

Numerical Exercises 1

Partial

1. A ~~nonlinear~~ differential equation like the given equation

$$u_t - a(t)u_x - \epsilon u_{xx} = 0, \text{ is linear if the}$$

dependent variable ~~is~~ in this case ~~x and t~~ and its partial derivatives are present linearly in the equation.

For example, for a second order linear PDE like we have here, it must take the form

$$S_1(x, t)u_{xx} + S_2(x, t)u_{xt} + S_3(x, t)u_{tx} + S_4(x, t)u_{tt} \dots$$

$$\dots + S_5(x, t)u_x + S_6(x, t)u_t + S_7(x, t)u = f(x, t).$$

Clearly this is satisfied with $S_6 = 1$, $S_5 = -a(t)$, $S_1 = -\epsilon$ and $S_2 = S_3 = S_4 = S_7 = f = 0$.

The equation includes the diffusive term ' $-\epsilon u_{xx}$ ' and describes how the dependent variable is distributed in a given region over time. There is an additional advective time term ' $-a(t)u_x$ ' which describes the motion of u as it is advected by the velocity field.

2. The Θ -scheme is given by

$$U_j^{n+1} - U_j^n = \Delta t [\Theta \delta_x^2 U_j^{n+1} + (1-\Theta) \delta_x^2 U_j^n]$$

we Taylor expand each term around the point (x_j, t_{n+k}) for this scheme. This gives:

$$u_j^{n+1} \approx u(x, t) + u_t\left(\frac{1}{2}\Delta t\right) + \frac{1}{2!} u_{tt}\left(\frac{1}{2}\Delta t\right)^2 + \frac{1}{3!} u_{ttt}\left(\frac{1}{2}\Delta t\right)^3 + \dots$$

This follows from the form of the Taylor Series

$$f(x) \approx f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \dots$$

where (in 2 independent variables) we take

$$a = (x, t) \text{ and } x = (x, t + \frac{1}{2}\Delta t). \text{ Similarly,}$$

$$u_j^n \approx u(x, t) + u_t\left(-\frac{1}{2}\Delta t\right) + \frac{1}{2!} u_{tt}\left(-\frac{1}{2}\Delta t\right)^2 + \frac{1}{3!} u_{ttt}\left(-\frac{1}{2}\Delta t\right)^3 + \dots$$

where $a = (x, t + \frac{1}{2}\Delta t)$ and $x = (x, t)$. Hence

$$\begin{aligned} u_j^{n+1} - u_j^n &= u(x, t + \frac{1}{2}\Delta t) - u(x, t - \frac{1}{2}\Delta t) + u_t\left(\frac{1}{2}\Delta t\right) - u_t\left(-\frac{1}{2}\Delta t\right) + \dots \\ &\quad + \frac{1}{2} u_{tt}\left(\frac{1}{4}\Delta t^2\right) - \frac{1}{2} u_{tt}\left(\frac{1}{4}\Delta t^2\right) + \dots \\ &= u_t \Delta t + \frac{1}{24} (\Delta t)^3 u_{ttt} + \dots O((\Delta t)^5). \end{aligned}$$

We can also Taylor expand $\delta_x^2 u_j^{n+1}$. Since

$$\delta_x^2 u(x, t) = u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)$$

we again expand around point $(x_j, t + \frac{1}{2}\Delta t)$ and therefore $a = (x, t + \frac{1}{2}\Delta t)$ in the expansion, giving:

$$u(x + \Delta x, t) \approx u(x, t + \frac{1}{2}\Delta t) + u_{xc} \Delta x + \frac{1}{2!} u_{xxx} (\Delta x)^2 + \dots$$

$$u(x, t) \approx u(x, t + \frac{1}{2}\Delta t) + u_{xc}$$

$$u(x - \Delta x, t) \approx u(x, t + \frac{1}{2}\Delta t) + u_{xc} (-\Delta x) + \frac{1}{2!} u_{ccc} (-\Delta x)^2 + \dots$$

Therefore we have

$$\delta_x^2 u(x, t + \Delta t) \approx u_{xc} (\Delta x)^2 + \frac{1}{12} (\Delta x)^4 u_{xxxcc} + \dots \Big|_j^{n+1}$$

We would get the same expansion for $\delta_x^2 u_j^n$ except

the time component would be n and not $n+1$.

We now expand each term in the two expressions for $\delta_{xc}^z u_j^{n+1}$ and $\delta_{xc}^z u_j^n$ above around the point $(x_j, t_{n+\frac{1}{2}\Delta t})$ but in powers of Δt . Therefore

$$\delta_{xc}^z u_j^{n+1} = \left[(\Delta x)^2 \frac{\partial^2 u(x, t + \frac{1}{2}\Delta t)}{\partial x^2} + \frac{1}{12} (\Delta x)^4 \frac{\partial^4 u(x, t + \frac{1}{2}\Delta t)}{\partial x^4} + \dots \right]$$

$$+ \frac{1}{2} \Delta t \left[(\Delta x)^2 u_{xxx} + \frac{1}{12} (\Delta x)^4 u_{xxxxx} + \dots \right]$$

$$+ \frac{1}{2!} \left(\frac{1}{2} \Delta t \right)^2 \left[(\Delta x)^2 u_{xxxx} + \frac{1}{12} (\Delta x)^4 u_{xxxxx} + \dots \right] + \dots$$

The expansion for $\delta_{xc}^z u_j^n$ would be similar except the ~~coefficient~~ powers of Δt would be on $t - (t + \frac{1}{2}\Delta t) = -\frac{1}{2}\Delta t$ hence giving

$$\delta_{xc}^z u_j^n = \left[(\Delta x)^2 u_{xx} + \frac{1}{12} (\Delta x)^4 u_{xxxxx} + \dots \right]$$

$$- \frac{1}{2} \Delta t \left[(\Delta x)^2 u_{xxx} + \frac{1}{12} (\Delta x)^4 u_{xxxxx} + \dots \right]$$

$$- \frac{1}{2!} \left(-\frac{1}{2} \Delta t \right)^2 \left[(\Delta x)^2 u_{xx} + \dots \right] - \dots$$

Combining these gives in the context of the Θ -scheme gives:

$$\Theta \delta_{xc}^z u_j^{n+1} + (1-\Theta) \delta_{xc}^z u_j^n =$$

$$\left[(\Delta x)^2 u_{xx} + \frac{1}{12} (\Delta x)^4 u_{xxxxx} + \dots \right]$$

$$+ (\Theta - \frac{1}{2}) \Delta t \left[(\Delta x)^2 u_{xxx} + \frac{1}{12} (\Delta x)^4 u_{xxxxx} + \dots \right]$$

$$+ \frac{1}{2!} \left(-\frac{1}{2} \Delta t \right)^2 \left[(\Delta x)^2 u_{xx} + \frac{1}{12} (\Delta x)^4 u_{xxxxx} + \dots \right]$$

+ ...

using the definition of the truncation error we therefore have:

$$\begin{aligned} T_j^{n+\frac{1}{2}} &:= \frac{u_j^{n+1} - u_j^n}{\Delta t} - \frac{\theta \delta x^2 u_j^{n+1} + (1-\theta) \delta x^2 u_j^n}{(\Delta x)^2} \\ &= u_t + \frac{1}{24} (\Delta t)^2 u_{ttt} + \dots \\ &\quad - [u_{xx} + \frac{1}{12} (\Delta x)^2 u_{xxxxx} + \dots] \\ &\quad - \frac{1}{6} (\theta - \frac{1}{2}) \Delta t [u_{xxx} + \frac{1}{12} (\Delta x)^2 u_{xxxxx} + \dots] \\ &\quad - \frac{1}{2!} (-\frac{1}{2} \Delta t)^2 [u_{xxxxt} + \frac{1}{12} (\Delta x)^2 u_{xxxxxt}] + \dots \\ &= (u_t - u_{xx}) + \left[\left(\frac{1}{2} - \theta \right) \Delta t u_{xxt} - \frac{1}{12} (\Delta x)^2 u_{xxxxx} \right] \\ &\quad + \left[\frac{1}{24} (\Delta t)^2 u_{ttt} - \frac{1}{2!} (-\frac{1}{2} \Delta t)^2 u_{xxxxt} \right] \\ &\quad + \frac{1}{12} \left(\frac{1}{2} - \theta \right) \Delta t (\Delta x)^2 u_{xxxxxt} - \dots \end{aligned}$$



3. The Θ -discretisation for the equation

$$u_t - a(t)u_{xx} - \epsilon u_{xxx} = 0$$

is done as follows:

Using an ~~upwind~~ we can use a forward difference scheme for the time derivative approximation, and so

$$u_t \approx \frac{u_j^{n+1} - u_j^n}{\Delta t}.$$

For the advective term an ^{Spatial} upwind scheme is used in conjunction with the weight Θ , therefore

$$u_x \approx \Theta \frac{u_{j+1}^{n+1} - u_j^{n+1}}{\Delta x} + (1-\Theta) \frac{u_{j+1}^n - u_j^n}{\Delta x}, \text{ assuming } a(t) < 0.$$

Finally, the diffusive term is weighted using the same Θ as follows

$$u_{xx} \approx \Theta \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} + (1-\Theta) \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}$$

Putting this together we can discretise our equation

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} - \frac{a(t)}{\Delta x} \left(\Theta(u_{j+1}^{n+1} - u_j^{n+1}) + (1-\Theta)(u_{j+1}^n - u_j^n) \right) - \frac{\epsilon}{(\Delta x)^2} \left(\Theta(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) + (1-\Theta)(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \right) = 0.$$

Defining two constant variables $k_1 = \frac{a(t)\Delta t}{\Delta x}$ and $k_2 = \frac{\epsilon \Delta t}{(\Delta x)^2}$ we can simplify the discretisation,

assuming $a(t)$ is constant, to

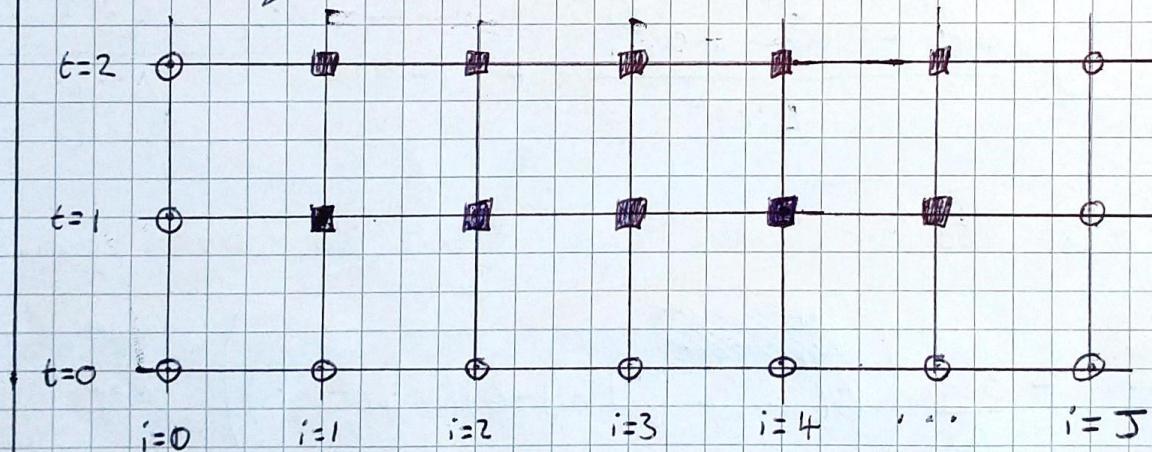
$$u_j^{n+1} - u_j^n = k_1 \left(\theta (u_{j+1}^{n+1} - u_j^{n+1}) + (1-\theta) (u_{j+1}^n - u_j^n) \right) + k_2 \left(\theta (u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) + (1-\theta) (u_{j+1}^n - 2u_j^n + u_{j-1}^n) \right)$$

Since all points on the boundary timestep $t=n$ will be known and points on the timestep $t=n+1$ will be unknown quantities to be derived we can collect known and unknown terms on either side of the discretisation, giving

$$u_{j+1}^{n+1} (-k_1 \theta - k_2 \theta) + u_j^{n+1} (1 + k_1 \theta + 2k_2 \theta) + u_{j-1}^{n+1} (-k_2 \theta) = \dots$$

$$\dots u_{j+1}^n (k_1 - k_1 \theta + k_2 - k_2 \theta) + u_j^n (1 - k_1 + k_1 \theta - 2k_2 + 2k_2 \theta) + u_{j-1}^n (k_2 - k_2 \theta)$$

If we draw a stencil for the θ -scheme at the boundary where circles denote the known boundary points and squares the interior unknowns we have



The first unknown in the scheme is indexed by $i=1, t=1$. The last unknown in each row (i.e. for each timestep) will be indexed by $i=J-1$. Hence, the Scheme can be written in the form $\underline{A} \underline{x} = \underline{b}$ as follows:

$$\begin{bmatrix} S_1 & S_2 & 0 & 0 & \cdots \\ S_3 & S_4 & S_5 & 0 & \cdots \\ 0 & S_6 & S_7 & S_8 & \cdots \\ 0 & 0 & S_9 & S_{10} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ S_n & & & & \end{bmatrix} = \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ \vdots \\ u_{j-1}^{n+1} \\ u_j^n \end{bmatrix} = \begin{bmatrix} s(u_0^*, u_1^*, u_2^* \dots) \\ s(u_0^*, u_1^*, u_2^* \dots) \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

~~At~~ Note that the first and last elements in the b vector will have an extra boundary condition term u_0^{n+1} and u_j^{n+1} respectively.



4. For the explicit scheme we have the discretised equation $U_j^{n+1} = U_j^n + M(U_{j+1}^n - 2U_j^n + U_{j-1}^n)$ for the linear diffusion equation $u_t = u_{xx}$. We can now perform a Fourier analysis of the scheme. Suppose we substitute into our scheme

$$U_j^n = (\lambda)^n e^{ik(j\Delta x)}, \text{ then we also know that}$$

$$U_j^{n+1} = \lambda U_j^n \quad \text{and similarly}$$

$$U_{j+1/j-1}^n = e^{\pm ik\Delta x} U_j^n. \text{ Substituting these terms into}$$

the explicit scheme equation we have

$$\lambda U_j^n = U_j^n + M(e^{ik\Delta x} U_j^n - 2U_j^n + e^{-ik\Delta x} U_j^n). \text{ Dividing}$$

by U_j^n we have

$$\lambda = 1 + M(e^{ik\Delta x} - 2 + e^{-ik\Delta x}),$$

$$\lambda = 1 - 2M(1 - \cos(k\Delta x)),$$

$$\lambda = 1 - 4M \sin^2\left(\frac{k\Delta x}{2}\right). \text{ As time } n \text{ increases}$$

$\lambda(k)$ will diverge so long as $|\lambda(k)| > 1$ and thus the stability condition becomes

$$\left| 1 - 4M \sin^2\left(\frac{k\Delta x}{2}\right) \right| \leq 1. \text{ Taking the mode most}$$

likely to be unstable i.e. $k\Delta x = \pi$ we have

$$|1 - 4M| \leq 1, \text{ since } M > 0 \text{ we look at}$$

the negative condition $1 - 4M \geq -1$ and so the stability condition becomes $M \leq \frac{1}{2}$.

This explains the question 4 python plot since for $\Delta x = 0.05$ we have

$$M_{0.0013} = \frac{\Delta t}{(\Delta x)^2} = \frac{0.0013}{(0.05)^2} = 0.52 \quad (\text{i.e. unstable}) \text{ and}$$

$$M_{0.0012} = \frac{\Delta t}{(\Delta x)^2} = \frac{0.0012}{(0.05)^2} = 0.48 \quad (\text{i.e. stable}).$$

In addition, in question 4 we can observe that the initial condition gives $U_{\min} = 0$ and $U_{\max} = 1$ and the graphs show that all U_j^n satisfy the maximum principle

$$0 \leq U_j^n \leq 1.$$

5. Turning our attention to the Θ -Scheme we can similarly perform a Fourier analysis of the advective and diffusive parts of the equation in separation.

Let us first rewrite the Θ -scheme discretisation without the advective term i.e. setting $a=0$:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{\epsilon}{(\Delta x)^2} \left(\Theta(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) + (1-\Theta)(U_{j+1}^n - 2U_j^n + U_{j-1}^n) \right)$$

Defining $\mu = \frac{\epsilon \Delta t}{(\Delta x)^2}$ and again using $U_j^n = (\lambda)^n e^{ik(j\Delta x)}$ and all ^{it's} derived equalities we can rewrite the equation as

$$\lambda v_j^n - v_j^n = m \left(\theta \left(\lambda \left(e^{ik\Delta x} v_j^n - 2v_j^n + e^{-ik\Delta x} v_j^n \right) \right) \dots \right. \\ \left. \dots + (1-\theta) \left(e^{ik\Delta x} v_j^n - 2v_j^n + e^{-ik\Delta x} v_j^n \right) \right).$$

Again dividing through by v_j^n we have

$$\lambda = 1 - 2m \left(\theta \lambda (1 - \cos(k\Delta x)) + (1-\theta)(1 - \cos(k\Delta x)) \right),$$

$$\lambda \left(1 + 2m\theta (1 - \cos(k\Delta x)) \right) = 1 - 2m(1-\theta) \left(1 - \cos(k\Delta x) \right),$$

$$\lambda = \frac{1 - 4m(1-\theta) \left(\sin^2 \left(\frac{k\Delta x}{2} \right) \right)}{1 + 4m\theta \left(\sin^2 \left(\frac{k\Delta x}{2} \right) \right)}.$$

~~Since $\mu > 0$~~ If we assume $\epsilon > 0$ then
~~and~~ we have also defined θ in
the domain $0 \leq \theta \leq 1$. Hence we can never
have $\lambda > 1$ and so we only have instability if
 $\lambda < -1$, therefore

$$1 - 4m(1-\theta) \left(\sin^2 \left(\frac{k\Delta x}{2} \right) \right) < - \left(1 + 4m\theta \left(\sin^2 \left(\frac{k\Delta x}{2} \right) \right) \right)$$

a condition of instability. This simplifies to

$$m(1-2\theta) \sin^2 \left(\frac{k\Delta x}{2} \right) > \frac{1}{2}, \text{ and taking the}$$

mode $k\Delta x = \pi$ that is most likely to violate
the condition we have

$$m(1-2\theta) > \frac{1}{2}$$

as the instability condition.

Now, if $\frac{1}{2} \leq \theta \leq 1$ then the stability condition is in the interval $[-M, 0]$ and since we assume $M > 0$ then this can never be greater than $\frac{1}{2}$, hence the scheme is stable for all M . In contrast, when we have $0 \leq \theta < \frac{1}{2}$ then the stability condition is in the interval $(0, M]$ and therefore the scheme is only stable if and only if

$$M \leq \frac{1}{2(1-\theta)}.$$

We can perform a similar analysis for the advection term by setting $\epsilon = 0$ and writing out the θ -scheme discretisation for just the advection term,

$$\frac{v_j^{n+1} - v_j^n}{\Delta t} = a \left(\frac{\theta(v_{j+1}^n - v_j^n)}{\Delta x} + \frac{(1-\theta)(v_{j-1}^n - v_j^n)}{\Delta x} \right).$$

Defining $M = \frac{a \Delta t}{\Delta x}$, $a < 0$ and again using the Fourier mode $v_j^n = (\lambda)^n e^{ik(j\Delta x)}$ and it's derived equalities we can rewrite the equation as

$$\lambda v_j^{n+1} - v_j^n = M \left(\theta(\lambda e^{ik\Delta x} v_j^n - \lambda v_j^n) + (1-\theta)(e^{ik\Delta x} v_j^n - v_j^n) \right),$$

and again dividing by v_j^n we have

$$\lambda = 1 + M\theta(\lambda e^{ik\Delta x} - 1) + M(1-\theta)(e^{ik\Delta x} - 1),$$

$$\lambda(1 - M\theta(e^{ik\Delta x} - 1)) = 1 + M(1-\theta)(e^{ik\Delta x} - 1),$$

$$\lambda = \frac{1 + M(1-\theta)(e^{ik\Delta x} - 1)}{1 - M\theta(e^{ik\Delta x} - 1)}.$$

This leads to

$$|\lambda|^2 = \frac{1 - 2m(1-\theta)[1-m(1-\theta)][1 - \cos(k\Delta x)]}{1 + 2m\theta[1+m\theta][1 - \cos(k\Delta x)]}$$

$$|\lambda|^2 = \frac{1 - 4m(1-\theta)[1-m(1-\theta)] \sin^2\left(\frac{k\Delta x}{2}\right)}{1 + 4m\theta[1+m\theta] \sin^2\left(\frac{k\Delta x}{2}\right)}$$

For stability we must have $|\lambda| \leq 1$ and so we can write an instability condition as

$$\left| 1 - 4m(1-\theta)(1-m(1-\theta)) \sin^2\left(\frac{k\Delta x}{2}\right) \right| > \left| 1 + 4m\theta(1+m\theta) \sin^2\left(\frac{k\Delta x}{2}\right) \right|.$$

The term on the left-hand side is always positive since $m < 0$. Therefore we can split the condition into two cases:

$$1 - 4m(1-\theta)(1-m(1-\theta)) \sin^2\left(\frac{k\Delta x}{2}\right) > 1 + 4m\theta(1+m\theta) \sin^2\left(\frac{k\Delta x}{2}\right),$$
$$\cancel{1 - 4m(1-\theta)(1-m(1-\theta))} \sin^2\left(\frac{k\Delta x}{2}\right) > \cancel{1 + 4m\theta(1+m\theta)} \sin^2\left(\frac{k\Delta x}{2}\right),$$
$$-4m^2\theta \sin^2\left(\frac{k\Delta x}{2}\right) - 4m(1+m\theta-m) \sin^2\left(\frac{k\Delta x}{2}\right) > 0.$$

Taking the mode most likely to be unstable, i.e. $k\Delta x = \pi$, we have

~~$$4m[m\theta + 1 - m(1-\theta)] < 0,$$~~

$$+m(1+2m\theta-m) < 0,$$

$$m(1+m(2\theta-1)) < 0.$$

If we have $0 \leq \theta \leq \frac{1}{2}$ then because $m < 0$ the scheme is always unstable. If $\frac{1}{2} < \theta \leq 1$ then again since $m < 0$ we must have

$$1+m(2\theta-1) > 0, \text{ which is always satisfied}$$

for $\frac{1}{2} < \theta \leq 1$ and again the scheme is unstable.

Taking the other case we have

$$1 - 4m(1-\theta)(1-m(1-\theta)) \left(\sin^2 \left(\frac{k\Delta x}{2} \right) \right) < - \left[1 + 4m\theta(1+m\theta) \sin^2 \left(\frac{k\Delta x}{2} \right) \right],$$

$$\cancel{2 + 4m^2 \sin^2 \left(\frac{k\Delta x}{2} \right) + 4m}$$

$$2 + 8m\theta(1+m\theta) \sin^2 \left(\frac{k\Delta x}{2} \right) - 4m^2 \theta \sin^2 \left(\frac{k\Delta x}{2} \right) - 4m(1-m(1-\theta)) \sin^2 \left(\frac{k\Delta x}{2} \right) < 0,$$

and again taking the most unstable mode i.e $k\Delta x = \pi$ we have

$$2 + 8m\theta(1+m\theta) - 4m^2\theta - 4m(1-m(1-\theta)) < 0,$$

$$2 + 8m\theta + 8m^2\theta^2 - 4m^2\theta - 4m + 4m^2 - 4m^2\theta < 0,$$

$$8m^2\theta^2 - 8m^2\theta + 8m\theta + 4m^2 - 4m < -2,$$

$$8m\theta(m\theta - m + 1) + 4m(m-1) < -2,$$

$$2m\theta(m\theta - m + 1) + m(m-1) < -\frac{1}{2}.$$

