Computing in Sciences - 2.   16-April 2020.

- distribution of momenta: initialisation.

Momentum Distribution.

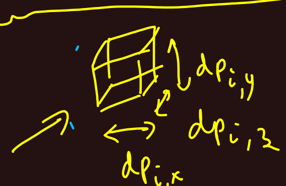
$$\mathrm{prob}(\bar{p}) \propto \prod_{i=1}^{N} e^{-\frac{1}{kT}\frac{\bar{p}_i\cdot\bar{p}_i}{2m_i}}$$

$\bar{p} \in \mathbb{R}^f$

$$\boxed{\mathrm{Prob}(\bar{p}_i)} \propto e^{-\frac{1}{kT}\frac{\bar{p}_i\cdot\bar{p}_i}{2m_i}}$$

Probability Density.

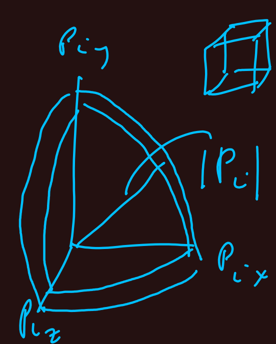
$$\boxed{\mathrm{prob}(\bar{p}_i, \bar{p}_i + d\bar{p}_i) \propto e^{-\frac{1}{kT}\frac{\bar{p}_i\cdot\bar{p}_i}{2m_i}} \cdot d\bar{p}_i}$$



SAME

$$\boxed{dp_{i,x} \cdot dp_{i,y}\, dp_{i,z}}$$

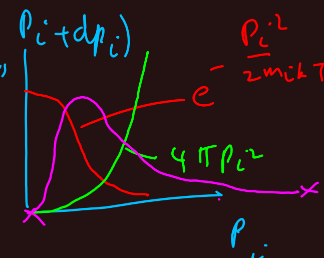
$$\boxed{4\pi p_i^2 \cdot dp_i}$$



$$\propto e^{-\frac{1}{kT}\frac{p_i^2}{2m_i}}\, 4\pi p_i^2\, dp_i$$

$$\boxed{\boxed{4\pi p_i^2}\ \boxed{e^{-\frac{1}{2m_ikT}p_i^2}}\ dp_i}$$

$\mathrm{Prob}(p_i, p_i + dp_i)$



$P_{acc} = \min(1, \exp(-\beta\Delta E)) \longrightarrow$ prob-accept $\leftarrow$

event : 1 w/ prob = prob-accept

0 w/ prob = 1 − prob-accept

prob-accept

① $\rightarrow$ $\mathrm{Prob}(x_u \leq p) = \int_0^p \rho_u(x)\,dx = cp$

$$② \rightarrow \text{Prob}(x_u > p) = \int_p^1 dx\, \rho_u(x) = c(1-p)$$

$$①+② = 1 \rightarrow c=1 \rightarrow \quad \text{prob}(x_u < p) = p.$$

$$\text{prob}(x_u < \text{prob-acc}) = \text{prob-accept}$$

Class Models: Dyanamical Models { COVID 19, SIR Model

EPIDEMIOLOGICAL MODEL   Prey-Predator   Lokta-Volterra

Prey: Rabbits: X - size of population of rabbits. | $X(t)$ Dynamical

Predator: Fox: Y | $Y(t)$

Chemical Kinetics

α - parameter | feild

Interaction: Procreation, Food in Forerst

$$X \xrightarrow{\cancel{\alpha}\, a} 2X$$

$$\frac{dX(t)}{dt} = +\alpha X(t)$$

~~Fox~~

$$\cancel{Y \rightarrow 2Y}$$

$$X + Y \xrightarrow{\cancel{\beta}\, b} 2Y \quad : \quad \frac{dX}{dt} = -\beta XY, \quad \frac{dY}{dt} = +\beta XY$$

$\boxed{\text{X and Y are coupled}}$

Death

Natural $\boxed{X \xrightarrow{\cancel{\gamma}\, c} \phi}$

$$Y \xrightarrow{\cancel{\delta}\, d} \phi$$

$$\frac{dX}{dt} = -\gamma X$$

$$\frac{dY}{dt} = -\delta Y$$

$aX - cX$ $\boxed{\alpha = a - c}$

$$\frac{dX}{dt} = \alpha X - \beta XY$$

$$\frac{dY}{dt} = \beta XY - \delta Y$$

d

α, β } +ve

γ

δ

FIELD DATA

OBSERVATIONS

Rate Eqns.

$$\frac{dX(t)}{dt} = \alpha X(t) - \beta X(t) Y(t)$$

$$\frac{dY(t)}{dt} = \gamma X(t) Y(t) - \delta Y(t)$$

① Task $\alpha, \beta, \gamma, \delta, X(0), Y(0)$

$X(t)$
$Y(t)$

Steady State $X(t) = X^*$ and $Y(t) = Y^*$

$\frac{dX(t)}{dt} = 0$ $\quad \frac{dY}{dt} = 0$; LHS of Rate Eqns $= 0$

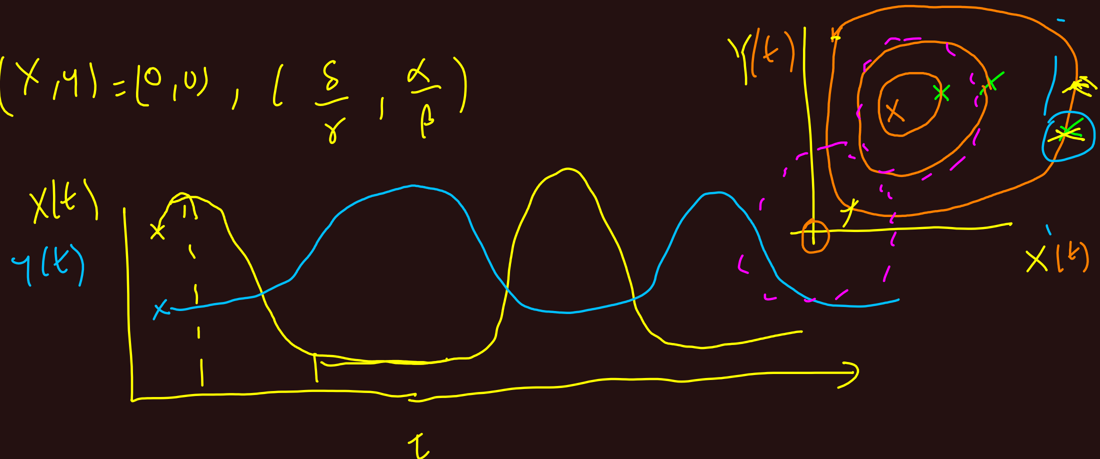
$(X^*, Y^*) = (0, 0)$,

→ $\alpha X - \beta X Y = 0 \to X(\alpha - \beta Y) = 0 \to X = 0$ or $Y = \alpha/\beta$

and $\gamma X Y - \delta Y = 0 \to Y(\gamma X - \delta) = 0 \to Y = 0$ or $X = \delta/\gamma$

4 possibilities

$(X, Y) = (0, 0)$, $\left(\frac{\delta}{\gamma}, \frac{\alpha}{\beta}\right)$



$\left(\frac{\delta}{\gamma}, \frac{\alpha}{\beta}\right)$

$\frac{dX}{dt} = \alpha X - \beta X Y$

$\frac{dY}{dt} = \gamma X Y - \delta Y$

$\bar{R} = (X, Y)$

$$\frac{d\bar{R}}{dt} = \begin{pmatrix} f_1(\bar{R}) \\ f_2(\bar{R}) \end{pmatrix}$$

about Steady State

$f_1(\bar{R}) = \alpha X - \beta X Y$, $\quad f_2(\bar{R}) = \gamma X Y - \delta Y$

At steady state, $f_1(\bar{R}) = 0$, $f_2(\bar{R}) = 0$

$$f(x) = f(x_0) + \underbrace{f'(x_0)(x - x_0)}_{\text{LINEAR}} + \underbrace{\frac{1}{2} f''(x_0)(x - x_0)^2}_{\text{QUADRATIC}} + \cdots$$

Taylor expansion about x_0

MULTIVARIABLE FUNCTION

$$f(x, y) = f(x_0, y_0) + (x - x_0)\left(\frac{\partial f}{\partial x}\right)(x_0, y_0) + (y - y_0)\frac{\partial f}{\partial y}(x_0, y_0)$$

HIGHER ORDER THAN LINEAR

$$\left\{ \begin{aligned} &+ \frac{1}{2}(x-x_0)^2 \frac{\partial^2 f}{\partial x^2}(x_0,y_0) + (x-x_0)(y-y_0)\cdot\frac{\partial^2 f}{\partial x \partial y}(x_0,y_0) \\ &+ \frac{1}{2}(y-y_0)^2 \frac{\partial^2 f}{\partial y^2}(x_0,y_0) \\ &+ \dots \end{aligned} \right.$$

LINEAR ANALYSIS $(0,0)$, $\left(\frac{\delta}{\gamma}, \frac{\alpha}{\beta}\right)$ $(X_0, Y_0) \to f_{1,2}(X_0,Y_0) = 0$

$$\frac{dX}{dt} = \alpha X - \beta XY = f_1(X,Y) \cong \underline{f_1(X_0,Y_0)} + (X-X_0)\,[\alpha - \beta Y_0] + (Y-Y_0)\cdot[-\beta X_0]$$

$$\frac{dY}{dt} = \gamma XY - \delta Y = f_2(X,Y) \cong f_2(X_0,Y_0) + (X-X_0)\,[\gamma Y_0 - 0] + (Y-Y_0)\cdot(\gamma X_0 - \delta)$$

$$\begin{Bmatrix} \alpha,\beta,\gamma,\delta \\ X_0, Y_0 \end{Bmatrix} \quad \frac{dX}{dt} = \underline{(X-X_0)}\,[\alpha - \beta Y_0] + \underline{(Y-Y_0)}\,[-\beta Y_0]$$

$$\frac{dY}{dt} = \underline{(X-X_0)}\,[\gamma Y_0] + \underline{(Y-Y_0)}\,(\gamma X_0 - \delta)$$

11, 12, 21, 22

$\bar R - \bar R_0$

$$\frac{d}{dt}(\bar R - \bar R_0) = \begin{bmatrix} 11 & 12 \\ 21 & 22 \end{bmatrix} (\bar R - \bar R_0)$$

$$\frac{d\bar R}{dt} - \cancel{\frac{d\bar R_0}{dt}} \to 0$$

$$\bar R = \begin{pmatrix} X \\ Y \end{pmatrix} ; \quad \bar R' = \bar R - \bar R_0 \longrightarrow \frac{d\bar R'}{dt} = \bar{\bar J}\,\bar R'$$

Vector Eqn

2×1 $\quad 2\times2 \quad 2\times1$

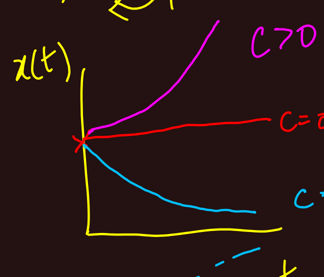
Matrix of constants

$$\rightarrow \boxed{\frac{d\bar R'}{dt} = \bar{\bar J}_0\,\bar R'}$$

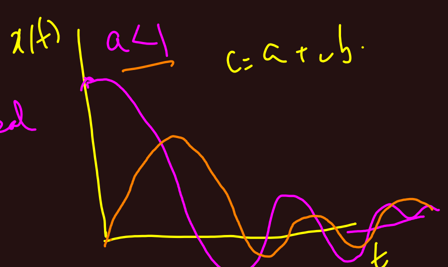
Behavior of dynamical system in near neighbourhood of steady state (X_0, Y_0)

RHS $\bar{\bar M}\,\bar V$

$$\frac{d x(t)}{dt} = c\,x(t) \leftarrow \boxed{x(t) = x(0)\,e^{+ct}}$$



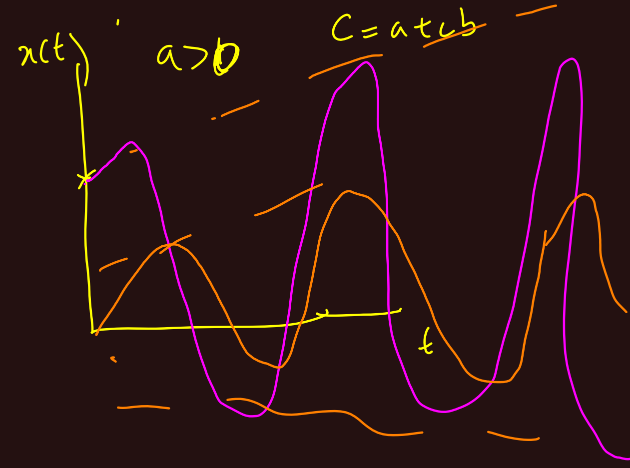
C = 0
C < 0
C > 0



$C = a + ib$

$$x(t) = \underbrace{x_0 e^{at}}\cdot\underbrace{e^{ibt}}$$

$$= x_0 e^{at}\cos bt + i x_0 a^t \sin bt$$



$$\boxed{\frac{d\bar{R}}{dt} = \bar{\bar{J}}_0 \cdot \bar{R} \,?}$$

Solving eigen system

$$\bar{\bar{J}}_0 \bar{R} = \lambda \bar{R}$$

$$\bar{\bar{M}}\,\bar{v} = \lambda \bar{v} \qquad \lambda_1 \leftrightarrow \bar{v}_1 \qquad \lambda_2 \leftrightarrow \bar{v}_2$$

$$\bar{R}(t) = c_1^{(t)}\bar{v}_1 + c_2^{(t)}\bar{v}_2 + \dots \longleftrightarrow \bar{\bar{M}}$$ Rank N, eigenvectors $\leftrightarrow$ linearly independent basis

$$\frac{d\bar{R}}{dt} = \bar{\bar{J}}_0 \bar{R} \; ; \quad \bar{R} = \underset{\lambda_1}{c_1}\bar{v}_1 + \underset{\lambda_2}{c_2\bar{v}_2}$$

$$\boxed{\bar{\bar{J}}_0 \bar{v}_i = \lambda_i \bar{v}_i}$$

LHS $\frac{d}{dt}\left(c_1\bar{v}_1 + c_2\bar{v}_2\right) = \bar{v}_1 \cdot \frac{dc_1(t)}{dt} + \bar{v}_2 \frac{dc_2(t)}{dt}$

RHS $\bar{\bar{J}}_0\left(c_1\bar{v}_1 + c_2\bar{v}_2\right) = c_1\bar{\bar{J}}_0\bar{v}_1 + c_2\bar{\bar{J}}_0\bar{v}_2 = c_1\lambda_1\bar{v}_1 + c_2\lambda_2\bar{v}_2$

$$\bar{v}_1 \cdot \frac{dc_1}{dt} + \bar{v}_2\frac{dc_2}{dt} = \bar{v}_1\, c_1\lambda_1 + \bar{v}_2\, c_2\lambda_2$$

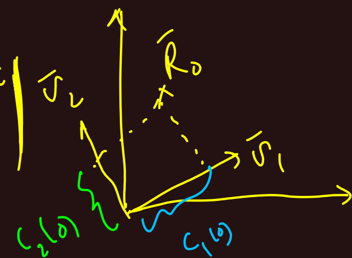
$$\bar{v}_1\left(\frac{dc_1}{dt} - c_1\lambda_1\right) + \bar{v}_2\left(\frac{dc_2}{dt} - c_2\lambda_2\right) = 0$$

$\bar{v}_1, \bar{v}_2$ are linearly independent

$$\frac{dc_i}{dt} - c_i\lambda_i = 0 \quad \forall\, i = 1, 2$$

$$\frac{dc_i(t)}{dt} = \lambda_i c_i(t) \qquad i = 1,2$$

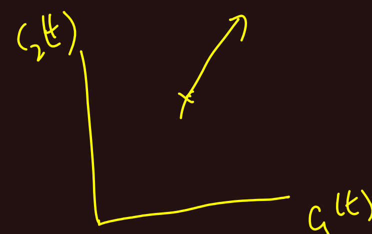
$$c_i(t) = c_i(0)\, e^{\lambda_i (t)} \quad \Big| \quad c_1(t) = c_1(0)\, e^{\lambda_1 t}$$

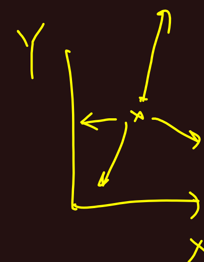


~~$\lambda_1 = 0$, $\lambda_2 = 0$~~

Excluded

$\lambda_1, \lambda_2 \neq 0$. $\lambda_1, \lambda_2 \to$ +ve





Tasks

① $X(t)$, $Y(t)$ vs time → scipy.integrate.odeint

② $X(t)$ vs $Y(t)$

③ Linearise J_0 $\begin{cases} (0,0) \to \lambda_1, \lambda_2, \bar{v}_1, \bar{v}_2 \\ \left(\frac{\delta}{\gamma}, \frac{\alpha}{\beta}\right), \lambda_1, \lambda_2, \bar{v}_1, \bar{v}_2 \end{cases}$ | Compute

$\boxed{\alpha, \beta, \gamma, \delta = 1}$

numpy.linalg.eig

GOOD SOURCE: WIKIPEDIA ARTICLE "LOTKA-VOLTERRA MODEL".