline{\underline{J}}_{\begin{bmatrix}0\\0\\0\end{bmatrix}} = \begin{bmatrix} -\sigma & \sigma & 0 \\ r & -1 & 0 \\ 0 & 0 & -b \end{bmatrix}$$

$$\lambda_1 = -b$$

$$\lambda_2 = \frac{1}{2}\left[-(\sigma+1) + \sqrt{(\sigma+1)^2 - 4\sigma(1-r)}\right]$$

$$\lambda_3 = \frac{1}{2}\left[-(\sigma+1) - \sqrt{(\sigma+1)^2 - 4\sigma(1-r)}\right]$$

b is always +ve

$\Rightarrow$ λ_1 is always -ve

if $0 < r < 1$; λ_2 & λ_3 < 0

$\longrightarrow$ SINK SOLUTION @ $\begin{bmatrix}0\\0\\0\end{bmatrix}$

$$J = \begin{bmatrix} \sqrt{b(r-1)} \\ \sqrt{b(r-1)} \\ (r-1) \end{bmatrix} =$$

Let $\sigma = 10$

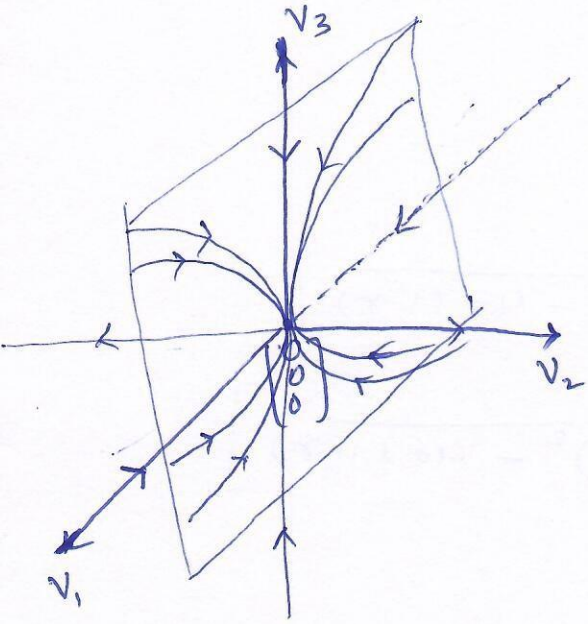
$b = 8/3$

$r = 28$

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} ; \begin{bmatrix} 6\sqrt{2} \\ 6\sqrt{2} \\ 27 \end{bmatrix} ; \begin{bmatrix} -6\sqrt{2} \\ -6\sqrt{2} \\ 27 \end{bmatrix}$$

$\lambda_1 = -8/3$

$\lambda_2, \lambda_3 = \frac{-11}{2} \pm \frac{\sqrt{1201}}{2}$



$\lambda_1 < 0$

$\lambda_2 > 0$

$\lambda_3 < 0$

Saddle solution

$\lambda_{1,2} = Re + i\,Im$

$Re > 0$

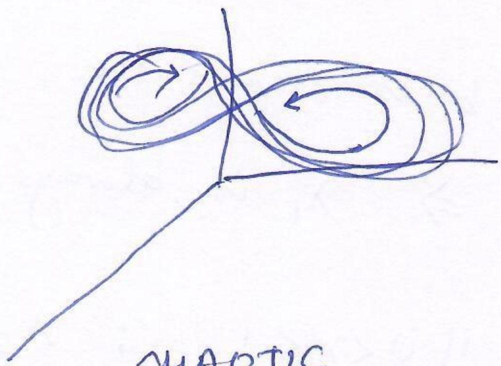
$\lambda_3 = -ve$

$\downarrow$

~~osillatory~~

circular / spiral solution

+ Sink



CHAOTIC SYSTEM