MA261 Assignment 2.

Q 1.1 (1)

$$\frac{dA}{dt} = -k_f A^2 + k_r A^* A$$

$$\frac{dA^*}{dt} = k_f A^2 - k_r A A^* - cA^*$$

$$\frac{dP}{dt} = cA^*$$

Can see $A + A^* + P$ is conserved as

$$\frac{dA}{dt} + \frac{dA^*}{dt} + \frac{dP}{dt} = (-k_f A^2 + k_r A^* A) + (k_f A^2 - k_r A^* A - cA^*) + cA^*$$
$$= 0$$

So $A(t) + A^*(t) + P(t) = A(0) + A^*(0) + P(0)$
$$= A_0 + A_0^* + P_0$$

So $A^*(t) = A_0 + A_0^* + P_0 - A(t) - P(t)$

So
$$\frac{dA}{dt} = -k_f A^2 + k_r (A_0 + A_0^* + P_0 - A(t) - P(t)) A$$
$$= -k_f A^2 - (k_r A - k_r P + k_r A_0 + k_r A_0^* + k_r P_0) A$$

$$\frac{dP}{dt} = cA^* = c(A_0 + A_0^* + P_0 - A - P)$$
$$= cA_0 + cA_0^* + cP_0 - cA - cP$$

2) $\frac{dA^*}{dt} = 0 \Rightarrow k_f A^2 - k_r AA^* - CA^* = 0$

$\Leftrightarrow k_f A^2 = k_r AA^* + CA^*$

$\Rightarrow A^* = \frac{k_f A^2}{k_r A + C}$

$\frac{dA}{dt} = -k_f A^2 + k_r A^* A = -k_f A^2 + k_r A\left(\frac{k_f A^2}{k_r A + C}\right)$

$= -k_f A^2 + \frac{k_r k_f A^3}{k_r A + C}$

$\frac{dP}{dt} = CA^* = C\left(\frac{k_f A^2}{k_r A + C}\right) = \frac{C k_f A^2}{k_r A + C}$

Q1.2 (1) $y_{n+1} = y_n + h\sum_{i=1}^{m} \gamma_i k_i(t_n, y_n; h)$

$k_1 = f(t + \alpha_1 h, y + h\sum_{i=1}^{m} B_{1,i} k_i(t, y; h)) = f(t, y) = \lambda y_n$

$k_2 = f(t + ah, y + h\sum_{i=1}^{m} B_{2,i} k_i(t, y; h)) = f(t + ah, y + hak_1) = \lambda y + \lambda a k_1 h$

$= \lambda y_n + \lambda^2 a y_n h$

$y_{n+1} = y_n + h((1-\gamma)k_1 + \gamma k_2)$

$= y_n + h((1-\gamma)\lambda y_n + \gamma(\lambda y_n + h\lambda^2 a y_n))$

$= y_n + h(\lambda y_n - \gamma\lambda y_n + \gamma\lambda y_n + h\gamma\lambda^2 a y_n)$

$= y_n + h\lambda y_n + h^2\gamma\lambda^2 a y_n$

$= (1 + h\lambda + h^2\gamma\lambda^2 a) y_n$

$R(\lambda h) = 1 + h\lambda + h^2\gamma\lambda^2 a$

$R(\mu) = 1 + \mu + a\gamma\mu^2$

stable if $|R(\lambda h)| < 1$ $\quad \mu = \lambda h \quad x \in [0,1]$

$\Leftrightarrow$

$$|1 + h\lambda + h^2\gamma\lambda^2 a| < 1 \qquad |1+\mu+x\mu^2| < 1$$

$-1 < 1 + h\lambda + h^2\gamma\lambda^2 a < 1$

$-2 < h\lambda + h^2\gamma\lambda^2 a < 0$

$-2 < h\lambda(1 + \gamma\lambda h a) < 0$

$-2 < h\lambda(1+h\lambda x) < 0$

so need $1+h\lambda x > 0$

$-2 < h\lambda(1+\lambda x)$

$-1 < 1+\mu+x\mu^2 < 1$

$-2 < \mu + a\mu^2 < 0$

$x := a\gamma \quad -2 < \mu(1+x\mu) < 0$

$h\lambda < 0 \quad 2 > 1+x\mu > 0$

$1 > x\mu > -1$

$h\lambda x > -1 \quad \frac{1}{x} > \mu > -\frac{1}{x}$

$h > \frac{-1}{x\lambda} = \frac{1}{x|\lambda|} \quad \frac{1}{x} > h\lambda > -\frac{1}{x}$

$h_0 = \frac{1}{x}$ //

$|h\lambda| < \frac{1}{x}$

$h|\lambda| < \frac{1}{x}$

$h < \frac{1}{x|\lambda|}$

$h_0 = \frac{1}{x}$ //

(2) Don't get the question

$|y_n| < R \Rightarrow |R(\lambda h)| \leq 1$

(3) $\lambda = \alpha i, \alpha \neq 0$

Solve inequality $|1 + h\lambda + xh^2\lambda^2| \leq 1$

$|1 + h\alpha i - xh^2\alpha^2| \leq 1$

$\Rightarrow$

$1 - h^2\alpha^2 = (1+h\alpha)(1-h\alpha)$

$(1 - xh^2\alpha^2)^2 + h^2\alpha^2 \leq 1$

$1 - 2xh^2\alpha^2 + x^2h^4\alpha^4 + h^2\alpha^2 \leq 1$

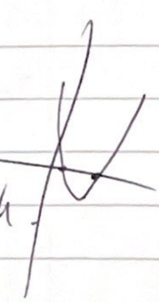
$h^2\alpha^2(x^2h^2\alpha^2 + 1 - 2x) \leq 0$

$x^2h^2\alpha^2 + 1 - 2x \leq 0$

$\Rightarrow$

$x = \frac{2 \pm \sqrt{4 - 4h^2\alpha^2}}{2h^2\alpha^2} = \frac{1 \pm \sqrt{1-h^2\alpha^2}}{h^2\alpha^2} \quad \frac{1-\sqrt{1-h^2\alpha^2}}{h^2\alpha^2} \leq x \leq \frac{1+\sqrt{1-h^2\alpha^2}}{h^2\alpha^2}$

$\frac{1-\sqrt{1-h^2\alpha^2}}{h^2\alpha^2} \leq x \leq \frac{1+\sqrt{1-h^2\alpha^2}}{h^2\alpha^2}$



Good enough

Don't have α again

$$\partial_p H = p$$
$$\partial_x H = \alpha x$$

1.3 (1) FE: $x_{n+1} = x_n + h\partial_p H(x_n, p_n)$
$p_{n+1} = p_n - h\partial_x H(x_n, p_n)$

$$H_n = H(x_n, p_n) = H\left(x_{n-1} + h\partial_p H(x_{n-1}, p_{n-1}),\ p_{n-1} - h\partial_x H(x_{n-1}, p_{n-1})\right)$$

$$= \frac{\left(p_{n-1} - h\partial_x H(x_{n-1}, p_{n-1})\right)^2}{2} + \frac{\alpha\left(x_{n-1} + h\partial_p H(x_{n-1}, p_{n-1})\right)^2}{2}$$

$$= \frac{p_{n-1}^2 - 2p_{n-1} h\partial_x H(x_{n-1}, p_{n-1}) + h^2\left(\partial_x H(x_{n-1}, p_{n-1})\right)^2}{2}$$

$$+ \frac{\alpha x_{n-1}^2 + 2\alpha x_{n-1} h\partial_p H(x_{n-1}, p_{n-1}) + \alpha h^2\left(\partial_p H(x_{n-1}, p_{n-1})\right)^2}{2}$$

$$= H(x_{n-1}, p_{n-1}) - \frac{\cancel{2} p_{n-1} h\partial_x H(x_{n-1}, p_{n-1})}{\cancel{2}} + \frac{h^2\left(\partial_x H(x_{n-1}, p_{n-1})\right)^2}{2}$$

$$+ \frac{\cancel{2}\alpha x_{n-1} h\partial_p H(x_{n-1}, p_{n-1})}{\cancel{2}} + \frac{\alpha h^2\left(\partial_p H(x_{n-1}, p_{n-1})\right)^2}{2}$$

$$= H(x_{n-1}, p_{n-1}) - p_{n-1} h\alpha x_{n-1} + \frac{h^2\alpha^2 x_{n-1}^2}{2}$$

$$+ \alpha x_{n-1} h p_{n-1} + \frac{\alpha h^2 p_{n-1}^2}{2}$$

$$= H(x_{n-1}, p_{n-1}) + \alpha h^2 H(x_{n-1}, p_{n-1}) = (1 + \alpha h^2) H(x_{n-1}, p_{n-1})$$

Iterating we see $H_n = (1 + \alpha h^2)^n H_0$ //

(2) $x_{n+1} = x_n + h\partial_p H(x_n, p_n) = x_n + hp_n$

$$p_{n+1} = p_n - h\partial_x H(x_{n+1}, p_n) = p_n - h\alpha x_{n+1}$$
$$= p_n - h\alpha(x_n + hp_n)$$
$$= p_n - h\alpha x_n - h^2\alpha p_n$$

So $\begin{pmatrix} x_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} 1 & h \\ -h\alpha & 1-h^2\alpha \end{pmatrix} \begin{pmatrix} x_n \\ p_n \end{pmatrix}$

So $A = \begin{pmatrix} 1 & h \\ -h\alpha & 1-h^2\alpha \end{pmatrix}$ //

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(3)h $\frac{d}{dt} H(x,p) = \partial_x H(x,p) x' + \partial_p H(x,p) p'$

$= \partial_x H(x,p) \partial_p H(x,p) - \partial_p H(x,p) \partial_x H(x,p) = 0$ //

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(3) $H_n = H(x_n, p_n) = H\left(x_{n-1} + h \frac{H(x_{n-1}, p_n) - H(x_{n-1}, p_{n-1})}{p_n - p_{n-1}}, p_{n-1} - h \frac{H(x_n, p_n) - H(x_{n-1}, p_n)}{x_n - x_{n-1}}\right)$

$$= \frac{\left(p_{n-1} - h \frac{H(x_n,p_n) - H(x_{n-1}, p_n)}{x_n - x_{n-1}}\right)^2}{2} + \frac{\alpha \left(x_{n-1} + h \frac{H(x_{n-1},p_n) - H(x_{n-1}, p_{n-1})}{p_n - p_{n-1}}\right)^2}{2}$$

$$= \frac{p_{n-1}^2 - 2hp_{n-1} \frac{(H(x_n,p_n) - H(x_{n-1},p_n))}{(x_n - x_{n-1})} + h^2 \cdot \frac{(H(x_n,p_n) - H(x_{n-1},p_n))^2}{(x_n - x_{n-1})^2}}{2}$$

$$+ \frac{\alpha x_{n-1}^2 + 2\alpha h x_{n-1} \frac{H(x_{n-1},p_n) - H(x_{n-1},p_{n-1})}{p_n - p_{n-1}} + \alpha h^2 \frac{(H(x_{n-1},p_n) - H(x_{n-1},p_{n-1}))^2}{(p_n - p_{n-1})^2}}{2}$$

$$= H(x_{n-1}, p_{n-1}) - hp_{n-1} \frac{\left(\frac{p_n^2}{2} + \frac{\alpha x_n^2}{2} - \frac{p_n^2}{2} - \frac{\alpha x_{n-1}^2}{2}\right)}{x_n - x_{n-1}} + \alpha h x_{n-1} \frac{\left(\frac{p_n^2}{2} + \frac{\alpha x_{n-1}^2}{2} - \frac{p_{n-1}^2}{2} - \frac{\alpha x_{n-1}^2}{2}\right)}{p_n - p_{n-1}}$$

$$+ \frac{h^2}{2} \frac{\left(\frac{p_n^2}{2} + \frac{\alpha x_n^2}{2} - \frac{p_n^2}{2} - \frac{\alpha x_{n-1}^2}{2}\right)^2}{(x_n - x_{n-1})^2} + \frac{\alpha h^2}{2} \frac{\left(\frac{p_n^2}{2} + \frac{\alpha x_{n-1}^2}{2} - \frac{p_{n-1}^2}{2} - \frac{\alpha x_{n-1}^2}{2}\right)^2}{(p_n - p_{n-1})^2}$$

$$= H(x_{n-1}, p_{n-1}) - hp_{n-1}\left(\frac{\frac{\alpha}{2}\left(x_n^2 - x_{n-1}^2\right)}{x_n - x_{n-1}}\right) + \alpha h x_{n-1}\left(\frac{\frac{1}{2}\left(p_n^2 - p_{n-1}^2\right)}{p_n - p_{n-1}}\right)$$

$$+ \frac{h^2}{2}\left(\frac{\frac{\alpha}{2}\left(x_n^2 - x_{n-1}^2\right)^2}{\left(x_n - x_{n-1}\right)^2} + \frac{\alpha h^2}{2}\left(\frac{\frac{1}{2}\left(p_n^2 - p_{n-1}^2\right)^2}{\left(p_n - p_{n-1}\right)^2}\right)\right)$$

$$= H(x_{n-1}, p_{n-1}) - \frac{h\alpha p_{n-1}}{2}\left(x_n + x_{n-1}\right) + \frac{h\alpha x_{n-1}}{2}\left(p_n + p_{n-1}\right)$$

$$+ \frac{h^2\alpha}{4}\left(x_n + x_{n-1}\right)^2 + \frac{h^2\alpha}{4}\left(p_n + p_{n-1}\right)^2$$ Stuck here.

All wrong used a specific Hamiltonian

$$(x_{n+1} - x_n)(p_{n+1} - p_n) = h\left(H(x_n, p_{n+1}) - H(x_n, p_n)\right)$$

$$\frac{(x_{n+1} - x_n)(p_{n+1} - p_n)}{h} + H(x_n, p_n) = H(x_n, p_{n+1}) \quad (1)$$

$$\frac{(p_{n+1} - p_n)(x_{n+1} - x_n)}{-h} + H(x_{n+1}, p_{n+1}) = H(x_n, p_{n+1}) \quad (2)$$

(2) − (1)

$$\Rightarrow H(x_{n+1}, p_{n+1}) - H(x_n, p_n) = 0$$

$$\Rightarrow H(x_{n+1}, p_{n+1}) = H(x_n, p_n)$$

i.e. $H_{n+1} = H_n$

Iterating it is clear that $H_n = H_0 \ \forall n$.

$$x_{n+1} = x_n + h\,\frac{H(x_n, p_{n+1}) - H(x_n, p_n)}{p_{n+1} - p_n} = x_n + h\,\frac{\frac{p_{n+1}^2}{2} + V(x_n) - V(x_n) - \frac{p_n^2}{2}}{p_{n+1} - p_n} = x_n + \frac{h}{2}(p_{n+1} + p_n)$$

$$p_{n+1} = p_n - h\,\frac{H(x_{n+1}, p_{n+1}) - H(x_n, p_{n+1})}{x_{n+1} - x_n} = p_n - h\,\frac{\frac{p_{n+1}^2}{2} + V(x_{n+1}) - V(x_n) - \frac{p_{n+1}^2}{2}}{x_{n+1} - x_n} = p_n - h\,\frac{V(x_{n+1}) - V(x_n)}{x_{n+1} - x_n}$$

$$x_{n+1} = x_n + \frac{h}{2}\left(2p_n - h\,\frac{V(x_{n+1}) - V(x_n)}{x_{n+1} - x_n}\right) = x_n + h\delta_n$$

$$= x_n + h p_n - \frac{h^2}{2}\,\frac{V(x_{n+1}) - V(x_n)}{x_{n+1} - x_n}$$

$$\delta_n = p_n - \frac{h}{2}\,\frac{V(x_{n+1}) - V(x_n)}{x_{n+1} - x_n} = p_n - \frac{1}{2}\,\frac{V(x_n + h\delta_n) - V(x_n)}{\delta_n}$$

$$F_n(\delta) = \delta - p_n + \frac{V(x_n + h\delta) - V(x_n)}{2\delta}$$

$$DF = I_m + \frac{h\delta\, DV(x_n + h\delta) - V(x_n + h\delta) + V(x_n)}{2\delta^2}$$