AM213B Numerical Methods for the Solution of Differential Equations

Lecture 06

List of topics in this lecture

- Runge-Kutta methods: stability function, region of absolute stability, A-stability and L-stability; necessary conditions for p-th order accuracy, for A-stability, and for L-stability
- Linear multi-step methods: stability polynomial, region of absolute stability, A-stability and L-stability; first Dahlquist barrier and second Dahlquist barrier
- No explicit method is both consistent and A-stable.
- How to find numerically the region of absolute stability of an LMM

A-stability and L-stability of Runge-Kutta methods

Recall that we studied behaviors of numerical methods for model ODE $u' = -\lambda u$.

To define A-stability, we consider a slightly more general model ODE:

$u' = \gamma u$

where $\gamma = a + i b$ is <u>complex</u>.

We are interested in the case of $\mathrm{Re}(\gamma) < 0$. Our old model ODE is simply $\gamma = -\lambda$.

<u>The exact solution:</u>

$$u(t) = \exp(\gamma t) = \exp(at + ibt) = \exp(at)\Big(\cos(bt) + i\sin(bt)\Big)$$

<u>Two properties of the exact solution for $\mathrm{Re}(z) < 0$</u>:

1. $u(t) \to 0$ as $t \to \infty$
2. For a fixed value of $t > 0$ (no matter how small it is),

   $u(t) \to 0$ as $\mathrm{Re}(\gamma) \to -\infty$.

We like to preserve these two properties in numerical soliutions.

We consider behaviors of Runge-Kutta methods applied to model ODE $u' = \gamma u$.

<u>Claim 1:</u>

An RK method applied to $u' = \gamma u$ has the form

$$u_{n+1} = u_n \phi(z), \qquad z = h\gamma$$

Question: Why does it depend on only the combination of $(h\gamma)$?

Answer:

- In the model ODE, $f(u) = \gamma\, u$
- In the RK method, h and $f(u)$ are always multiplied together.

Claim 2:

- For an explicit method, $\phi(z)$ = polynomial of z.
- For an implicit method, $\phi(z)$ = rational function of z (i.e., polynomial/polynomial)

Example:

Euler method:

$$u_{n+1} = u_n + h\gamma u_n = u_n(1+h\gamma) = u_n(1+z), \qquad z = h\gamma$$

==> $\phi(z) = 1+z$, a polynomial of z

Backward Euler:

$$u_{n+1} = u_n + h\gamma u_{n+1}$$

==> $u_{n+1}(1-h\gamma) = u_n$ ==> $u_{n+1}(1-z) = u_n$, $z = h\gamma$

==> $\phi(z) = \dfrac{1}{1-z}$, a rational function of z

Trapezoidal method:

$$u_{n+1} = u_n + \frac{1}{2}h\gamma u_n + \frac{1}{2}h\gamma u_{n+1}$$

==> $u_{n+1}\left(1-\dfrac{h\gamma}{2}\right) = u_n\left(1+\dfrac{h\gamma}{2}\right)$ ==> $u_{n+1}\left(1-\dfrac{z}{2}\right) = u_n\left(1+\dfrac{z}{2}\right)$, $z = h\gamma$

==> $\phi(z) = \dfrac{1+z/2}{1-z/2}$, a rational function of z

The numerical solution of $u' = \gamma\, u$ with an RK method has the expression

$$u_n = u_0\left(\phi(z)\right)^n, \qquad z = h\gamma$$

As $n \to \infty$, u_n decreases to 0 if and only if $\left|\phi(z)\right| < 1$.

Definition (stability function):

Function $\phi(z)$ is called the stability function.

Definition (region of absolute stability)

$S \equiv \left\{ z \in \mathbb{C} \,\middle|\, \left|\phi(z)\right| < 1 \right\}$ is called the region of absolute stability

(Or is simply referred to as stability region).

Remarks:

Here the region of absolute stability is defined based on

"u_n decreases to 0 as $n \to \infty$".

In some literature, the region of absolute stability is defined based on

"u_n remains bounded as $n \to \infty$".

$S_2 \equiv \left\{ z \in \mathbb{C} \,\middle|\, \left|\phi(z)\right| \le 1 \right\}$

For single step methods, we always have,

$$\left(\underbrace{S_2}_{\substack{\text{based on} \\ |u_n| \le C}} \right) = \text{cl}\left(\underbrace{S}_{\substack{\text{based on} \\ u_n \to 0}} \right) \qquad \text{closure of set S.}$$

For multi-step methods, this is not always true.

Definition (A-stability)

A method is called A-stable if the region of absolute stability contains the entire left half of the complex plane:

$$\left\{ z \in \mathbb{C} \,\middle|\, \text{Re}(z) < 0 \right\} \subseteq \left\{ z \in \mathbb{C} \,\middle|\, \left|\phi(z)\right| < 1 \right\}$$

In other words, a method is A-stable if the stability function $\phi(z)$ satisfies

$$\boxed{\left|\phi(z)\right| < 1 \quad \text{for all } \text{Re}(z) < 0}$$

Definition (L-stability)

A method is called L-stable if

- it is A-stable and
- $\phi(z) \to 0$ as $z \to \infty$.

Question: Why do we specify the limit as $z \to \infty$, instead of the limit as $\mathrm{Re}(z) \to -\infty$?

Answer:

Recall that $\phi(z)$ is a rational function: $\phi(z) = \dfrac{P(z)}{Q(z)}$.

"$\phi(z) \to 0$ as $z \to \infty$" and "$\phi(z) \to 0$ as $\mathrm{Re}(z) \to -\infty$" are both equivalent to

"degree of $P(z)$ < degree of $Q(z)$"

Example: (Region of absolute stability, A-stability, L-stability)

Euler method:

Stability function:

$$\phi(z) = 1 + z$$

Region of absolute stability:

$$S = \left\{ z \in \mathbb{C} \,\middle|\, |\phi(z)| < 1 \right\} = \left\{ z \in \mathbb{C} \,\middle|\, |z - (-1)| < 1 \right\}$$

= interior of the circle centered at $z_c = -1$ with radius 1.

(Show the region of absolute stability for Euler method.)

==> Euler method is not A-stable

(and, of course, it is not L-stable.)

Backward Euler method:

Stability function:

$$\phi(z) = \frac{1}{1 - z}$$

Region of absolute stability:

$$S = \left\{ z \in \mathbb{C} \,\middle|\, |\phi(z)| < 1 \right\} = \left\{ z \in \mathbb{C} \,\middle|\, |z - 1| > 1 \right\}$$

= exterior of the circle centered at $z_c = 1$ with radius 1.

(Show the region of absolute stability for backward Euler method.)

==> Backward Euler method is A-stable.

In addition, it satisfies $\phi(z) = \dfrac{1}{1 - z} \to 0$ as $z \to \infty$.

==> Backward Euler method is L-stable.

Trapezoidal method:

Stability function:

$$\phi(z)=\frac{1+z/2}{1-z/2}$$

Region of absolute stability:

$$S=\left\{z\in\mathbb{C}\,\middle|\,|\phi(z)|<1\right\}=\left\{z\in\mathbb{C}\,\middle|\,\left|\frac{1+z/2}{1-z/2}\right|<1\right\}$$

$$=\left\{z\in\mathbb{C}\,\middle|\,|z-(-2)|<|z-2|\right\}$$

(The boundary of S is the perpendicular bisector of [–2, 2])

$$=\left\{z\in\mathbb{C}\,\middle|\,\mathrm{Re}(z)<0\right\}$$

==> Trapezoidal method is A-stable.

But $\phi(z)=\dfrac{1+z/2}{1-z/2}\to -1$ as $z\to\infty$

==> Trapezoidal method is not L-stable.

Theorem

(This theorem is about necessary conditions for p-th order accuracy, A-stability, and L-stability of Runge-Kutta methods.)

1. If an RK method is p-th order accurate, then it must satisfies

   $$\phi(z)=e^{z}+O(|z|^{p+1})\quad \text{for small } |z|$$

2. If a method is A-stable, then it must be implicit.
3. If a method is L-stable, then it must also satisfy

   degree of $P(z)$ < degree of $Q(z)$ where $\phi(z)=\dfrac{P(z)}{Q(z)}$

Proof: (skip in lecture)

Part 1: Suppose the RK method is p-th order accurate.

==> Error of one step is $e_n(h) = O(h^{p+1})$

==> $u_1 - u(h) = O(h^{p+1})$

Applying the RK method to the model ODE $u' = \gamma u$

==> $u_0\,\phi(h\gamma) - u_0\exp(h\gamma) = O(h^{p+1})$

Set $u_0 = 1$ and $|\gamma| = 1$.

==> $\phi(h\gamma) = \exp(h\gamma) + O(|h\gamma|^{p+1})$ for h = real > 0

==> $\phi(z) = e^z + O(|z|^{p+1})$ for small $|z|$

Part 2: Suppose the method is A-stable.

==> $|\phi(z)| < 1$ for all $\mathrm{Re}(z) < 0$

==> $\phi(z) = \dfrac{P(z)}{Q(z)}$ remains bounded as $\mathrm{Re}(z) \to -\infty$

==> degree of $P(z)$ ≤ degree of $Q(z)$.

==> degree of $Q(z) \geq 1$.

==> The method must be implicit.

Part 3: Suppose the method is L-stable

==> $\phi(z) = \dfrac{P(z)}{Q(z)} \to 0$ as $z \to \infty$

==> degree of $P(z)$ < degree of $Q(z)$

A-stability and L-stability of LMM (linear multi-step methods)

The general form of LMM:

$$\sum_{j=0}^{r} \alpha_j u_{n+j} = h \sum_{j=0}^{r} \beta_j f(u_{n+j}, t_{n+j}), \qquad \alpha_r = 1$$

Apply it to the model ODE, $u' = \gamma u$, we get

$$\sum_{j=0}^{r} \alpha_j u_{n+j} = h\gamma \sum_{j=0}^{r} \beta_j u_{n+j}$$

Consider solutions of the form $\{u_k = \xi^k$, k=0, 1, 2, …$\}$

Substituting $u_k = \xi^k$ into the LMM yields a polynomial equation for ξ.

$$\sum_{j=0}^{r} \alpha_j \xi^{n+j} - z \sum_{j=0}^{r} \beta_j \xi^{n+j} = 0, \qquad z = h\gamma$$

==> $$\sum_{j=0}^{r}\alpha_j\xi^j - z\sum_{j=0}^{r}\beta_j\xi^j = 0$$

In terms of characteristic polynomials, the equation for ξ becomes

$$\rho(\xi) - z\sigma(\xi) = 0$$

<u>Definition</u> (stability polynomial of LMM):

Function $\pi(\xi, z) \equiv \rho(\xi) - z\sigma(\xi)$ is called the stability polynomial of the LMM.

We view $\pi(\xi, z) = 0$ as <u>an equation for ξ</u> with <u>z as a parameter</u>. Let

{ $\xi_j(z)$ } denote simple roots of $\pi(\xi, z) = 0$, and

{ $q_i(z)$ } denote roots of $\pi(\xi, z) = 0$ with multiplicity > 1.

The numerical solution of $u' = \gamma u$ with the LMM has the form

$$u_n = \left(c_1\xi_1^n(z) + c_2\xi_2^n(z) + \cdots\right) + \left(b_1^{(0)} + b_1^{(1)}n + \cdots\right)q_1^n(z) + \left(b_2^{(0)} + b_2^{(1)}n + \cdots\right)q_2^n(z) + \cdots$$

As $n \to \infty$, u_n decreases to 0

if and only if $\left|\xi_j(z)\right| < 1$ and $\left|q_i(z)\right| < 1$

if and only if |all roots| < 1 <u>regardless of multiplicity</u>.

<u>Definition</u> (region of absolute stability of LMM):

$$S \equiv \left\{ z \in \mathbb{C} \,\middle|\, \text{All roots of } \pi(\xi, z) \text{ satisfy } \left|\xi_j(z)\right| < 1 \right\}$$

is called the region of absolute stability

(Or is simply referred to as stability region).

<u>Remark:</u>

In some literature, the region of absolute stability is defined based on

"u_n remains bounded as $n \to \infty$".

$$S_2 \equiv \left\{ z \in \mathbb{C} \,\middle|\, \begin{array}{l} \text{All simple roots of } \pi(\xi, z) \text{ satisfy } \left|\xi_j(z)\right| \le 1 \\ \text{All roots of } \pi(\xi, z) \text{ with multiplicity above 1 satisfy } \left|q_i(z)\right| < 1 \end{array} \right\}$$

For multi-step methods, it is not always true that

$$\left(\underbrace{S_2}_{\substack{\text{based on} \\ |u_n| \le C}} \right) = \mathrm{cl}\left(\underbrace{S}_{\substack{\text{based on} \\ u_n \to 0}} \right)$$

Definition (A-stability of LMM)

A method is called A-stable if the region of absolute stability contains the entire left half of the complex plane:

$$\left\{ z \in \mathbb{C} \,\middle|\, \mathrm{Re}(z) < 0 \right\} \subseteq \left\{ z \in \mathbb{C} \,\middle|\, \text{All roots of } \pi(\xi, z) \text{ satisfy } \left|\xi_j(z)\right| < 1 \right\}$$

In other words, a method is called A-stable if

$$\boxed{\text{all roots of } \pi(\xi, z) \text{ satisfy } \left|\xi_j(z)\right| < 1 \quad \text{for all } \ \mathrm{Re}(z) < 0}$$

Definition (L-stability of LMM)

A method is called L-stable if

- it is A-stable and
- all roots of $\pi(\xi, z)$ satisfy $\xi_j(z) \to 0$ as $z \to \infty$.

Next we discuss the theoretical limits on the order of accuracy and on the A-stability of LMM. Swedish mathematician Germund Dahlquist established these theoretical limits in two theorems, known as first Dahlquist barrier and second Dahlquist barrier.

Theorem (First Dahlquist barrier on LMM)

Let p denote the order of accuracy of a zero-stable LMM.

p is constrained by the number of steps, r, as follows:

For explicit r-step LMMs, $p \le r$.

For implicit r-step LMMs, $p \le r + 1$ if r = odd

$p \le r + 2$ if r = even

Proof: The proof of this theorem is beyond the scope of this course.

Remark:

Adams-Bashforth methods (explicit) achieve $p = r$.

Adams-Moulton methods (implicit) achieve $p = r + 1$.

Theorem (Second Dahlquist barrier on LMM)

1. There is no explicit LMM that is both A-stable and consistent.
2. For an implicit A-stable LMM, the order of accuracy is limited by: $p \le 2$.

   Furthermore, the trapezoidal method (1-step Adams-Moulton) has the smallest error among all implicit A-stable LMMs.

Proof: We present the proof for part 1 in Appendix A.

The proof for part 2 is outside the scope of this course.

Remark:

It is trivial to write out an explicit LMM that is A-stable but is not consistent.

We can do so by just completely ignoring the ODE we are solving.

$$u_{n+2} - \frac{1}{2} u_n = 0$$

Example: Region of absolute stability of the 2-step midpoint method

$$u_{n+2} - u_n = 2hf(u_{n+1}, t_{n+1})$$

Two characteristic polynomials:

$$\rho(\xi) = \xi^2 - 1, \qquad \sigma(\xi) = 2\xi$$

Stability polynomial:

$$\pi(\xi, z) \equiv \rho(\xi) - z\sigma(\xi) = (\xi^2 - 1) - z2\xi = \xi^2 - z2\xi - 1$$

We can write out the two roots using the quadratic formula and then analyze the two roots. But that is unnecessary. We notice that the two roots satisfy $\xi_1 \xi_2 = -1$ for any z.

Thus, for any z, it is impossible to have

both $|\xi_1| < 1$ and $|\xi_2| < 1$

It follows that the region of absolute stability is empty

$$S \equiv \left\{ z \in \mathbb{C} \,\middle|\, |\xi_1(z)| < 1 \text{ and } |\xi_2(z)| < 1 \right\} = \text{EMPTY}$$

Example: Region of absolute stability of the 2-step Adams-Moulton method

$$u_{n+2} - u_{n+1} = h\left[\frac{5}{12} f(u_{n+2}, t_{n+2}) + \frac{8}{12} f(u_{n+1}, t_{n+1}) - \frac{1}{12} f(u_n, t_n) \right]$$

Two characteristic polynomials:

$$\rho(\xi) = \xi^2 - \xi, \qquad \sigma(\xi) = \frac{5}{12}\xi^2 + \frac{8}{12}\xi - \frac{1}{12}$$

Stability polynomial:

$$\pi(\xi,z)\equiv\rho(\xi)-z\sigma(\xi)=\left(\xi^2-\xi\right)-z\left(\frac{5}{12}\xi^2+\frac{8}{12}\xi-\frac{1}{12}\right)$$
$$=\left(1-\frac{5}{12}z\right)\xi^2-\left(1+\frac{8}{12}z\right)\xi+\frac{1}{12}z$$

We first show <u>analytically</u> that the region of absolute stability is <u>non-empty.</u>

Let $z = -\varepsilon$ (real) with small $\varepsilon > 0$. Recall that $z = h\gamma$. So $z = -\varepsilon$ corresponds to solving

$u' = -u$ with time step ε. This is the most likely situation where the method will behave well. For that reason, $z = -\varepsilon$ is the most likely member of the region of absolute stability if the region is non-empty.

For $z = -\varepsilon$, the stability polynomial has the expression

$$\pi(\xi,-\varepsilon)=\left(1+\frac{5\varepsilon}{12}\right)\xi^2-\left(1-\frac{8\varepsilon}{12}\right)\xi-\frac{\varepsilon}{12}$$

The two roots of $\pi(\xi, -\varepsilon)$ are

$$\xi_{1,2}=\frac{1}{2\left(1+\frac{5\varepsilon}{12}\right)}\left[\left(1-\frac{8\varepsilon}{12}\right)\pm\sqrt{\left(1-\frac{8\varepsilon}{12}\right)^2+4\cdot\frac{\varepsilon}{12}\left(1+\frac{5\varepsilon}{12}\right)}\right]$$

Expanding the two roots in terms of ε, we have

$$\xi_{1,2}=\frac{1}{2}\left(1-\frac{5\varepsilon}{12}+O(\varepsilon^2)\right)\left[\left(1-\frac{8\varepsilon}{12}\right)\pm\sqrt{1-\frac{12\varepsilon}{12}+O(\varepsilon^2)}\right]$$

==> $\xi_1=1-\varepsilon+O(\varepsilon^2)$, $\quad\xi_2=\frac{-\varepsilon}{12}+O(\varepsilon^2)$

==> $|\xi_{1,2}| < 1$ for small $\varepsilon > 0$.

Thus, the region of absolute stability, S, contains $z = -\varepsilon$ for small $\varepsilon>0$.

Next, we consider ∂S, the boundary of S.

<u>A necessary condition</u> for ∂S:

Suppose z is on ∂S. Then one root of $\pi(\xi, z)$ has absolute value = 1.

==> one root of $\pi(\xi, z)$ can be written as $\xi = e^{i\theta}$ for some value of θ.

==> $\pi(e^{i\theta}, z) = 0$ for some value of θ (depending on z).

==> z satisfies $\rho(e^{i\theta})-z\,\sigma(e^{i\theta}) = 0$ for some value of θ.

==> $\boxed{z \text{ has the expression } z = \dfrac{\rho(e^{i\theta})}{\sigma(e^{i\theta})} \text{ for some value of } \theta.}$

We point out that this is only <u>a necessary condition</u>, <u>NOT a sufficient condition</u>.

When θ varies from 0 to 2π, $z = \rho(e^{i\theta})/\sigma(e^{i\theta})$ traces a curve in the complex plane. Not all segments of this curve are part of ∂S. This curve is merely a <u>candidate</u> for ∂S. Going across a segment of this curve, there are at least two possibilities:

1. The absolute value of one root goes from below 1 to above 1 while the absolute value of the other root stays <u>below 1</u>.
2. The absolute value of one root goes from below 1 to above 1 while the absolute value of the other root stays <u>above 1</u>.

Only possibility #1 corresponds to a part of ∂S.

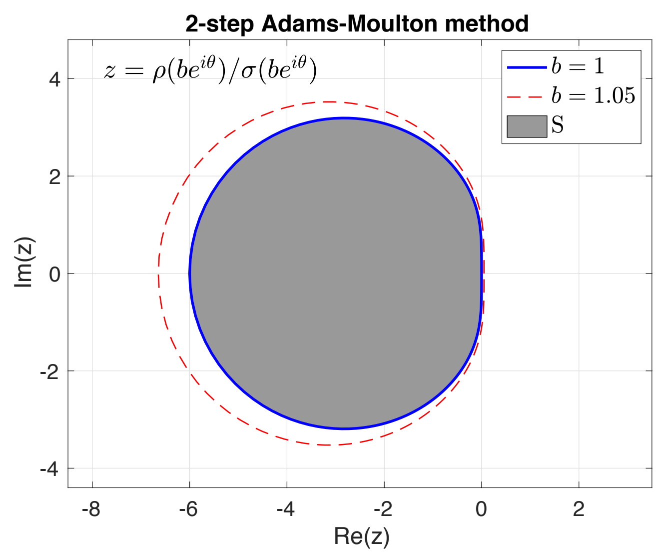

Figure 1 plots a <u>candidate</u> of ∂S for the 2-step Adams-Moulton method, traced out by $z = \rho(e^{i\theta})/\sigma(e^{i\theta})$, shown as the solid blue line. The dashed red line shows the curve traced by $z = \rho(be^{i\theta})/\sigma(be^{i\theta})$ with $b = 1.05$. The shaded region is the region of absolute stability, S.

<u>Example:</u> Region of absolute stability of the 4-step Adams-Bathforth method

$$u_{n+4} = u_{n+3} + \frac{h}{24}\left[-9f(u_n,t_n) + 37f(u_{n+1},t_{n+1}) - 59f(u_{n+2},t_{n+2}) + 55f(u_{n+3},t_{n+3})\right]$$

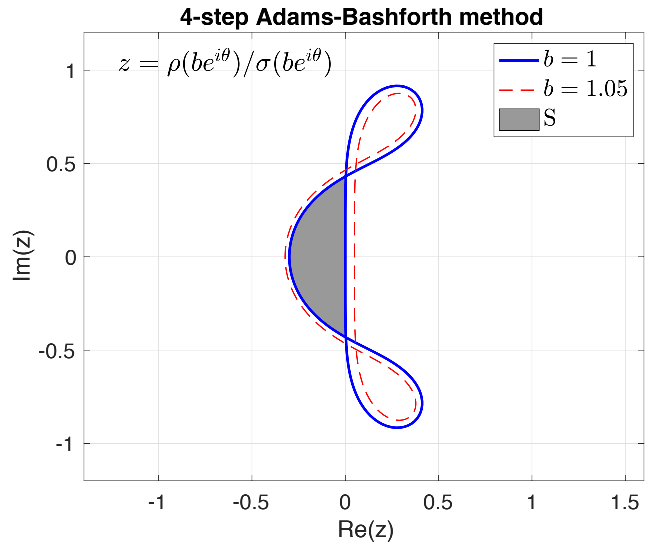

Figure 2 plots a candidate of ∂S for the 4-step Adams-Bashforth method, traced out by $z = \rho(e^{i\theta})/\sigma(e^{i\theta})$, shown as the solid blue line. The dashed red line shows the curve traced by $z = \rho(be^{i\theta})/\sigma(be^{i\theta})$ with $b = 1.05$. The shaded region is the region of absolute stability, S, whose boundary contains only part of the solid blue line.

Appendix A: Proof of second Dahlquist barrier on LMM

Theorem (Second Dahlquist barrier on LMM)

1. There is no explicit LMM that is both A-stable and consistent.
2. ...

Proof for part 1: Recall the general form of the r-step LMM

$$\sum_{j=0}^{r} \alpha_j u_{n+j} = h \sum_{j=0}^{r} \beta_j f\left(u_{n+j}, t_{n+j}\right), \qquad \alpha_r = 1$$

Suppose there is an explicit LMM that is both A-stable and consistent. We have

$\alpha_r = 1$ (by convention)

$\beta_r = 0$ (since the LMM is explicit)

By definition, the stability polynomial $\pi(\xi, z)$ of the LMM has the expression

$$\begin{aligned}\pi(\xi, z) &= \xi^r + \sum_{j=0}^{r-1} (\alpha_j - z\beta_j)\xi^j \\ &\equiv \xi^r + a_{r-1}(z)\xi^{r-1} + a_{r-2}(z)\xi^{r-2} + \cdots + a_0(z)\end{aligned}$$

where $a_j(z) \equiv (\alpha_j - z\,\beta_j)$ for $j \le r-1$.

On the other hand, $\pi(\xi, z)$ is expressed in terms of its roots.

$$\pi(\xi,z) = \prod_{k=1}^{r}\left(\xi - \xi_k(z)\right)$$

$$= \xi^r - \left(\sum_k \xi_k(z)\right)\xi^{r-1} + \left(\sum_{k_1,k_2} \xi_{k_1}(z)\xi_{k_2}(z)\right)\xi^{r-2} + \cdots + (-1)^r \prod_{k=1}^{r}\xi_k(z)$$

Comparing these two expressions of $\pi(\xi, z)$, we obtain

$$a_{r-1}(z) = -\left(\sum_k \xi_k(z)\right)$$

$$a_{r-2}(z) = \left(\sum_{k_1,k_2} \xi_{k_1}(z)\xi_{k_2}(z)\right)$$

…

The A-stability of the LMM implies that all roots of $\pi(\xi, z)$ satisfy

$$\left|\xi_k(z)\right| < 1 \quad \text{for all } \operatorname{Re}(z) < 0$$

==> $\left|\xi_k(z)\right|$ remains bounded as $\operatorname{Re}(z) \to -\infty$

==> $\left|a_j(z)\right|$ remains bounded as $\operatorname{Re}(z) \to -\infty$ for $j \le r-1$

Combining this result with $a_j(z) \equiv (\alpha_j - z\,\beta_j)$, we obtain

$\beta_j = 0$ for $j \le r-1$ and we already have $\beta_r = 0$.

Thus, we have $\sigma(\xi) \equiv 0$, and $\pi(\xi, z) = \rho(\xi)$, independent of z.

The consistency condition, $\rho(1) = 0$, $\rho'(1) = \sigma(1)$, implies

$\rho(1) = 0$, $\rho'(1) = 0$

==> $\xi = 1$ is a double root of $\rho(\xi)$.

==> $\xi = 1$ is a double root of $\pi(\xi, z)$, independent of z,

which contradicts the A-stability.

End of proof