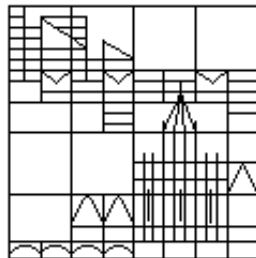


Some aspects
of
consistency and stability
for
lattice Boltzmann methods

Workshop Lattice Boltzmann schemes – Methods and Applications

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Sufficient condition for stability of LB schemes

Stability-structure for collision operator: \rightarrow [Junk & Yong, 07] and [MRh, 08]

$$\left. \begin{array}{l} \text{i) } \quad BJ = -\text{diag}(\lambda_1, \dots, \lambda_q)B \\ \text{ii) } \quad B^\top B = \text{diag}(b_1, \dots, b_q) \\ \text{iii) } \quad \lambda_k \in [0, 2] \quad \text{for all } k \in \{1, \dots, q\} \end{array} \right\} \quad B \text{ invertible}$$

Question: BGK *collision operators* with *stability-structure*

\longrightarrow MRT *collision operators* with *stability-structure*?

$$J_{\text{BGK}} = \frac{1}{\omega}(G - I) \quad \leftrightarrow \quad J_{\text{MRT}} = A(G - I)$$

Properties of A :

$$\ker A^\top = \ker(G^\top - I) = \ker J_{\text{BGK}}^\top \quad (\Rightarrow J_{\text{MRT}} \text{ has same conserved moments as } J_{\text{BGK}})$$

symmetric ($A = A^\top$) and *positive semidefinite*

$$J \text{ admits stability structure} \quad \Leftrightarrow \quad JD = DJ^\top \quad (D \text{ diagonal \& positive definite})$$

Construction: BGK \rightarrow MRT

[MRh, 08]

$$1) \quad G = WS \quad (\text{positive definite \& diagonal weight matrix } W, \text{ symmetric } S)$$

$$2) \text{ no specific assumptions: } J_{\text{BGK}}\tilde{D} = \tilde{D}J_{\text{BGK}}^\top$$

$$(G-I)\tilde{D} = \tilde{D}(G-I)^\top \quad \underbrace{A(G-I)}_{J_{\text{MRT}}} D = D \underbrace{(G-I)^\top A}_{J_{\text{MRT}}^\top} \quad A, D = ?$$

$$\left. \begin{array}{l} J_{\text{BGK}}\tilde{D} \text{ symmetric} \\ D := \tilde{D} \end{array} \right\} \Rightarrow [A, J_{\text{BGK}}\tilde{D}] = 0$$

$$A \text{ symmetric} \Rightarrow \text{eigenspaces of } A = \text{eigenspaces of } J_{\text{BGK}}\tilde{D}$$

$$\ker A^\top = \ker (J_{\text{BGK}}\tilde{D})^\top = \ker (DJ_{\text{BGK}}^\top) \Rightarrow \ker A^\top = \ker J_{\text{BGK}}^\top$$

Observe: $\text{spec}(J_{\text{MRT}}) = \text{spec}(A)$

- Advantage of MRT w.r.t. BGK:

more parameters \leftrightarrow more flexibility

\Rightarrow Hope to improve stability behavior.

- However, modification \rightarrow *consistency check*.

Does the algorithm still what it is intended to do?

- Example to be studied exemplarily:

D1Q3 lattice Boltzmann algorithm discretizing
advection diffusion equation.

\rightarrow admits *advection velocity* as additional parameter *affecting stability*.

$$\mathbf{e} := (1, 1, 1)^\top \qquad \mathbf{c} := (-1, 1, 0)^\top$$

LB equation: $\hat{f}_k(t + h^2, x + \mathbf{c}_k h) = \hat{f}_k(t, x) + \left[J \hat{\mathbf{f}}(t, x) \right]_k$

Collision and equilibrium operator:

$$\left\{ \begin{array}{l} J = \underbrace{A}_{\text{relaxation}} \left(\underbrace{G}_{\text{equilibrium}} - \underbrace{I}_{\text{identity}} \right) \qquad J = J_d + hAG_a \\ G\mathbf{f} := G_d\mathbf{f} + hG_a\mathbf{f} := \langle \mathbf{e}, \mathbf{f} \rangle \mathbf{w} + ah\theta \langle \mathbf{e}, \mathbf{f} \rangle \mathbf{c}\mathbf{w} \quad \text{for } \mathbf{f} \in \mathbb{R}^3 \end{array} \right.$$

Regular expansion: $\underbrace{\hat{\mathbf{f}}}_{\text{discrete arguments}} = \underbrace{\mathbf{f}^{(0)} + h\mathbf{f}^{(1)} + h^2\mathbf{f}^{(2)} + h^3\mathbf{f}^{(3)} + \dots}_{\text{continuously varying arguments}}$

Taylor expansion: $\left[f_k^{(j)}(t + h^2, x + \mathbf{c}_k h) \right]_{k \in \{1,2,3\}} = \sum_{\alpha} h^{\alpha} D_{\alpha}(\partial_t, \mathbf{c}\partial_x) \mathbf{f}^{(j)}$

$$D_{\alpha}(\vartheta, \varsigma) := \sum_{2\beta + \gamma = \alpha} \frac{\vartheta^{\beta} \varsigma^{\gamma}}{\beta! \gamma!}$$

$$D_0(\partial_t, \mathbf{c}\partial_x) = 1, \quad D_1(\partial_t, \mathbf{c}\partial_x) = \mathbf{c}\partial_x, \quad D_2(\partial_t, \mathbf{c}\partial_x) = \partial_t + \frac{1}{2}\mathbf{c}^2\partial_x^2,$$

$$D_3(\partial_t, \mathbf{c}\partial_x) = \mathbf{c}\partial_x\partial_t + \frac{1}{6}\mathbf{c}^3\partial_x^3, \quad D_4(\partial_t, \mathbf{c}\partial_x) = \frac{1}{2}\partial_t^2 + \frac{1}{2}\mathbf{c}^2\partial_x^2\partial_t + \frac{1}{24}\mathbf{c}^4\partial_x^4$$

Equating terms of order h^ℓ :

$$h^\ell : \quad J_d \mathbf{f}^{(\ell)} = -AG_a \mathbf{f}^{(\ell-1)} + \sum_{j=1}^{\ell} D_j (\partial_t, \mathbf{c} \partial_x) \mathbf{f}^{(\ell-j)}$$

$$h^0 : \quad J_d \mathbf{f}^{(0)} = 0$$

$$h^1 : \quad J_d \mathbf{f}^{(1)} = -AG_a \mathbf{f}^{(0)} + \mathbf{c} \partial_x \mathbf{f}^{(0)}$$

$$h^2 : \quad J_d \mathbf{f}^{(2)} = -AG_a \mathbf{f}^{(1)} + \mathbf{c} \partial_x \mathbf{f}^{(1)} + \partial_t \mathbf{f}^{(0)} + \frac{1}{2} \mathbf{c}^2 \partial_x^2 \mathbf{f}^{(0)}$$

- Discussion of eqn. (h^0)

$$\mathbf{f}^{(0)} \in \ker J_d = \ker A(G_d - I) \quad \Rightarrow \quad \mathbf{f}^{(0)} = \rho^{(0)} \mathbf{w} \quad \text{with } \rho^{(0)}(t, x) = ?$$

- Discussion of eqn. (h^1)

$$\text{solution exists} \quad \Leftrightarrow \quad \text{RHS} \in \text{im} J_d \quad \Leftrightarrow \quad \text{RHS} \in (\ker J_d^\top)^\perp = \text{span}(\mathbf{e})^\perp$$

$$0 = \langle \mathbf{e}, -AG_a \mathbf{f}^{(0)} + \mathbf{c} \partial_x \mathbf{f}^{(0)} \rangle \quad \Leftarrow \quad \mathbf{f}^{(0)} = \rho^{(0)} \mathbf{w}.$$

$$\text{Formal solution:} \quad \begin{cases} \mathbf{f}^{(1)} &= \rho^{(1)} \mathbf{w} + J_d^\dagger \left(-AG_a \mathbf{f}^{(0)} + (\mathbf{c} \partial_x \mathbf{f}^{(0)}) \right) \\ &= \rho^{(1)} \mathbf{w} - a\theta \rho^{(0)} J_d^\dagger A(\mathbf{c} \mathbf{w}) + \partial_x \rho^{(0)} J_d^\dagger (\mathbf{c} \mathbf{w}) \end{cases}$$

$J : \mathbb{R}^q \rightarrow \mathbb{R}^q$ not invertible (neither *injective* nor *surjective*)

$$J\mathbf{x} = \mathbf{y} \quad \text{difficulty: } \begin{cases} \mathbf{y} \in \text{im}J \Rightarrow \text{not unique solution} \\ \mathbf{y} \notin \text{im}J \Rightarrow \text{no solution} \end{cases} \quad \mathbf{x} = \cancel{J^{-1}\mathbf{y}}$$

Best *approximate* solution of *minimal* norm:

$$\bar{\mathbf{x}} \in \left\{ \mathbf{a} : \|J\mathbf{a} - \mathbf{y}\| = \min_{\mathbf{z}} \|J\mathbf{z} - \mathbf{y}\| \right\} =: \mathcal{A}, \quad \|\bar{\mathbf{x}}\| \leq \|\mathbf{a}\| \text{ for all } \mathbf{a} \in \mathcal{A}$$

Pseudo-inverse: $J^\dagger \mathbf{y} := \bar{\mathbf{x}}$ (well-defined & linear)

Explicit construction: $J|_{(\ker J)^\perp} =: \tilde{J} : (\ker J)^\perp \rightarrow \text{im}J$ (invertible restriction)

$$J^\dagger = \tilde{E}_{(\ker J)^\perp} \tilde{J}^{-1} \tilde{P}_{\text{im}J}$$

$$J = \tilde{E}_{\text{im}J} \tilde{J} \tilde{P}_{(\ker J)^\perp}$$

Some properties:

$$\mathbf{y} \in \text{im}J \Rightarrow \text{exact solution } J^\dagger \mathbf{y} + \ker J$$

$$J^\dagger J = P_{(\ker J)^\perp} \in \text{End}(\mathbb{R}^q) \text{ but } J J^\dagger = P_{\text{im}J} \in \text{End}(\mathbb{R}^q), \quad (AB)^\dagger \neq B^\dagger A^\dagger$$

- J symmetric: $J = J^\top$ (orthogonal eigenspaces)

$$\ker J = \text{eig}(J, 0) \perp \text{im} J \quad \Leftrightarrow \quad \ker(J)^\perp = \text{im} J \quad (\Rightarrow \quad J^\dagger J = J J^\dagger = P_{\text{im} J})$$

$$\begin{aligned} J &= M \text{diag}(0, \dots, 0, \lambda_1, \dots, \lambda_{\dim(\text{im} J)}) M^{-1} \\ \Rightarrow J^\dagger &= M \text{diag}(0, \dots, 0, \lambda_1^{-1}, \dots, \lambda_{\dim(\text{im} J)}^{-1}) M^{-1} \end{aligned} \quad (M^{-1} = M^\top)$$

$\Rightarrow J^\dagger$ symmetric

- J projection: $J = J^2$ (BGK: $J_d = \frac{1}{\omega}(G_d - I)$)

Two possibilities for solving $J\mathbf{x} = \mathbf{y} \in \text{im} J$

$$\text{i) } \mathbf{x} = \mathbf{y} + \ker J \quad (\mathbf{y} \in \text{im} J \Leftrightarrow \mathbf{y} = J\mathbf{z} \Rightarrow J\mathbf{y} = J^2\mathbf{z} = J\mathbf{z} = \mathbf{y})$$

$$\text{ii) } \mathbf{x} = J^\dagger \mathbf{y} + \ker J$$

$$\mathbf{y} - J^\dagger \mathbf{y} \in \ker J \quad \Leftrightarrow \quad \underbrace{J\mathbf{y}}_{=\mathbf{y}} - \underbrace{J J^\dagger \mathbf{y}}_{=\mathbf{y}} = \mathbf{0}$$

$$J_d \mathbf{f}^{(2)} = -AG_a \mathbf{f}^{(1)} + \mathbf{c} \partial_x \mathbf{f}^{(1)} + \partial_t \mathbf{f}^{(0)} + \frac{1}{2} \mathbf{c}^2 \partial_x^2 \mathbf{f}^{(0)}$$

- Discussion of eqn. (h^2)

Solvability condition for $\mathbf{f}^{(2)}$: $\text{RHS} \in \text{im} J_d \Leftrightarrow \text{RHS} \in (\ker J_d^\top)^\perp = \text{span}(\mathbf{e})^\perp$

$$0 = \langle \mathbf{e}, -AG_a \mathbf{f}^{(1)} + \mathbf{c} \partial_x \mathbf{f}^{(1)} + \partial_t \mathbf{f}^{(0)} + \frac{1}{2} \mathbf{c}^2 \partial_x^2 \mathbf{f}^{(0)} \rangle = \langle \mathbf{e}, \mathbf{c} \partial_x \mathbf{f}^{(1)} + \partial_t \mathbf{f}^{(0)} + \frac{1}{2} \mathbf{c}^2 \partial_x^2 \mathbf{f}^{(0)} \rangle$$

$$\downarrow \quad \begin{aligned} \mathbf{f}^{(0)} &= \rho^{(0)} \mathbf{w} \\ \mathbf{f}^{(1)} &= \rho^{(1)} \mathbf{w} - a\theta \rho^{(0)} J_d^\dagger A(\mathbf{c}\mathbf{w}) + \partial_x \rho^{(0)} J_d^\dagger(\mathbf{c}\mathbf{w}) \end{aligned}$$

$$0 = \partial_t \rho^{(0)} \underbrace{-a\theta \langle \mathbf{c}, J_d^\dagger A \mathbf{c}\mathbf{w} \rangle}_{\text{advection velocity}} \partial_x \rho^{(0)} + \underbrace{\left(\langle \mathbf{c}, J_d^\dagger \mathbf{c}\mathbf{w} \rangle + \frac{1}{2\theta} \right)}_{\text{-diffusivity}} \partial_x^2 \rho^{(0)}$$

$\Rightarrow \rho^{(0)}$ has to satisfy a drift-diffusion equation.

- Turns out:

Transport coefficients (almost) independent of specific A and thus of J_d .

- $A = \begin{pmatrix} \dot{\omega} \\ \dot{\omega} \\ \dot{\omega} \end{pmatrix}$ or $A = \omega I \Rightarrow J = \frac{1}{\omega}(G - I)$ (BGK)

$$\langle \mathbf{c}, J_d^\dagger A \mathbf{c} \mathbf{w} \rangle = -\langle \mathbf{c}, \mathbf{c} \mathbf{w} \rangle = -\frac{1}{\theta}, \quad \langle \mathbf{c}, J_d^\dagger \mathbf{c} \mathbf{w} \rangle = -\frac{1}{\omega} \langle \mathbf{c}, \mathbf{c} \mathbf{w} \rangle = -\frac{1}{\theta \omega}$$

- $A = M^{-1} \begin{pmatrix} \dot{\omega} \\ \dot{\omega} \\ \dot{\lambda} \end{pmatrix} M$ $M := \begin{pmatrix} \mathbf{e}^\top \\ \mathbf{c}^\top \\ (\mathbf{c}^2 - \frac{1}{\theta} \mathbf{e})^\top \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ -1 & 1 & 0 \\ 1-1/\theta & 1-1/\theta & -1/\theta \end{pmatrix}$

$$M \text{ has } W\text{-orthogonal rows} \Rightarrow J_d^\dagger = -A^\dagger$$

$$\langle \mathbf{c}, J_d^\dagger A \mathbf{c} \mathbf{w} \rangle = -\langle \mathbf{c}, A^\dagger A \mathbf{c} \mathbf{w} \rangle = -\frac{1}{\theta}, \quad \langle \mathbf{c}, J_d^\dagger \mathbf{c} \mathbf{w} \rangle = -\langle \mathbf{c}, A^\dagger \mathbf{c} \mathbf{w} \rangle = -\frac{1}{\theta \omega}$$

- $A = M^{-1} \begin{pmatrix} \dot{\omega} \\ \dot{\omega} \\ \dot{\lambda} \end{pmatrix} M$ $M := \begin{pmatrix} \mathbf{e}^\top / \sqrt{3} \\ \mathbf{c}^\top / \sqrt{2} \\ (3\mathbf{c}^2 - 2\mathbf{e})^\top / \sqrt{6} \end{pmatrix} = \begin{pmatrix} (1 & 1 & 1) / \sqrt{3} \\ (-1 & 1 & 0) / \sqrt{2} \\ (1 & 1 & -2) / \sqrt{6} \end{pmatrix}$

$$A \text{ is symmetric} \Leftrightarrow M \text{ is orthonormal, } J_d^\dagger \neq -A^\dagger \text{ but}$$

$$\langle \mathbf{c}, J_d^\dagger A \mathbf{c} \mathbf{w} \rangle = -\langle \mathbf{c}, A^\dagger A \mathbf{c} \mathbf{w} \rangle = -\frac{1}{\theta}, \quad \langle \mathbf{c}, J_d^\dagger \mathbf{c} \mathbf{w} \rangle = -\langle \mathbf{c}, A^\dagger \mathbf{c} \mathbf{w} \rangle = -\frac{1}{\theta \omega}$$

$$\partial_t \rho^{(0)} \underbrace{- a\theta \langle \mathbf{c}, J_d^\dagger A \mathbf{c} \omega \rangle}_{\text{advection velocity}} \partial_x \rho^{(0)} + \underbrace{\left(\langle \mathbf{c}, J_d^\dagger \mathbf{c} \omega \rangle + \frac{1}{2\theta} \right)}_{\text{-diffusivity}} \partial_x^2 \rho^{(0)} = 0$$

$$\partial_t \rho^{(0)} + a \partial_x \rho^{(0)} - \underbrace{\frac{1}{\theta} \left(\frac{1}{\omega} - \frac{1}{2} \right)}_{=\nu} \partial_x^2 \rho^{(0)} = 0$$

- $A \sim \begin{pmatrix} \dot{\omega} \\ \dot{\lambda} \end{pmatrix}$, $A = A^\top$, $[A, GD] = 0$ $(GD) = (GD)^\top = DG^\top$

$$A \text{ symmetric, } J_d^\dagger \neq -A^\dagger \text{ still}$$

$$\langle \mathbf{c}, J_d^\dagger A \mathbf{c} \omega \rangle = -\langle \mathbf{c}, A^\dagger A \mathbf{c} \omega \rangle = -\frac{1}{\theta} \quad \langle \mathbf{c}, J_d^\dagger \mathbf{c} \omega \rangle = -\langle \mathbf{c}, A^\dagger \mathbf{c} \omega \rangle$$

$$\text{but } \langle \mathbf{c}, A^\dagger \mathbf{c} \omega \rangle = -\nu(a, h, \theta, \omega, \lambda)$$

i.e. diffusivity \rightarrow (complicated) function of all algorithmic parameters

A has same eigenspaces as GD depending on ah

- Evolution of $\rho^{(\ell)}$:

Drift-diffusion equation ← driven by derivatives of lower orders

- Unlike BGK, in general: $\rho^{(\ell)} \neq \langle \mathbf{e}, \mathbf{f}^{(\ell)} \rangle \quad \ell > 0$

$$J_d \mathbf{f}^{(\ell)} = \underbrace{-AG_a \mathbf{f}^{(\ell-1)} + \sum_{j=1}^{\ell} D_j (\partial_t, \mathbf{c} \partial_x) \mathbf{f}^{(\ell-j)}}_{\text{RHS}^{(\ell)}}$$

$$\text{RHS}^{(\ell)} \in \text{im} J_d \Leftrightarrow \text{RHS}^{(\ell)} \perp \ker J_d^\top \Rightarrow \langle \mathbf{e}, \text{RHS}^{(\ell)} \rangle = 0$$

$$\mathbf{f}^{(\ell)} = \rho^{(\ell)} \mathbf{w} + J_d^\dagger \text{RHS}^{(\ell)} \Rightarrow \langle \mathbf{e}, \mathbf{f}^{(\ell)} \rangle = \rho^{(\ell)} + \underbrace{\langle (J^\top)^\dagger \mathbf{e}, \text{RHS}^{(\ell)} \rangle}_{=0 \text{ if } J_d \text{ sym.}}$$

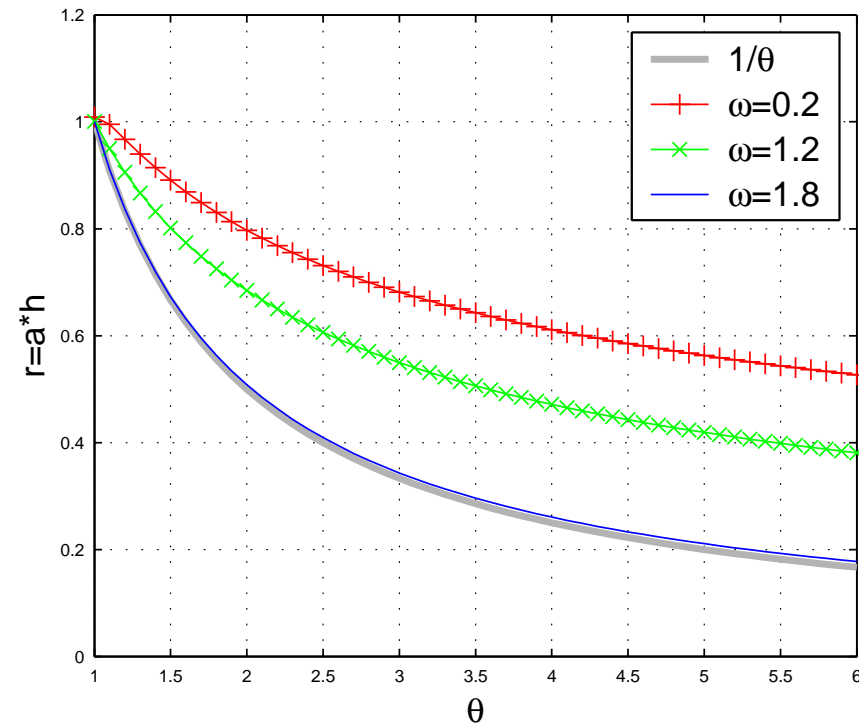
$$J^\dagger = \tilde{E}_{(\ker J)^\perp} \tilde{J}^{-1} \tilde{P}_{\text{im} J} \Rightarrow \begin{cases} \ker J^\dagger = (\text{im} J)^\perp = \ker J^\top & \Rightarrow \ker (J^\top)^\dagger = (\text{im} J^\top)^\perp = \ker J \\ \text{im} J^\dagger = (\ker J)^\perp = \text{im} J^\top & \Rightarrow \text{im} (J^\top)^\dagger = (\ker J^\top)^\perp = \text{im} J \end{cases}$$

- **Avoid this** → successive solution: $J_d \mathbf{f}^\ell = A(G - I) \mathbf{f}^{(\ell)} = \text{RHS}^{(\ell)}$ (A symmetric)

$$\langle \mathbf{e}, \text{RHS}^{(\ell)} \rangle = 0 \Rightarrow (G - I) \mathbf{f}^{(\ell)} = A^\dagger \text{RHS}^{(\ell)} \quad (\text{not general solution})$$

$$\underbrace{\langle \mathbf{e}, A^\dagger \text{RHS}^{(\ell)} \rangle = 0}_{\text{automatically satisfied}} \Rightarrow \mathbf{f}^{(\ell)} = \rho^{(\ell)} \mathbf{w} - A^\dagger \text{RHS}^{(\ell)} \quad (G - I \text{ negative projector})$$

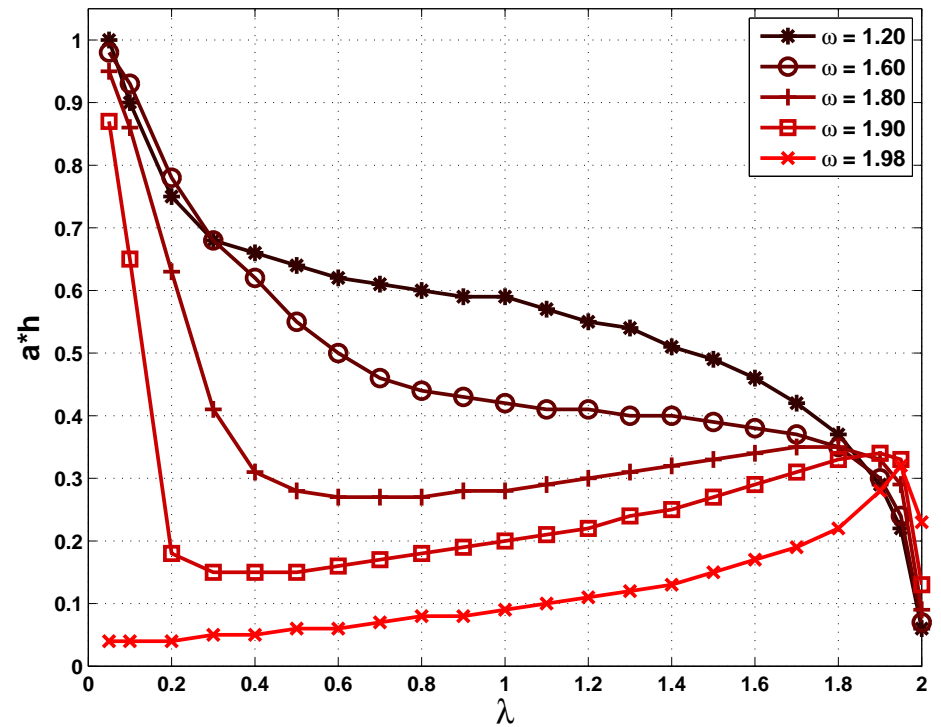
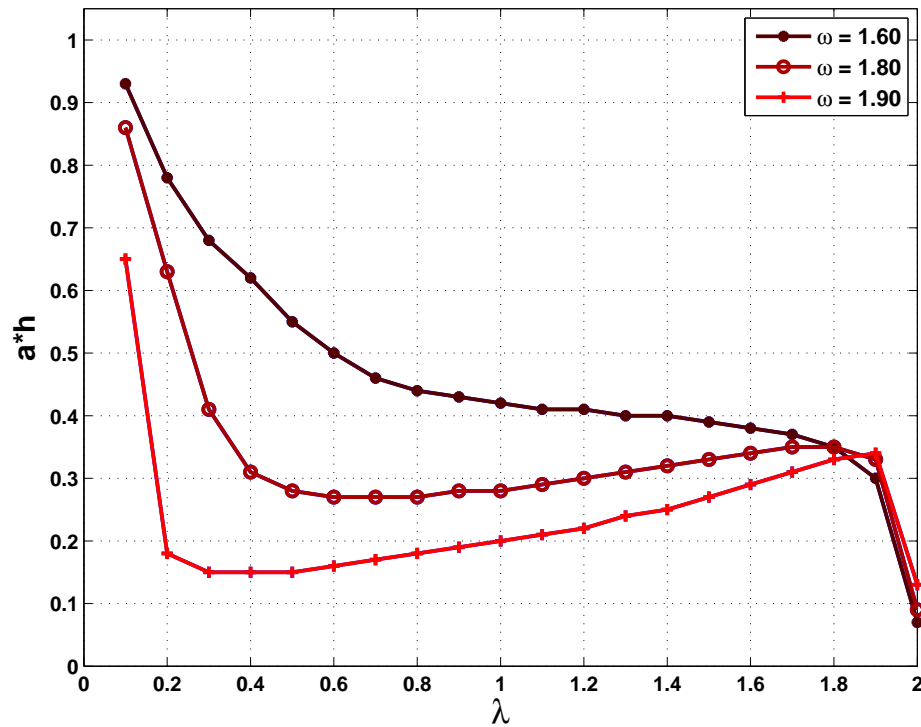
automatically satisfied



Stability-structure: guarantees stability for $|ah| < \frac{1}{\theta}$.

W -orthogonal moment generating vectors:

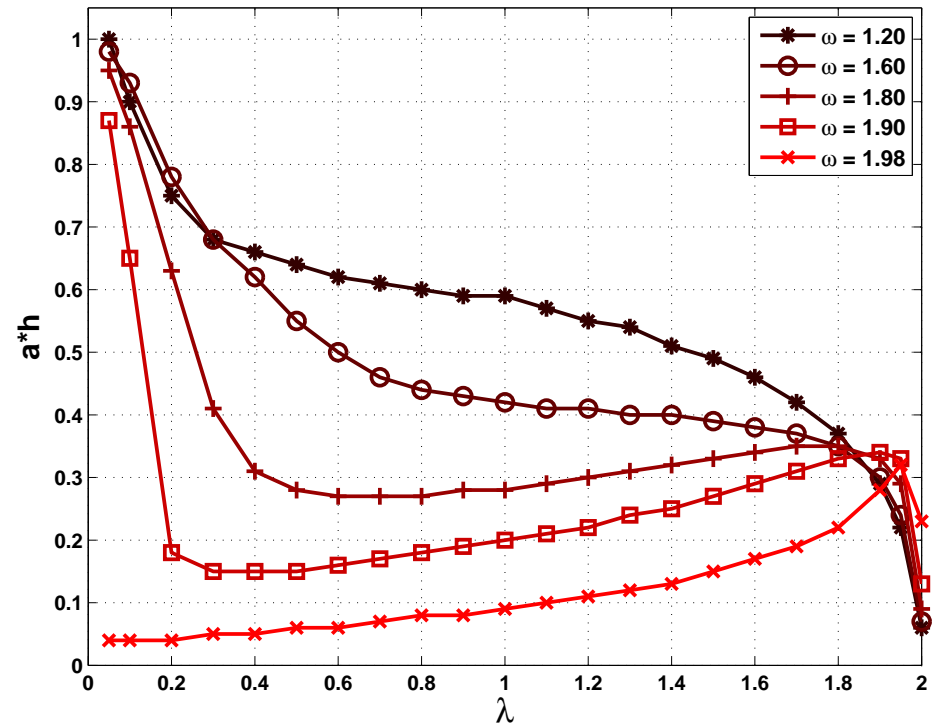
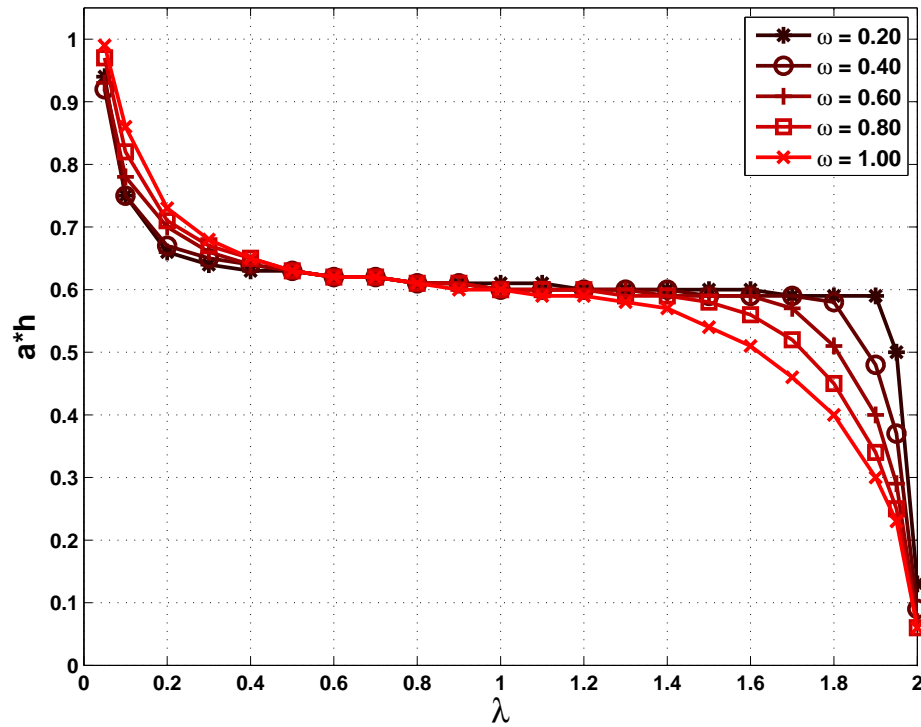
$$M := \begin{pmatrix} \mathbf{e}^\top \\ \mathbf{c}^\top \\ (\mathbf{c}^2 - \frac{1}{\theta}\mathbf{e})^\top \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ -1 & 1 & 0 \\ 1 - \frac{1}{\theta} & 1 - \frac{1}{\theta} & -\frac{1}{\theta} \end{pmatrix} \quad A = M^{-1} \begin{pmatrix} 0 & \omega & \\ \cdot & \cdot & \\ \cdot & \cdot & \lambda \end{pmatrix} M$$



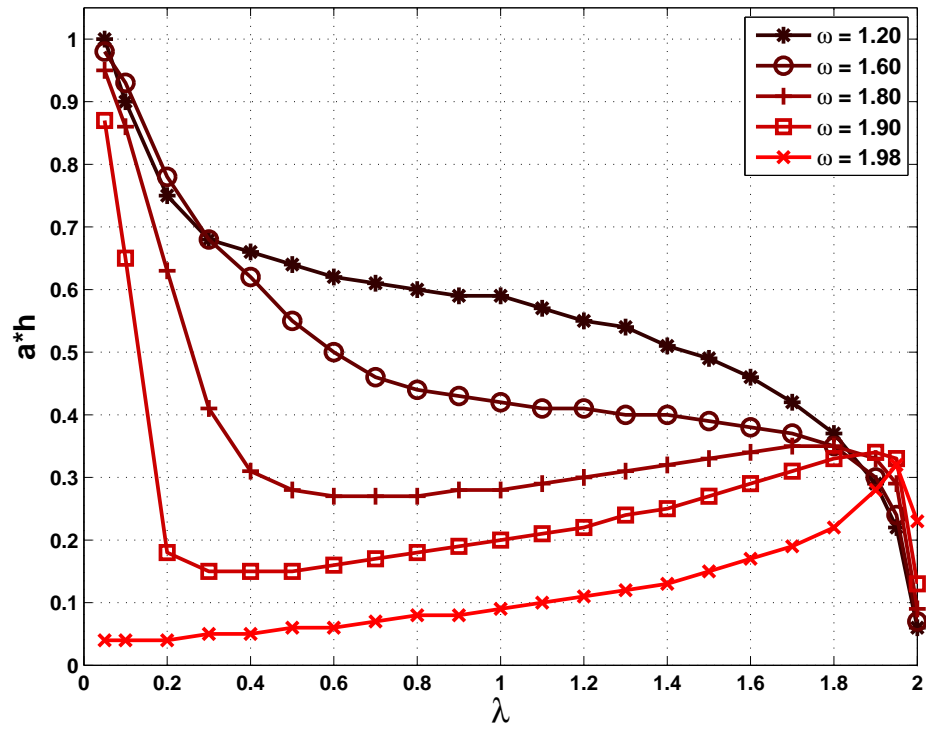
Observation:

Orthonormal moment generating vectors:

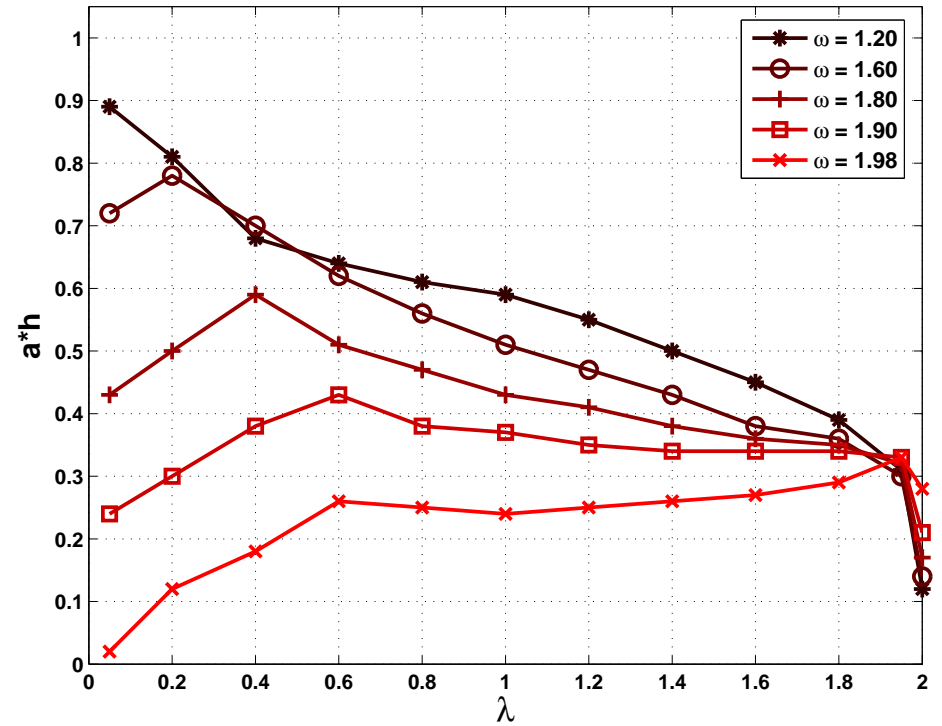
$$M := \begin{pmatrix} \mathbf{e}^\top / \sqrt{3} \\ \mathbf{c}^\top / \sqrt{2} \\ (3\mathbf{c}^2 - 2\mathbf{e})^\top / \sqrt{6} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \end{pmatrix} \quad A = M^{-1} \begin{pmatrix} 0 & \dot{\omega} & \dot{\omega} \\ \cdot & \cdot & \lambda \end{pmatrix} M$$



Observation:



standard MRT



cascaded MRT ([Geier],[Asinari])