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特征值问题的预变换方法 (I): 杨辉三角阵变换与二阶 PDE 特征多项式

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摘要　本文提出一类求解特征值问题的下三角预变换方法, 目标是通过相似变换后矩阵下三角元素平方和明显减少、且变换后的特征值及其特征向量较易求解, 使变换后的对角线可作为全体特征值很好的一组初值, 其作用如同对于解方程组找到好的预条件子, 加速迭代收敛. 以二阶 PDE 数值计算为例, 对于以 Laplace 方程为代表的特征波向量组及正交多项式组有广泛的应用前景.

杨辉三角是我国古代数学家的一项重要成就. 本文引入杨辉三角矩阵作为预变换子, 给出一般矩阵用杨辉三角矩阵作为左、右预变换子时变为上三角矩阵的充要条件, 给出了元素为行指标二次多项式的两个矩阵类 (三对角线阵与五对角线阵) 中特征值何时保持二次多项式的充要条件, 并应用于构造新的二元 PDE 正交多项式.

关键词　特征问题预变换　二阶 PDE 特征多项式　杨辉三角矩阵

MSC (2000) 主题分类　65F15, 65D99, 65N25, 15A18, 35P99

1　引言

众所周知, 方程组与特征值问题是科学计算研究与解法器的两大重要内容. 求解线性方程组的预条件子方法自上世纪七十年代末引入以来[1,2], 已在算法效率与大规模实际计算中取得巨大的进展. 其基本思想是把原始的病态方程 $Au = f$ 变为另一个等价方程组 $BAu = Bf$ 的求解, 以期改善条件数 $\kappa(BA) \ll \kappa(A)$ 加速迭代. 预条件子的思想也正推广到某些稀疏非线性方程组求解[3]. 2010 年 11 月, 作者所在研究所的青年学者杨超在国产千万亿次计算机 "天河一号" 上测试 "地球外核热流动模拟" 时主要用区域分解预条子已解出百亿未知数的方程组[4].

如何处理特征值问题则要复杂得多. 特征值问题是一种特殊的非线性问题, 求解方式与相应的矩阵或 PDE 性质密切相关. 事实上, 基于第一原理, 不少物理学家想了很多办法构造特殊基底用以近似求解 Schrödinger 方程特征值问题. 如我国物理学家王鼎盛等应用自洽和全电子的线性化缀加平面波方法, 在密度泛函近似和间隙区完整势函数近似下, 计算了几十种元素晶体的结合能[5], 并与作者合作在国产机上实现了特征值并行计算[6,7]. 国际上计算少量较小特征值有效的 Jacobi-Davidson 算法首先也是计算化学家提出的[8].

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在数学上, 类似于求解线性方程组的预条件子方法, 一个特征值问题

$$Au = \lambda u, \quad A = (a_{jk}) \tag{1.1}$$

可以通过相似变换

$$u = Tv \tag{1.2}$$

变为另一个等价特征值问题[9–11]

$$(T^{-1}AT)v = \lambda v. \tag{1.3}$$

据此, 本文提出一类求解特征值问题的下三角预变换方法.

定义 1 等价特征值问题 (1.3) 称为原始特征值问题 (1.1) 的一个预变换, 是指

(1) 预变换后矩阵下三角 (或上三角) 元素平方和明显减少,

$$\mathrm{off}(T^{-1}AT)_L := \sum_{j>k} |(T^{-1}AT)_{jk}|^2 \ll \sum_{j>k} |(A)_{jk}|^2 = \mathrm{off}(A)_L, \tag{1.4}$$

或

$$\mathrm{off}(T^{-1}AT)_U := \sum_{j<k} |(T^{-1}AT)_{jk}|^2 \ll \sum_{j<k} |(A)_{jk}|^2 = \mathrm{off}(A)_R. \tag{1.5}$$

(2) 预变换后的特征值问题 (1.3) 及特征向量 (1.2) 较易求解.

满足这两个要求的变换 T 称为原始特征值问题的预变换子. 当 T 为下三角矩阵时可称为下三角预变换子, 简称为 LIAL.

一般可假定原始矩阵不是块三角, 否则特征值已显式给出. 特别地, 当 T 取为完备的特征向量阵时, 由上面所定义的 (1.3) 式即已给出特征值, 而 $u = Tv$ 即为特征向量. 更一般地, 对于特征值问题, 如果找到一个好的预变换子, 变换后的对角线可视为全体特征值很好的一组初值, 其作用如同对于解方程组找到好的预条件子, 能加速迭代收敛, 提高计算效率.

经典的 Lonczos 方法的数学基础是任意矩阵可通过相似变换变为三对角线阵[9, 12–14], 本文定义预变换的目标阵则为上三角阵. 与经典的 Givens 变换不同, 本文定义的预变换 (1.4)–(1.5) 只要求变换后矩阵下三角 (或上三角) 元素平方和明显减少, 而不要求所有非对角线平方和变换后严格下降; 采取的变换由正交变换放宽为相似变换, 不假定原始矩阵对称, 以期扩大可预变换的范围. 具体实施时不只限于个别元素, 着重于整体效应, 以期提高变换效果.

因此, 尽可能找到一批常用的精确特征向量阵, 对于有效实施特征值问题的预变换是必不可少的. 以二阶 PDE 数值计算为例, 以 Laplace 方程为代表的特征波向量组及正交多项式组有广泛的应用范围. 作者在专著 [15] 中对此作过专门探讨.

本文重点研究二元二阶 PDE 正交多项式存在性而引出的如下矩阵特征值问题: 设矩阵 A 的每条对角线均为其行指标或列指标的二次多项式, 即

$$A = (a_{jk})_{0\leqslant j,k\leqslant N}, \qquad a_{j,k}|_{j-k=i} \in \Pi_2(N-k, k). \tag{1.6}$$

问题是: 何时该矩阵 A 全部特征值也为其行、列指标的二次多项式? 即找出 $\lambda_{mn} \in \Pi_2(m,n)$ $(m+n = N)$ 的条件.

杨辉三角, 又称为贾宪三角形, 是我国古代数学家的一项重要成就, 我国古代文字记载就比国际文献称为的 Pascal 三角 [16] 要早三百年. 杨辉三角的一种表达式是无穷下三角阵, 基于其逆阵系数组成各阶差分算子的性质恰好能用于多项式消去的特性, 本文在第 2 节引入杨辉三角矩阵作为预变换子. 并分别给出一般矩阵用杨辉三角矩阵作为左、右预变换子时变为上三角矩阵的充要条件. 对于矩阵元素为二次多项式的三对角线矩阵类与五对角线矩阵类, 第 3 节分别给出能用杨辉三角矩阵作相似变换化为三角矩阵简单而实用的的充要条件, 是进一步开展特征值问题预变换有效算法研究的基础. 最后, 第 4 节回到二元 PDE 正交多项式, 作为本文预变换方法的应用, 验证了若干二元 PDE 正交多项式的存在性, 其中两个四次曲线域上的二元 PDE 正交多项式 (4.15) 与 (4.17), 作者尚未在国内外著名文献 (如 [17–19]) 中见过.

2　矩阵相似变换中的杨辉三角消去法

记矩阵 (有穷或无穷矩阵)

$$A=\begin{pmatrix}\boldsymbol{a}_0\\ \boldsymbol{a}_1\\ \vdots\\ \boldsymbol{a}_j\\ \vdots\end{pmatrix}=\begin{pmatrix}a_{00} & \boldsymbol{a}_0^{[1]}\\ a_{10} & \boldsymbol{a}_1^{[1]}\\ \vdots & \vdots\\ a_{j0} & \boldsymbol{a}_j^{[1]}\\ \vdots & \vdots\end{pmatrix}=\cdots=\begin{pmatrix}a_{00} & \cdots & a_{0,k-1} & \boldsymbol{a}_0^{[k]}\\ a_{10} & \cdots & a_{1,k-1} & \boldsymbol{a}_1^{[k]}\\ \vdots & \ddots & \vdots & \vdots\\ a_{j0} & \cdots & a_{j,k-1} & \boldsymbol{a}_j^{[k]}\\ \vdots & \cdots & \vdots & \vdots\end{pmatrix}, \tag{2.1}$$

这里 $\boldsymbol{a}_j^{[k]}$ 称为矩阵 A 截断 k 列后的第 j 个行向量.

定义 2　行向量 $\boldsymbol{a}_j$ 的 k 阶差分记号与该行向量的 k 阶求和记号分别定义为

$$\delta^k\boldsymbol{a}_j:=\sum_{l=0}^{k}(-1)^l\binom{k}{l}\boldsymbol{a}_{j-l}, \tag{2.2}$$

$$\sigma^k\boldsymbol{a}_j:=\sum_{l=0}^{k}\binom{k}{l}\boldsymbol{a}_{j-l}. \tag{2.3}$$

记初等矩阵系列

$$T_k=\begin{bmatrix}1 &&&&&&\\ & 1 &&&&&\\ && \ddots &&&&\\ &&& 1 &&&\\ &&& \binom{k+1}{k} & 1 &&\\ &&& \binom{k+2}{k} && 1 &\\ &&& \vdots &&& \ddots\\ &&& \binom{j}{k} &&&& 1\\ &&& \vdots &&&&& \ddots\end{bmatrix},\quad k=0,1,2,\dots \tag{2.4}$$

相应地, 记 T_k 中第 k 个下三角向量

$$\boldsymbol{e}^{[k]}=\left(1,\binom{k+1}{k},\binom{k+2}{k},\dots,\binom{j}{k},\dots\right),\quad \forall\, k=0,1,2,\dots \tag{2.5}$$

容易看出, 初等矩阵系列 (2.4) 的依次有限乘积即为杨辉三角矩阵

$$\prod_{k=0}^{N} T_k = \left(\binom{j}{k}\right)_{j,k=0,\dots,N}, \tag{2.6}$$

且初等矩阵系列 (2.4) 的逆为

$$T_k^{-1} = \begin{bmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & \ddots & & & & & \\ & & & 1 & & & & \\ & & & -\binom{k+1}{k} & 1 & & & \\ & & & -\binom{k+2}{k} & & 1 & & \\ & & & \vdots & & & \ddots & \\ & & & -\binom{j}{k} & & & & 1 & \\ & & & \vdots & & & & & \ddots \end{bmatrix}, \quad k = 0, 1, 2, \dots \tag{2.7}$$

下面利用初等矩阵系列 (2.4) 逐次对 A 施行相似变换. 首先, 令

$$A^{[1]} := T_0^{-1} A T_0 = T_0^{-1} \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}_0 \rangle & \boldsymbol{a}_0^{[1]} \\ \langle \boldsymbol{a}_1, \boldsymbol{e}_0 \rangle & \boldsymbol{a}_1^{[1]} \\ \vdots & \vdots \\ \langle \boldsymbol{a}_j, \boldsymbol{e}_0 \rangle & \boldsymbol{a}_j^{[1]} \\ \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \boldsymbol{a}_0^{[1]} \\ \langle \boldsymbol{a}_1 - \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]} \\ \vdots & \vdots \\ \langle \boldsymbol{a}_j - \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \boldsymbol{a}_j^{[1]} - \boldsymbol{a}_0^{[1]} \\ \vdots & \vdots \end{pmatrix}.$$

因而, 如果下面诸向量内积相等,

$$\langle \boldsymbol{a}_j,\ \boldsymbol{e}^{[0]} \rangle = \langle \boldsymbol{a}_0,\ \boldsymbol{e}^{[0]} \rangle, \quad \forall\, j = 1, 2, \dots, \tag{2.8}$$

则 $A^{[1]}$ 的第一列除第一个元素外均能消成零,

$$A^{[1]} := T_0^{-1} A T_0 = \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \boldsymbol{a}_0^{[1]} \\ 0 & \boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]} \\ \vdots & \vdots \\ 0 & \boldsymbol{a}_j^{[1]} - \boldsymbol{a}_0^{[1]} \\ \vdots & \vdots \end{pmatrix}. \tag{2.9}$$

其次,

$$A^{[2]} := T_1^{-1} A^{[1]} T_1 = T_1^{-1} \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \boldsymbol{a}_0^{[1]} \\ \langle \boldsymbol{a}_1 - \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]} \\ \vdots & \vdots \\ \langle \boldsymbol{a}_j - \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \boldsymbol{a}_j^{[1]} - \boldsymbol{a}_0^{[1]} \\ \vdots & \vdots \end{pmatrix} \begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & 2 & 1 & & & & \\ & 3 & & 1 & & & \\ & 4 & & & 1 & & \\ & \vdots & & & & \ddots & \\ & k & & & & & 1 \\ & \vdots & & & & & & \ddots \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & & & & & \\ 1 & & & & & & \\ -2 & 1 & & & & & \\ -3 & & 1 & & & & \\ -4 & & & 1 & & & \\ \vdots & & & & \ddots & & \\ -j & & & & & 1 & \\ \vdots & & & & & & \ddots \end{bmatrix} \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_0^{[2]} \\ \langle \boldsymbol{a}_1 - \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_1^{[2]} - \boldsymbol{a}_0^{[2]} \\ \langle \boldsymbol{a}_2 - \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_2^{[1]} - \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_2^{[2]} - \boldsymbol{a}_0^{[2]} \\ \vdots & \vdots & \vdots \\ \langle \boldsymbol{a}_j - \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_j^{[1]} - \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_j^{[2]} - \boldsymbol{a}_0^{[2]} \\ \vdots & \vdots & \vdots \end{pmatrix}.$$

由假定 (2.8), $A^{[2]}$ 可化简为

$$A^{[2]} = \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_0^{[2]} \\ 0 & \langle \boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_1^{[2]} - \boldsymbol{a}_0^{[2]} \\ 0 & \langle (\boldsymbol{a}_2^{[1]} - \boldsymbol{a}_0^{[1]}) - 2(\boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]}), \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_2^{[2]} - 2\boldsymbol{a}_1^{[2]} + \boldsymbol{a}_0^{[2]} \\ \vdots & \vdots & \vdots \\ 0 & \langle (\boldsymbol{a}_j^{[1]} - \boldsymbol{a}_0^{[1]}) - j(\boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]}), \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_j^{[2]} - j\boldsymbol{a}_1^{[2]} + (j-1)\boldsymbol{a}_0^{[2]} \\ \vdots & \vdots & \vdots \end{pmatrix}.$$

于是, 如果附加条件

$$\langle \boldsymbol{a}_j, \boldsymbol{e}^{[0]} \rangle = \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle, \quad \langle \boldsymbol{a}_j^{[1]} - \boldsymbol{a}_{j-1}^{[1]}, \boldsymbol{e}^{[1]} \rangle = \langle \boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle, \quad \forall\, j = 1, 2, \dots \tag{2.10}$$

则 $A^{[2]}$ 的第二列除前两个元素外均消成零. 事实上, 这时,

$$\langle (\boldsymbol{a}_2^{[1]} - \boldsymbol{a}_0^{[1]}) - 2(\boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]}), \boldsymbol{e}^{[1]} \rangle = \langle (\boldsymbol{a}_2^{[1]} - \boldsymbol{a}_1^{[1]}, \boldsymbol{e}^{[1]} \rangle - \langle \boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle = 0.$$

一般地, 由归纳假定可知

$$\begin{aligned} &\langle (\boldsymbol{a}_j^{[1]} - j\boldsymbol{a}_1^{[1]} + (j-1)\boldsymbol{a}_0^{[1]}), \boldsymbol{e}^{[1]} \rangle \\ &\quad = \langle (\boldsymbol{a}_{j-1}^{[1]} - (j-1)\boldsymbol{a}_1^{[1]} + (j-2)\boldsymbol{a}_0^{[1]}), \boldsymbol{e}^{[1]} \rangle + \langle ((\boldsymbol{a}_j^{[1]} - \boldsymbol{a}_{j-1}^{[1]}) - (\boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]})), \boldsymbol{e}^{[1]} \rangle = 0, \end{aligned}$$

及

$$R_2^{[j]} := \boldsymbol{a}_j - j\boldsymbol{a}_1 + (j-1)\boldsymbol{a}_0 = \sum_{\mu=2}^{j} \delta^2 \boldsymbol{a}_\mu \sum_{\nu=\mu}^{j} = \sum_{\nu=2}^{j} (j-\nu+1)\delta^2 \boldsymbol{a}_\nu.$$

这表示在假定 (2.10) 之下, $A^{[2]}$ 可简化为

$$A^{[2]} = \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \boldsymbol{a}_0^{[2]} \\ 0 & \langle \boldsymbol{a}_1^{[1]} - \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \delta \boldsymbol{a}_1^{[2]} \\ 0 & 0 & \delta^2 \boldsymbol{a}_2^{[2]} \\ \vdots & \vdots & \vdots \\ 0 & 0 & \sum_{\nu=2}^{j} (j-\nu+1)\delta^2 \boldsymbol{a}_\nu \\ \vdots & \vdots & \vdots \end{pmatrix}. \tag{2.11}$$

进而, 容易验明, 如果在条件 (2.10) 基础上再加上如下约束

$$\langle \delta^2 \boldsymbol{a}_j, \boldsymbol{e}^{[2]} \rangle = \langle \delta^2 \boldsymbol{a}_2, \boldsymbol{e}^{[2]} \rangle, \qquad \forall j = 2, 3, \dots, \tag{2.12}$$

则

$$\begin{aligned} A^{[3]} :&= (T_0 T_1 T_2)^{-1} A (T_0 T_1 T_2) = T_2^{-1} A^{[2]} T_2 \\ &= \begin{pmatrix} U_2 & (\delta^\nu \boldsymbol{a}_\nu^{[3]})_{\nu=0,1,2} \\ & \delta^3 \boldsymbol{a}_3^{[3]} \\ & (\boldsymbol{a}_j^{[3]} - j\boldsymbol{a}_1^{[3]} + (j-1)\boldsymbol{a}_0^{[3]})_{j=4,5,\dots} \end{pmatrix} \\ &= \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \langle \boldsymbol{a}_0^{[2]}, \boldsymbol{e}^{[2]} \rangle & \boldsymbol{a}_0^{[3]} \\ & \langle \delta \boldsymbol{a}_1^{[1]}, \boldsymbol{e}^{[1]} \rangle & \langle \delta \boldsymbol{a}_1^{[2]}, \boldsymbol{e}^{[2]} \rangle & \delta \boldsymbol{a}_1^{[3]} \\ & & \langle \delta^2 \boldsymbol{a}_2^{[2]}, \boldsymbol{e}^{[2]} \rangle & \delta^2 \boldsymbol{a}_2^{[3]} \\ & & & \delta^3 \boldsymbol{a}_3^{[3]} \\ & & & \vdots \\ & & & \tilde{\boldsymbol{a}}_j^{[3]} \\ & & & \vdots \end{pmatrix}, \end{aligned} \tag{2.13}$$

其中

$$\tilde{\boldsymbol{a}}_j^{[3]} = (\boldsymbol{a}_j^{[3]} - \boldsymbol{a}_j^{[0]}) - j\delta \boldsymbol{a}_1^{[3]} - \binom{j}{2} \delta^2 \boldsymbol{a}_2^{[3]} = \sum_{\nu=2}^{j} (j - \nu + 1)(\delta^2 \boldsymbol{a}_\nu^{[3]} - \delta^2 \boldsymbol{a}_2^{[3]}), \quad \forall j \geqslant 4.$$

更一般地, 可归结为如下定理.

定理 1　如果 (2.1) 给定的矩阵 A (有穷或无穷矩阵) 满足假定

$$\langle \delta^\nu \boldsymbol{a}_j^{[\nu]}, \boldsymbol{e}^{[\nu]} \rangle = \langle \delta^\nu \boldsymbol{a}_\nu^{[\nu]}, \boldsymbol{e}^{[\nu]} \rangle, \qquad \forall j \geqslant k > \nu = 0, 1, 2, \dots, \tag{2.14}$$

则通过一系列 k 个型如 (2.4) 的下三角相似变换可将矩阵 A 的前 k 列变为如下的上三角阵,

$$A^{[k]} := \left(\prod_{l=0}^{k-1} T_l \right)^{-1} A \left(\prod_{l=0}^{k-1} T_l \right) = T_{k-1}^{-1} A^{[k-1]} T_{k-1} = \begin{pmatrix} U_{k-1} & (\delta^\nu \boldsymbol{a}_\nu^{[k]})_{1 \leqslant \nu \leqslant k-1} \\ 0 & (\boldsymbol{R}_j^{[k]})_{j \geqslant k} \end{pmatrix}, \tag{2.15}$$

其中 $\delta^\nu \boldsymbol{a}_j$ 表示由 (2.2) 定义的向量 $\boldsymbol{a}_j$ 的 ν 阶差分, U_{k-1} 是 $k-$ 阶的上三角阵

$$U^{[k-1]} = \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \cdots & \langle \boldsymbol{a}_0^{[k-1]}, \boldsymbol{e}^{[k-1]} \rangle \\ & \langle \delta \boldsymbol{a}_1^{[1]}, \boldsymbol{e}^{[1]} \rangle & \cdots & \langle \delta \boldsymbol{a}_1^{[k-1]}, \boldsymbol{e}^{[k-1]} \rangle \\ & & \ddots & \vdots \\ & & & \langle \delta^{k-1} \boldsymbol{a}_{k-1}^{[k-1]}, \boldsymbol{e}^{[k-1]} \rangle \end{pmatrix}, \tag{2.16}$$

余项通式

$$\boldsymbol{R}_j^{[k]} = \sum_{\nu=k}^{j} \binom{j - \nu + k - 1}{k - 1} \delta^k \boldsymbol{a}_\nu, \quad \forall j = k, k+1, \dots \tag{2.17}$$

证明 由 (2.8), (2.11), (2.13) 式, 可知该定理对于 $k=0,1,2$ 成立. 归纳假定该定理对于 $k-1$ 真, 则由

$$
\begin{aligned}
A^{[k+1]} &:= T_k^{-1}\begin{pmatrix} U_{k-1} & (\delta^\nu \boldsymbol{a}_\nu^{[k]})_{0\leqslant\nu\leqslant k-1} \\ & (\boldsymbol{R}_j^{[k]}) \end{pmatrix}\begin{bmatrix} I_{k-1} & & & \\ & \binom{k+1}{k}^{1} \; 1 & & \\ & \vdots & \ddots & \\ & \binom{j}{k} & & 1 \\ & \vdots & & & \ddots \end{bmatrix} \\
&= \begin{bmatrix} I_{k-1} & & & \\ & -\binom{k+1}{k}^{1} \; 1 & & \\ & \vdots & \ddots & \\ & -\binom{j}{k} & & 1 \\ & \vdots & & & \ddots \end{bmatrix}\begin{pmatrix} U_{k-1} & (\langle \delta^\nu \boldsymbol{a}_\nu^{[k]}, \boldsymbol{e}^{[k]}\rangle) & (\delta^\nu \boldsymbol{a}_\nu^{[k+1]})_{0\leqslant\nu\leqslant k-1} \\ & \langle \delta^k \boldsymbol{a}_k^{[k]}, \boldsymbol{e}^{[k]}\rangle & \delta^k \boldsymbol{a}_k^{[k+1]} \\ & \vdots & \vdots \\ & (\langle \boldsymbol{R}_j^{[k]}, \boldsymbol{e}^{[k]}\rangle) & \vdots \end{pmatrix} \\
&= \begin{pmatrix} U_{k-1} & (\langle \delta^\nu \boldsymbol{a}_l^{[k]}, \boldsymbol{e}^{[k]}\rangle) & \delta^\nu \boldsymbol{a}_l^{[k+1]} \\ & \langle \delta^k \boldsymbol{a}_k^{[k]}, \boldsymbol{e}^{[k]}\rangle & \delta^k \boldsymbol{a}_k^{[k+1]} \\ & \vdots & \vdots \\ & (\langle \boldsymbol{R}_j^{[k]} - \binom{j}{k}\delta^k \boldsymbol{a}_k^{[k]}, \boldsymbol{e}^{[k]}\rangle) & \boldsymbol{R}_j^{[k+1]} \end{pmatrix},
\end{aligned}
$$

这里下三角矩阵 L_k 及余项 $\boldsymbol{R}_j^{[k]}$ 分别已由 (2.16) 及 (2.17) 定义.

利用下面的恒等式

$$
\sum_{\nu=k}^{j}\binom{j-\nu+k-1}{k-1} = \sum_{\nu=0}^{j-k}\binom{j-1-\nu}{k-1} = \binom{j}{k},
$$

及归纳假定 (2.17), 当 $j\geqslant k+1$ 时, 有

$$
\begin{aligned}
\boldsymbol{R}_j^{[k+1]} &:= \boldsymbol{R}_j^{[k]} - \binom{j}{k}\delta^k \boldsymbol{a}_k^{[k]} = \sum_{\nu=k}^{j}\binom{j-\nu+k-1}{k-1}\delta^k \boldsymbol{a}_\nu^{[k]} - \binom{j}{k}\delta^k \boldsymbol{a}_k^{[k]} \\
&= \sum_{\nu=k}^{j}\binom{j-\nu+k-1}{k-1}(\delta^k \boldsymbol{a}_\nu^{[k]} - \delta^k \boldsymbol{a}_k^{[k]}) = \sum_{\nu=k}^{j}\binom{j-\nu+k-1}{k-1}\sum_{\mu=k+1}^{\nu}\delta^{k+1}\boldsymbol{a}_\mu^{[k]} \\
&= \sum_{\mu=k+1}^{j}\delta^{k+1}\boldsymbol{a}_\mu^{[k]}\sum_{\nu=k}^{j}\binom{j-\nu+k-1}{k-1} = \sum_{\nu=k+1}^{j}\binom{j-\nu+k}{k}\delta^{k+1}\boldsymbol{a}_\nu^{[k]}.
\end{aligned}
$$

特别地, 若当 $j>k$ 时,

$$
\langle \delta^k \boldsymbol{a}_j^{[k]}, \boldsymbol{e}^{[k]}\rangle = \langle \delta^k \boldsymbol{a}_k^{[k]}, \boldsymbol{e}^{[k]}\rangle,
$$

则有

$$
\begin{aligned}
\langle \delta^{k+1}\boldsymbol{a}_j^{[k]}, \boldsymbol{e}^{[k]}\rangle &= \langle \delta^k(\boldsymbol{a}_j^{[k]} - \boldsymbol{a}_{j-1}^{[k]}), \boldsymbol{e}^{[k]}\rangle \\
&= \langle \delta^k(\boldsymbol{a}_j^{[k]} - \boldsymbol{a}_k^{[k]}), \boldsymbol{e}^{[k]}\rangle - \langle \delta^k(\boldsymbol{a}_{j-1}^{[k]} - \boldsymbol{a}_k^{[k]}), \boldsymbol{e}^{[k]}\rangle = 0.
\end{aligned}
$$

因而

$$\langle \boldsymbol{R}_j^{[k+1]}, \boldsymbol{e}^{[k]} \rangle = \sum_{\nu=k+1}^{j} \binom{j-\nu+k}{k} \langle \delta^{k+1} \boldsymbol{a}_\nu^{[k]}, \boldsymbol{e}^{[k]} \rangle = 0.$$

最后, 我们得到

$$A^{[k+1]} = \begin{pmatrix} U_k & (\delta^\nu \boldsymbol{a}_\nu^{[k]})_{1 \leqslant \nu \leqslant k} \\ 0 & (\boldsymbol{R}_j^{[k+1]})_{j \geqslant k+1} \end{pmatrix}.$$

这样就完成了定理 1 的证明. □

定理 2 如果 $(N+1) \times (N+1)$ 阶矩阵 A 满足如下 $\binom{N}{2}$ 个约束

$$\langle \delta^{k+1} \boldsymbol{a}_j^{[k]}, \boldsymbol{e}^{[k]} \rangle = 0, \quad \forall\, 0 \leqslant k < j \leqslant N, \tag{2.18}$$

则矩阵 A 的 $N+1$ 个特征值为

$$\lambda_j(A) = \langle \delta^j \boldsymbol{a}_j^{[j]},\ \boldsymbol{e}^{[j]} \rangle, \quad \forall\, j = 0, 1, \ldots, N. \tag{2.19}$$

此外, 该矩阵可以通过杨辉三角作如下的左相似变换变到上三角矩阵

$$\boldsymbol{L}^{-1} A \boldsymbol{L} = \boldsymbol{U}, \tag{2.20}$$

这里 $\boldsymbol{L}$ 是 $N+1$ 阶杨辉下三角矩阵, $\boldsymbol{L}^{-1}$ 是其逆,

$$\boldsymbol{L} = \left(\binom{j}{k} \right)_{j,k=0,\ldots,N}, \qquad \boldsymbol{L}^{-1} = \left((-1)^{j-k} \binom{j}{k} \right)_{j,k=0,\ldots,N}. \tag{2.21}$$

且变换后的上三角矩阵

$$\boldsymbol{U} = \begin{pmatrix} \langle \boldsymbol{a}_0, \boldsymbol{e}^{[0]} \rangle & \langle \boldsymbol{a}_0^{[1]}, \boldsymbol{e}^{[1]} \rangle & \cdots & \langle \boldsymbol{a}_0^{[N]}, \boldsymbol{e}^{N]} \rangle \\ & \langle \delta \boldsymbol{a}_1^{[1]}, \boldsymbol{e}^{[1]} \rangle & \cdots & \langle \delta \boldsymbol{a}_1^{[N]}, \boldsymbol{e}^{[N]} \rangle \\ & & \ddots & \vdots \\ & & & \langle \delta^N \boldsymbol{a}_N^{[N]}, \boldsymbol{e}^{[N]} \rangle \end{pmatrix}. \tag{2.22}$$

证明 为此只需指出, 杨辉三角矩阵可以分解成形如 (2.4) 的初等矩阵乘积

$$\boldsymbol{L} = T_0 \times T_1 \cdot \times T_N = \prod_{\nu=0}^{N} T_\nu. \tag{2.23}$$

证明完毕. □

注 杨辉三角与杨辉矩阵在国外文献分别被称为 Pascal 三角与 Pascal 矩阵 [16].

类似于解线性方程组的预条件子方法, 矩阵相似变换中的变换阵也可以有左、右之分. 如果前面的预变换称为左变换, 则下面探讨的将称为右变换. 注意到

$$\boldsymbol{L}^{-1} = \left((-1)^{j-k} \binom{j}{k} \right)_{j,k=0,\ldots,N} = \prod_{\nu=0}^{N} \tilde{T}_k,$$

$$\tilde{T}_k = \begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & \ddots & & & & \\ & & & 1 & & & \\ & & & -\binom{k+1}{k} & 1 & & \\ & & & \binom{k+2}{k} & & 1 & \\ & & & \vdots & & & \ddots \\ & & & (-1)^{j-k}\binom{j}{k} & & & & 1 \\ & & & \vdots & & & & & \ddots \end{bmatrix}, \quad \tilde{T}_k^{-1} = \begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & \ddots & & & & \\ & & & 1 & & & \\ & & & \binom{k+1}{k} & 1 & & \\ & & & -\binom{k+2}{k} & & 1 & \\ & & & \vdots & & & \ddots \\ & & & -(-1)^{j-k}\binom{j}{k} & & & & 1 \\ & & & \vdots & & & & & \ddots \end{bmatrix},$$

定义

$$\tilde{A}^{[k]} := \bigg(\prod_{l=0}^{k-1} \tilde{T}_l\bigg)^{-1} \tilde{A} \bigg(\prod_{l=0}^{k-1} \tilde{T}_l\bigg) = \tilde{T}_{k-1}^{-1} \tilde{A}^{[k-1]} \tilde{T}_{k-1}. \tag{2.24}$$

记 $\tilde{\boldsymbol{e}}^{[0]} = (1, -1, \dots, (-1)^j, \dots)$, 若

$$\langle \boldsymbol{a}_\nu + \boldsymbol{a}_{\nu-1}, \tilde{\boldsymbol{e}}^{[0]} \rangle = 0, \quad \forall\, \nu = 1, 2, \dots, \tag{2.25}$$

则 $\tilde{A}^{[1]}$ 的第一列除第一个元素外均能消成零

$$\tilde{A}^{[1]} := \tilde{T}_0^{-1} A \tilde{T}_0 = \begin{bmatrix} 1 & & & & & & \\ 1 & 1 & & & & & \\ & & \ddots & & & & \\ -1 & & & & & & \\ 1 & & & 1 & & & \\ \vdots & & & & \ddots & & \\ -(-1)^j & & & & & 1 & \\ \vdots & & & & & & \ddots \end{bmatrix} \begin{bmatrix} \langle \boldsymbol{a}_0, \tilde{\boldsymbol{e}}_0 \rangle & \boldsymbol{a}_0^{[1]} \\ \langle \boldsymbol{a}_1, \tilde{\boldsymbol{e}}_0 \rangle & \boldsymbol{a}_1^{[1]} \\ \langle \boldsymbol{a}_2, \tilde{\boldsymbol{e}}_0 \rangle & \boldsymbol{a}_2^{[1]} \\ \vdots & \vdots \\ \langle \boldsymbol{a}_j, \tilde{\boldsymbol{e}}_0 \rangle & \boldsymbol{a}_j^{[1]} \\ \vdots & \vdots \end{bmatrix} = \begin{bmatrix} \langle \boldsymbol{a}_0, \tilde{\boldsymbol{e}}^{[0]} \rangle & \boldsymbol{a}_0^{[1]} \\ 0 & \boldsymbol{a}_1^{[1]} + \boldsymbol{a}_0^{[1]} \\ 0 & \boldsymbol{a}_2^{[1]} - \boldsymbol{a}_0^{[1]} \\ \vdots & \vdots \\ 0 & \boldsymbol{a}_j^{[1]} - (-1)^j \boldsymbol{a}_0^{[1]} \\ \vdots & \vdots \end{bmatrix},$$

其中

$$\boldsymbol{a}_j^{[1]} - (-1)^j \boldsymbol{a}_0^{[1]} = \sum_{\nu=1}^{j} (-1)^{j-\nu} (\boldsymbol{a}_\nu^{[1]} + \boldsymbol{a}_{\nu-1}^{[1]}). \tag{2.26}$$

一般地, 引入记号

$$\tilde{\boldsymbol{e}}^{[k]} = \left(1, \binom{k+1}{k}, -\binom{k+2}{k}, \dots, (-1)^{j-k+1}\binom{j}{k}, \dots\right), \quad \forall\, k = 0, 1, 2, \dots, \tag{2.27}$$

则有如下定理.

定理 3 如果 (2.1) 给定的矩阵 A (有穷或无穷矩阵) 满足假定

$$\langle \sigma^k \boldsymbol{a}_j^{[k]}, \tilde{\boldsymbol{e}}^{[k]} \rangle = \langle \sigma^k \boldsymbol{a}_k^{[k]}, \tilde{\boldsymbol{e}}^{[k]} \rangle, \qquad \forall\, j = k, k+1, \dots, \quad k = 0, 1, 2, \dots, \tag{2.28}$$

这里 $\sigma^\nu \boldsymbol{a}_j$ 表示由 (2.3) 定义的向量 $\boldsymbol{a}_j$ 的 ν 阶求和, 则通过一系列 k 个如下的下三角相似变换可将矩阵 A 的前 k 列变为如下的上三角矩阵,

$$\tilde{A}^{[k]} := \bigg(\prod_{l=0}^{k-1} \tilde{T}_l\bigg)^{-1} \tilde{A} \bigg(\prod_{l=0}^{k-1} \tilde{T}_l\bigg) = \tilde{T}_{k-1}^{-1} \tilde{A}^{[k-1]} \tilde{T}_{k-1} = \begin{pmatrix} \tilde{U}_{k-1} & (\sigma^\nu \boldsymbol{a}_\nu^{[k]})_{1 \leqslant \nu \leqslant k-1} \\ 0 & \tilde{R}_j^{[k]} \end{pmatrix}, \tag{2.29}$$

这里 $\tilde{U}_{k-1}$ 是 k 阶的上三角矩阵

$$\tilde{U}^{[k-1]} = \begin{pmatrix} \langle \boldsymbol{a}_0, \tilde{\boldsymbol{e}}^{[0]} \rangle & \langle \boldsymbol{a}_0^{[1]}, \tilde{\boldsymbol{e}}^{[1]} \rangle & \cdots & \langle \boldsymbol{a}_0^{[k-1]}, \tilde{\boldsymbol{e}}^{[k-1]} \rangle \\ & \langle \sigma \boldsymbol{a}_1^{[1]}, \tilde{\boldsymbol{e}}^{[1]} \rangle & \cdots & \langle \sigma \boldsymbol{a}_1^{[k-1]}, \tilde{\boldsymbol{e}}^{[k-1]} \rangle \\ & & \ddots & \vdots \\ & & & \langle \sigma^{k-1} \boldsymbol{a}_{k-1}^{[k-1]}, \tilde{\boldsymbol{e}}^{[k-1]} \rangle \end{pmatrix}, \tag{2.30}$$

余项通式

$$\tilde{R}_k^{[k]} = \sigma^k \boldsymbol{a}_k^{[k]}, \qquad \tilde{R}_j^{[k]} = \sum_{\nu=k}^{j} (-1)^{j-\nu} \binom{j+k-1-\nu}{k-1} \sigma^k \boldsymbol{a}_\nu^{[k]}. \tag{2.31}$$

证明 由上面推导可知该定理对于 $k = 0, 1, 2$ 成立. 归纳假定该定理对于 $k-1$ 真, 则由

$$\tilde{A}^{[k+1]} := \tilde{T}_k^{-1} \begin{pmatrix} \tilde{U}_{k-1} & (\sigma^\nu \boldsymbol{a}_\nu^{[k]})_{0 \leqslant \nu \leqslant k-1} \\ & (\tilde{\boldsymbol{R}}_j^{[k]}) \end{pmatrix} \begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & \ddots & & & & \\ & & & 1 & & & \\ & & & \binom{k+1}{k} & 1 & & \\ & & & -\binom{k+2}{k} & & 1 & \\ & & & \vdots & & & \ddots \\ & & & -(-1)^{j-k}\binom{j}{k} & & & & 1 \\ & & & \vdots & & & & & \ddots \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & \ddots & & & & \\ & & & 1 & & & \\ & & & -\binom{k+1}{k} & 1 & & \\ & & & \binom{k+2}{k} & & 1 & \\ & & & \vdots & & & \ddots \\ & & & (-1)^{j-k}\binom{j}{k} & & & & 1 \\ & & & \vdots & & & & & \ddots \end{bmatrix} \begin{pmatrix} \tilde{U}_{k-1} & (\langle \sigma^\nu \boldsymbol{a}_\nu^{[k]}, \tilde{\boldsymbol{e}}^{[k]} \rangle) & (\sigma^\nu \boldsymbol{a}_\nu^{[k+1]})_{0 \leqslant \nu \leqslant k-1} \\ & \langle \sigma^k \boldsymbol{a}_k^{[k]}, \tilde{\boldsymbol{e}}^{[k]} \rangle & \sigma^k \boldsymbol{a}_k^{[k+1]} \\ & \vdots & \vdots \\ & (\langle \tilde{\boldsymbol{R}}_j^{[k]}, \tilde{\boldsymbol{e}}^{[k]} \rangle) & \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \tilde{U}_{k-1} & (\langle \sigma^\nu \boldsymbol{a}_l^{[k]}, \tilde{\boldsymbol{e}}^{[k]} \rangle) & \sigma^\nu \boldsymbol{a}_l^{[k+1]} \\ & \langle \sigma^k \boldsymbol{a}_k^{[k]}, \tilde{\boldsymbol{e}}^{[k]} \rangle & \sigma^k \boldsymbol{a}_k^{[k+1]} \\ & \vdots & \vdots \\ & (\langle \tilde{\boldsymbol{R}}_j^{[k]} + (-1)^{j-k}\binom{j}{k} \sigma^k \boldsymbol{a}_k^{[k]}, \tilde{\boldsymbol{e}}^{[k]} \rangle) & \tilde{\boldsymbol{R}}_j^{[k+1]} \end{pmatrix},$$

其中下三角矩阵 $\tilde{L}_k$ 与通项 $\tilde{\boldsymbol{R}}_j^{[k]}$ 分别由 (2.30)、(2.31) 式确定. 归纳假定定理 3 对于给定 k 成立, 利用恒等式

$$\sum_{\nu=k}^{j} (-1)^{j-\nu} \binom{j-\nu+k-1}{k-1} = \sum_{\nu=0}^{j-k} (-1)^\nu \binom{j-1-\nu}{k-1} = (-1)^j \binom{j}{k},$$

及 (2.31), 则可导出

$$\tilde{\boldsymbol{R}}_j^{[k+1]} := \tilde{\boldsymbol{R}}_j^{[k]} + (-1)^{j-k} \binom{j}{k} \sigma^k \boldsymbol{a}_k^{[k]} = \sum_{\nu=k}^{j} (-1)^{j-\nu} \binom{j-\nu+k-1}{k-1} \sigma^k \boldsymbol{a}_\nu^{[k]} + (-1)^{j-k} \binom{j}{k} \sigma^k \boldsymbol{a}_k^{[k]}$$

$$= \sum_{\nu=k}^{j}(-1)^{j-\nu}\binom{j-\nu+k-1}{k-1}(\sigma^k \boldsymbol{a}_\nu^{[k]}+\sigma^k \boldsymbol{a}_{\nu-1}^{[k]})$$
$$= \sum_{\mu=k+1}^{j}(-1)^{j-\mu}\sigma^{k+1}\boldsymbol{a}_\mu^{[k]}\sum_{\nu=k}^{j}\binom{j-\nu+k-1}{k-1} = \sum_{\nu=k+1}^{j}(-1)^{j-\nu}\binom{j-\nu+k}{k}\sigma^{k+1}\boldsymbol{a}_\nu^{[k]}.$$

若当 $j>k$ 时

$$\langle \sigma^k \boldsymbol{a}_j^{[k]}, \tilde{\boldsymbol{e}}^{[k]}\rangle = \langle \sigma^k \boldsymbol{a}_k^{[k]}, \tilde{\boldsymbol{e}}^{[k]}\rangle,$$

则有

$$\begin{aligned}\langle \sigma^{k+1}\boldsymbol{a}_j^{[k]}, \tilde{\boldsymbol{e}}^{[k]}\rangle &= \langle \sigma^k(\boldsymbol{a}_j^{[k]}-\boldsymbol{a}_{j-1}^{[k]}), \tilde{\boldsymbol{e}}^{[k]}\rangle \\ &= \langle \sigma^k(\boldsymbol{a}_j^{[k]}-\boldsymbol{a}_k^{[k]}), \tilde{\boldsymbol{e}}^{[k]}\rangle - \langle \sigma^k(\boldsymbol{a}_{j-1}^{[k]}-\boldsymbol{a}_k^{[k]}), \tilde{\boldsymbol{e}}^{[k]}\rangle = 0.\end{aligned}$$

因此, 当 $j>k$ 时

$$\langle \tilde{\boldsymbol{R}}_j^{[k+1]}, \tilde{\boldsymbol{e}}^{[k]}\rangle = \sum_{\nu=k+1}^{j}(-1)^{j-\nu}\binom{j-\nu+k}{k}\langle \sigma^{k+1}\boldsymbol{a}_\nu^{[k]}, \tilde{\boldsymbol{e}}^{[k]}\rangle = 0.$$

于是, 我们得

$$A^{[k+1]} = \begin{pmatrix} \tilde{U}_k & (\sigma^\nu \boldsymbol{a}_\nu^{[k]})_{1\leqslant\nu\leqslant k} \\ 0 & (\tilde{\boldsymbol{R}}_j^{[k+1]})_{j\geqslant k+1}\end{pmatrix}.$$

这样就完成了定理 3 的证明. □

定理 4 如果 $(N+1)\times(N+1)$ 阶矩阵 A 满足如下 $\binom{N}{2}$ 个约束

$$\langle \sigma^{k+1}\boldsymbol{a}_j^{[k]}, \tilde{\boldsymbol{e}}^{[k]}\rangle = 0, \quad \forall\, 0\leqslant k<j\leqslant N, \tag{2.32}$$

则这时矩阵 A 的 $N+1$ 个特征值可表示成

$$\lambda_j(A) = \langle \sigma^j \tilde{\boldsymbol{a}}_j^{[j]},\ \tilde{\boldsymbol{e}}^{[j]}\rangle, \quad \forall\, j=0,1,\dots,N. \tag{2.33}$$

此外, 该矩阵可以通过杨辉三角作如下的右相似变换变到上三角矩阵

$$\boldsymbol{L}A\boldsymbol{L}^{-1} = \tilde{\boldsymbol{U}}, \tag{2.34}$$

这里 $\boldsymbol{L}$ 是 $N+1$ 阶杨辉下三角矩阵, $\boldsymbol{L}^{-1}$ 是其逆, 且变换后的上三角矩阵

$$\tilde{\boldsymbol{U}} = \begin{pmatrix} \langle \boldsymbol{a}_0, \tilde{\boldsymbol{e}}^{[0]}\rangle & \langle \boldsymbol{a}_0^{[1]}, \tilde{\boldsymbol{e}}^{[1]}\rangle & \cdots & \langle \boldsymbol{a}_0^{[N]}, \tilde{\boldsymbol{e}}^{N]}\rangle \\ & \langle \sigma\ ab_1^{[1]}, \tilde{\boldsymbol{e}}^{[1]}\rangle & \cdots & \langle \sigma\ ab_1^{[N]}, \tilde{\boldsymbol{e}}^{[N]}\rangle \\ & & \ddots & \vdots \\ & & & \langle \sigma^N\ ab_N^{[N]}, \tilde{\boldsymbol{e}}^{[N]}\rangle \end{pmatrix}. \tag{2.35}$$

3 元素为行指标二次多项式的两个矩阵类: 三对角线阵与五对角线阵

作为两个实例, 本节讨论元素为行指标二次多项式的两个矩阵类 (三对角线阵与五对角线阵) 中特征值何时保持二次多项式的条件.

先讨论 $(N+1)\times(N+1)$ 阶三对角线矩阵

$$A=\begin{bmatrix} c(N,0) & b(N,0) & & & & & \\ a(N-1,1) & c(N-1,1) & b(N-1,1) & & & & \\ & a(N-2,2) & c(N-2,2) & b(N-2,2) & & & \\ & & \cdots & \cdots & \cdots & & \\ & & & a(2,N-2) & c(2,N-2) & b(2,N-2) & \\ & & & & a(1,N-1) & c(1,N-1) & b(1,N-1) \\ & & & & & a(0,N) & c(0,N) \end{bmatrix}, \tag{3.1}$$

这里三条对角线元素均为行指标 n 的二次多项式 $(n+m=N)$,

$$\begin{aligned} a(m,n)&=n(\beta_{10}m+\beta_{11}n+\beta_{00}),\\ c(m,n)&=\alpha_{20}(m^2+n^2)+\alpha_{11}mn+\alpha_{10}(m+n)+\alpha_{00},\\ b(m,n)&=m(\beta_{10}n+\beta_{11}m+\beta_{00}). \end{aligned} \tag{3.2}$$

特别地, 当 $N=1$ 时, 二阶矩阵

$$A_2=\begin{pmatrix} \alpha_{20}+\alpha_{10}+\alpha_{00} & \beta_{11}+\beta_{00} \\ \beta_{11}+\beta_{00} & \alpha_{20}+\alpha_{10}+\alpha_{00} \end{pmatrix}$$

的两个特征值直接为

$$\lambda(A_2)=\alpha_{20}+\alpha_{10}+\alpha_{00}\pm(\beta_{11}+\beta_{00}).$$

而当 $N=2$ 时, 下面的结论是显然的: 如果

$$(2\alpha_{20}-\alpha_{11})^2=4(\beta_{11}-\beta_{10})^2, \tag{3.3}$$

则三阶矩阵

$$A_3=\begin{pmatrix} 4\alpha_{20}+2\alpha_{10}+\alpha_{00} & 2(2\beta_{11}+\beta_{00}) & 0 \\ \beta_{10}+\beta_{11}+\beta_{00} & 2\alpha_{20}+\alpha_{11}+2\alpha_{10}+\alpha_{00} & \beta_{10}+\beta_{11}+\beta_{00} \\ 0 & 2(2\beta_{11}+\beta_{00}) & 4\alpha_{20}+2\alpha_{10}+\alpha_{00} \end{pmatrix} \tag{3.4}$$

均为五个参数 $\{\alpha_{20},\alpha_{10},\alpha_{00},\beta_{11},\beta_{00}\}$ 的线性组合.

定理 5 对于任意 $m+n=N$, (3.1)–(3.2) 中元素为二次多项式的三对角线矩阵 A 的 N 个特征值 $\lambda_n(A)$ 恒为行指标 n 之二次多项式的充分必要条件是 (3.3) 式成立.

证明 记

$$\begin{aligned} \epsilon:&=2(\alpha_{20}+\beta_{11}-\beta_{10})-\alpha_{11},\\ \tilde{\epsilon}:&=2(\alpha_{20}-\beta_{11}+\beta_{10})-\alpha_{11}. \end{aligned}$$

给定 $n+m=N$, 由 (2.2) 与 (2.27) 两种求和公式, 得

$$S_{m,n}:=a(m,n)+c(m,n)+b(m,n)=\alpha_{00}+(\alpha_{10}+\beta_{00})N+(\alpha_{20}+\beta_{11})N^2+mn\epsilon,$$

$$\tilde{S}_{m,n} := -a(m,n) + c(m,n) - b(m,n) = \alpha_{00} + (\alpha_{10} - \beta_{00})N + (\alpha_{20} - \beta_{11})N^2 - mn\tilde{\epsilon}. \tag{3.5}$$

更一般地, 记

$$\begin{aligned} S^{[k]}_{m,n} &:= \binom{n-1}{k} a(m,n) + \binom{n}{k} c(m,n) + \binom{n+1}{k} b(m,n), \\ \tilde{S}^{[k]}_{m,n} &:= -\binom{n-1}{k} a(m,n) + \binom{n}{k} c(m,n) - \binom{n+1}{k} b(m,n). \end{aligned} \tag{3.6}$$

因为 A 是三对角线矩阵

$$\begin{aligned} &\boldsymbol{a}_{n-1} := (0,\ \ldots,\ 0,\ \ a(m+1,n-1),\ \ c(m+1,n-1),\ \ b(m+1,n-1),\ \ 0,\ \ldots,\ 0), \\ &\boldsymbol{a}_n := (0,\ \ldots,\ 0,\ \ a(m,n),\ \ c(m,n),\ \ b(m,n),\ \ 0,\ \ldots,\ 0), \\ &\delta^{[k]}\boldsymbol{a}_n = \sum_{\nu=0}^{k} (-1)^{\nu} \binom{k}{\nu} \boldsymbol{a}_{n-\nu}, \qquad \sigma^{[k]}\boldsymbol{a}_n = \sum_{\nu=0}^{k} \binom{k}{\nu} \boldsymbol{a}_{n-\nu}. \end{aligned}$$

易知

$$\begin{aligned} &\langle \boldsymbol{a}_n, \boldsymbol{e}^{[0]} \rangle = S_{m,n}, \quad \langle \delta\boldsymbol{a}_n, \boldsymbol{e}^{[0]} \rangle = S_{m,n} - S_{m+1,n-1} = -(N+1-2n)\epsilon, \\ &\langle \boldsymbol{a}_n, \tilde{\boldsymbol{e}}^{[0]} \rangle = (-1)^n \tilde{S}_{m,n}, \quad \langle \sigma\boldsymbol{a}_n, \tilde{\boldsymbol{e}}^{[0]} \rangle = (-1)^n (\tilde{S}_{m,n} - \tilde{S}_{m+1,n-1}) = -(N+1-2n)\tilde{\epsilon}, \end{aligned} \tag{3.7}$$

以及

$$\begin{aligned} &\langle \delta^2\boldsymbol{a}_n, \boldsymbol{e}^{[0]} \rangle = \delta^2 S_{m,n} = 2\epsilon, \quad \langle \sigma^2\boldsymbol{a}_n, \tilde{\boldsymbol{e}}^{[0]} \rangle = 2\tilde{\epsilon}, \\ &\langle \delta^k\boldsymbol{a}_n, \boldsymbol{e}^{[0]} \rangle = \delta^k S_{m,n} = 0, \quad \langle \sigma^3\boldsymbol{a}_n, \tilde{\boldsymbol{e}}^{[0]} \rangle = 0, \quad \forall\, k \geqslant 3. \end{aligned}$$

而且

$$\begin{aligned} \langle \delta^2\boldsymbol{a}_n, \boldsymbol{e}^{[1]} \rangle &= ((n-1)a(m,n) + n\ cc(m,n) + (n+1)b(m,n)) \\ &\quad - 2\,((n-2)a(m+1,n-1) + (n-1)cc(m+1,n-1) + n\ b(m+1,n-1)) \\ &\quad + ((n-3)a(m+2,n-2) + (n-2)cc(m+2,n-2) + (n-1)b(m+2,n-2)) \\ &= -2(N+3-3n)\epsilon. \end{aligned}$$

进而, 容易验证

引理 1 对于 $k = 1, 2, \ldots,$

$$\begin{aligned} &\delta^k n^{k-1} = 0, \qquad \delta^k n^k = k!, \qquad \delta^k n^{k+1} = (k+1)!\left(n - \frac{k}{2}\right), \\ &\delta^{k+1}\left(\binom{n-1}{k} n^2\right) = (k+1)((k+2)n - (k+1)^2). \end{aligned} \tag{3.8}$$

更一般地, 有

引理 2

$$\langle \delta^{k+1}\boldsymbol{a}^{[k]}_n, \boldsymbol{e}^{[k]} \rangle = -(k+1)(N+1+k(k+1)-(k+2)n)\epsilon, \quad \forall\, 0 \leqslant k < n \leqslant N. \tag{3.9}$$

证明 事实上, 该引理当 $k=1$ 时显然成立, 因为

$$\langle \boldsymbol{a}_n^{[k]}, \boldsymbol{e}^{[k]}\rangle = \binom{n-1}{k}a(m,n) + \binom{n}{k}c(m,n) + \binom{n+1}{k}b(m,n),$$

$$\langle \delta^{k+1}\boldsymbol{a}_n^{[k]}, \boldsymbol{e}^{[k]}\rangle = \delta^{k+1}\left(\binom{n-1}{k}a(m,n) + \binom{n}{k}c(m,n) + \binom{n+1}{k}b(m,n)\right) := \sigma_0+\sigma_c+\sigma_b.$$

归纳假定 (3.9) 对于 $\leqslant k$ 真, 则有

$$\begin{aligned}
\sigma_0 &= \delta^{k+1}\left(\binom{n-1}{k}\left(a(m,n)+c(m,n)+b(m,n)\right)\right) = \delta^{k+1}\left(\binom{n-1}{k}S_{m,n}\right)\\
&= \epsilon\ \delta^{k+1}\left(\binom{n-1}{k}(N-n)n\right) = -\epsilon\ \left(\delta^{k+1}\left(\binom{n-1}{k}n^2\right) - N\delta^{k+1}\left(\binom{n-1}{k}n\right)\right)\\
&= -\epsilon\ (k+1)(-(k+1)^2+(k+2)n-N),\\
\sigma_c &= \delta^{k+1}\left(\left(\binom{n}{k}-\binom{n-1}{k}\right)c(m,n)\right) = \delta^{k+1}\left(\binom{n-1}{k-1}c(m,n)\right)\\
&= \delta^{k+1}\left(\binom{n-1}{k-1}(2\alpha_{20}-\alpha_{11})n^2\right) = k(k+1)(2\alpha_{20}-\alpha_{11}),\\
\sigma_b &= \delta^{k+1}\left(\left(\binom{n+1}{k}-\binom{n-1}{k}\right)b(m,n)\right) = \delta^{k+1}\left(\left(\binom{n}{k-1}+\binom{n-1}{k-1}\right)b(m,n)\right)\\
&= \delta^{k+1}\left(\left(\binom{n}{k-1}+\binom{n-1}{k-1}\right)(2\beta_{11}-2\beta_{10})n^2\right) = 2k(k+1)(\beta_{11}-\beta_{10}),\\
\sigma_c+\sigma_b &= k(k+1)\epsilon.
\end{aligned}$$

证毕. □

类似地, 因为

$$\begin{aligned}
\langle \boldsymbol{a}_n^{[k]}, \tilde{\boldsymbol{e}}^{[k]}\rangle &= (-1)^{n-1}\binom{n-1}{k}a(m,n) + (-1)^n\binom{n}{k}c(m,n) + (-1)^{n+1}\binom{n+1}{k}b(m,n)\\
&= (-1)^n(-a(m,n)+c(m,n)-b(m,n)) = (-1)^n\tilde{S}_{m,n},\\
\langle \sigma^{k+1}\boldsymbol{a}_n^{[k]}, \tilde{\boldsymbol{e}}^{[k]}\rangle &= \sigma^{k+1}((-1)^n\tilde{S}_{m,n}) = (-1)^n\delta^{k+1}\tilde{S}_{m,n}^{[k]}\\
&= (-1)^n\delta^{k+1}\left(-\binom{n-1}{k}a(m,n)+\binom{n}{k}c(m,n)-\binom{n+1}{k}b(m,n)\right)\\
&:= (-1)^n(\tilde{\sigma}_0+\tilde{\sigma}_c+\tilde{\sigma}_b),
\end{aligned}$$

这里

$$\begin{aligned}
\tilde{\sigma}_0 &= \delta^{k+1}\left(\binom{n-1}{k}\tilde{S}_{m,n}\right) = -\tilde{\epsilon}\ \delta^{k+1}\left(\binom{n-1}{k}(N-n)n\right)\\
&= \tilde{\epsilon}\ (k+1)(-(k+1)^2+(k+2)n-N),\\
\tilde{\sigma}_c &= \delta^{k+1}\left(\left(\binom{n}{k}-\binom{n-1}{k}\right)c(m,n)\right) = \delta^{k+1}\left(\binom{n-1}{k-1}c(m,n)\right)\\
&= \delta^{k+1}\left(\binom{n-1}{k-1}(2\alpha_{20}-\alpha_{11})n^2\right) = k(k+1)(2\alpha_{20}-\alpha_{11}),\\
\tilde{\sigma}_b &= -\delta^{k+1}\left(\left(\binom{n+1}{k}-\binom{n-1}{k}\right)b(m,n)\right) = -\delta^{k+1}\left(\left(\binom{n}{k-1}+\binom{n-1}{k-1}\right)b(m,n)\right)
\end{aligned}$$

$$= -\delta^{k+1}\left(\left(\binom{n}{k-1}+\binom{n-1}{k-1}\right)(2\beta_{11}-2\beta_{10})n^2\right) = -2k(k+1)(\beta_{11}-\beta_{10}),$$

$$\tilde{\sigma}_c + \tilde{\sigma}_b = k(k+1)\tilde{\epsilon}.$$

综上所述, 我们得到

$$\begin{aligned}
\langle \delta^{k+1}\boldsymbol{a}_n, \boldsymbol{e}^{[k]}\rangle &= \sigma_0+\sigma_c+\sigma_b = -\epsilon(k+1)(k-(k+1)^2+(k+2)n-N)\\
&= -(k+1)(-k(k+1)+(k+2)n-N-1)\epsilon,\\
\langle \sigma^{k+1}\boldsymbol{a}_n, \tilde{\boldsymbol{e}}^{[k]}\rangle &= \tilde{\sigma}_0+\tilde{\sigma}_c+\tilde{\sigma}_b = \tilde{\epsilon}\ (k+1)(k-(k+1)^2+(k+2)n-N)\\
&= (k+1)(-k(k+1)+(k+2)n-N-1)\tilde{\epsilon}.
\end{aligned}$$

对于所有 $n>k$, 成立

$$\langle \delta^{k+1}\boldsymbol{a}_n^{[k]}, \boldsymbol{e}^{[k]}\rangle \times \langle \sigma^{k+1}\boldsymbol{a}_n^{[k]}, \tilde{\boldsymbol{e}}^{[k]}\rangle = C_{k,n}\ \epsilon\ \tilde{\epsilon} = C_{k,n}((2\alpha_{20}-\alpha_{11})^2-4(\beta_{11}-\beta_{10})^2),$$

其中常数 $C_{k,n}$ 只与 (n,k) 有关,

利用已证明的定理 1 与 3, 现在我们已完成了定理 5 的证明.

对于五对角线矩阵

$$A = \begin{bmatrix}
cc(N,0) & b_1(N,0) & b_2(N,0) & & & & & \\
a_1(N-1,1) & cc(N-1,0) & b_1(N-1,0) & b_2(N-1,0) & & & & \\
a_2(N-2,2) & a_1(N-2,2) & cc(N-2,2) & b_1(N-2,2) & b_2(N-2,2) & & & \\
 & a_2(N-3,3) & a_1(N-3,3) & cc(N-3,3) & b_1(N-3,3) & b_2(N-3,3) & & \\
 & \cdots & \cdots & \cdots & \cdots & \cdots & & \\
 & & a_2(2,N-2) & a_1(2,N-2) & cc(2,N-2) & b_1(2,N-2) & b_2(2,N-2) & \\
 & & & a_2(1,N-1) & a_1(1,N-1) & cc(1,N-1) & b_1(1,N-1) & \\
 & & & & a_2(0,N) & a_0(0,N) & cc(0,N) &
\end{bmatrix}, \tag{3.10}$$

其中五对角线元素为行 n 指标的二次多项式 $(m+n=N)$,

$$\begin{aligned}
&a_2(m,n) = n(n-1), \quad a_1(m,n) = n(\beta_{10}m+\beta_{11}n+\beta_{00}),\\
&cc(m,n) = \alpha_{20}(m^2+n^2)+\alpha_{11}mn+\alpha_{10}(m+n)+\alpha_{00},\\
&b_2(m,n) = m(m-1), \quad b_1(m,n) = m(\beta_{10}n+\beta_{11}m+\beta_{00}).
\end{aligned} \tag{3.11}$$

我们有

定理 6　对于任意 $m+n=N$, (3.10)–(3.11) 中元素为二次多项式的五对角线矩阵 A 的 N 个特征值 $\lambda_n(A)$ 恒为行指标 n 的二次多项式的充分必要条件为

$$(2+2\alpha_{20}-\alpha_{11})^2 = 4(\beta_{10}-\beta_{11})^2. \tag{3.12}$$

证明　记

$$\epsilon := 2+2\alpha_{20}-\alpha_{11}-2\beta_{10}+2\beta_{11}, \quad \tilde{\epsilon} := 2+2\alpha_{20}-\alpha_{11}+2\beta_{10}-2\beta_{11}.$$

对于 $n+m=N$, 记两种行和

$$\begin{aligned}
S_{m,n} :&= a_2(m,n)+a_1(m,n)+cc(m,n)+b_1(m,n)+b_2(m,n)\\
&= \alpha_{00}+(\alpha_{10}+\beta_{00}-1)N+(\alpha_{20}+\beta_{11}+1)N^2+mn\epsilon,\\
\tilde{S}_{m,n} :&= a_2(m,n)-a_1(m,n)+cc(m,n)-b_1(m,n)+b_2(m,n)
\end{aligned} \tag{3.13}$$

$$= \alpha_{00} + (\alpha_{10} - \beta_{00} - 1)N + (\alpha_{20} - \beta_{11} + 1)N^2 - mn\tilde{\epsilon}. \tag{3.14}$$

根据定理 2 和 4,

$$\tilde{\epsilon}\epsilon = (2 + 2\alpha_{20} - \alpha_{11})^2 - 4(\beta_{10} - \beta_{11})^2 = 0$$

成为定理 6 成立的必要条件. 我们只需证明, 该条件也是充分的.

因为矩阵 A 中五对角线的元素均为 (m,n) 的二次多项式, 其高于二次的差分恒为零. 记

$$\begin{aligned}\boldsymbol{a}_{n-1} &:= [0,\ \ldots,\ 0,\ \ a_2(m+1,n-1),\ \ a_1(m+1,n-1),\ \ cc(m+1,n-1),\ \ b_1(m+1,n-1),\\ &\qquad b_2(m+1,n-1),\ \ 0,\ \ldots,\ 0],\\ \boldsymbol{a}_n &:= [0,\ \ldots,\ 0,\ \ a_2(m,n),\ \ a_1(m,n),\ \ cc(m,n),\ \ b_1(m,n),\ \ b_2(m,n),\ \ 0,\ \ldots,\ 0].\end{aligned}$$

于是, 当 $k=1$ 时定理 6 显然成立. 对于一般的 k,

$$\begin{aligned}\langle \delta^{k+1}\boldsymbol{a}_n, \boldsymbol{e}^{[k]}\rangle &= \delta^{k+1}\left(\binom{n-2}{k}a_2(m,n) + \binom{n-1}{k}a_1(m,n) + \binom{n}{k}cc(m,n)\right.\\ &\qquad \left. + \binom{n+1}{k}b_1(m,n) + \binom{n+2}{k}b_2(m,n)\right)\\ &:= \sigma_0 + \sigma_{a2} + \sigma_{cc} + \sigma_{b1} + \sigma_{b2},\end{aligned}$$

其中

$$\begin{aligned}\sigma_0 &= \delta^{k+1}\left(\binom{n}{k}S_{mn}\right),\\ \sigma_{a2} &= \delta^{k+1}\left(\left(\binom{n-2}{k} - \binom{n}{k}\right)a_2(m,n)\right) = -\delta^{k+1}\left(\left(\binom{n-1}{k-1} + \binom{n-2}{k-1}\right)a_2(m,n)\right),\\ \sigma_{a1} &= \delta^{k+1}\left(\left(\binom{n-1}{k} - \binom{n}{k}\right)a_1(m,n)\right) = -\delta^{k+1}\left(\binom{n-1}{k-1}a_1(m,n)\right),\\ \sigma_{b1} &= \delta^{k+1}\left(\left(\binom{n+1}{k} - \binom{n}{k}\right)b_1(m,n)\right) = \delta^{k+1}\left(\binom{n}{k-1}b_1(m,n)\right),\\ \sigma_{b2} &= \delta^{k+1}\left(\left(\binom{n+2}{k} - \binom{n}{k}\right)b_2(m,n)\right) = \delta^{k+1}\left(\left(\binom{n}{k-1} + \binom{n+1}{k-1}\right)b_2(m,n)\right).\end{aligned}$$

由于

$$\begin{aligned}&\delta^{k+1}\left(\binom{n-1}{k-1}n\right) = (k+1), \quad \delta^{k+1}\left(\binom{n-1}{k-1}n^2\right) = (k+1)k,\\ &\delta^{k+1}\left(\binom{n-1}{k-1}n(n-1)\right) = (k+1)(k-1), \quad \delta^{k+1}\left(\binom{n-2}{k-1}n(n-1)\right) = (k+1)^2,\end{aligned}$$

从恒等式 (3.8) 可知

$$\sigma_0 = \epsilon\ \delta^{k+1}\left(\binom{n}{k}n(N-n)\right) = (k+1)\epsilon\ ((N+2) - (k+2)(n+1) + (k+1)^2).$$

因为

$$\sigma_{a2} = -\delta^{k+1}\left(\left(\binom{n-1}{k-1} + \binom{n-2}{k-1}\right)n(n-1)\right),$$

$$\sigma_{a1} = -2(\beta_{11} - \beta_{10})\delta^{k+1}\left(\binom{n-1}{k-1}n^2\right),$$
$$\sigma_{b1} = 2(\beta_{11} - \beta_{10})\delta^{k+1}\left(\binom{n}{k-1}n^2\right),$$
$$\sigma_{b2} = \delta^{k+1}\left(\left(\binom{n}{k-1} + \binom{n+1}{k-1}\right)(N-n)(N-n-1)\right)$$
$$= \delta^{k+1}\left(\left(\binom{n}{k-1} + \binom{n+1}{k-1}\right)n(n+1)\right),$$

利用指标 n 与 $m = N - n$ 的对称性,

$$\sigma_{a2} + \sigma_{b2} = \delta^{k+1}\left(\left(\binom{n}{k-1} + \binom{n+1}{k-1} - \binom{n-1}{k-1} - \binom{n-2}{k-1}\right)n(n+1)\right) = 0,$$
$$\sigma_{a1} + \sigma_{b1} = 2(\beta_{11} - \beta_{10})\delta^{k+1}\left(\left(\binom{n}{k-1} - \binom{n-1}{k-1}\right)n^2\right) = 0.$$

因此

$$\langle \delta^{k+1}\boldsymbol{a}_n, \boldsymbol{e}^{[k]}\rangle = \sigma_0 = (k+1)\epsilon\,\big((N+2) - (k+2)(n+1) + (k+1)^2\big).$$

定理得证. □

类似地, 有

$$\langle \sigma^{k+1}\boldsymbol{a}_n, \tilde{\boldsymbol{e}}^{[k]}\rangle = \sigma^{k+1}\left((-1)^n\left(\binom{n-2}{k}a_2(m,n) - \binom{n-1}{k}a_1(m,n) + \binom{n}{k}cc(m,n)\right.\right.$$
$$\left.\left. - \binom{n+1}{k}b_1(m,n) + \binom{n+2}{k}b_2(m,n)\right)\right)$$
$$:= (-1)^n(\tilde{\sigma}_0 + \tilde{\sigma}_{a2} + \tilde{\sigma}_{cc} + \tilde{\sigma}_{b1} + \tilde{\sigma}_{b2}),$$

这里

$$\tilde{\sigma}_0 = \delta^{k+1}\left(\binom{n}{k}\tilde{S}_{mn}\right),$$
$$\tilde{\sigma}_{a2} = \delta^{k+1}\left(\left(\binom{n-2}{k} - \binom{n}{k}\right)a_2(m,n)\right),$$
$$\tilde{\sigma}_{a1} = -\delta^{k+1}\left(\left(\binom{n-1}{k} - \binom{n}{k}\right)a_1(m,n)\right),$$
$$\tilde{\sigma}_{b1} = -\delta^{k+1}\left(\left(\binom{n+1}{k} - \binom{n}{k}\right)b_1(m,n)\right),$$
$$\tilde{\sigma}_{b2} = \delta^{k+1}\left(\left(\binom{n+2}{k} - \binom{n}{k}\right)b_2(m,n)\right).$$

由恒等式 (3.8) 可知

$$\tilde{\sigma}_0 = \tilde{\epsilon}\ \delta^{k+1}\left(\binom{n}{k}n(N-n)\right) = \tilde{\epsilon}\ \delta^{k+1}\left(\binom{n}{k}(-(n+1)^2 + (n+1)(N+2) - (N+1))\right)$$
$$= (k+1)\tilde{\epsilon}\ ((N+2) - (k+2)(n+1) + (k+1)^2).$$

利用指标 n 与 $m=N-n$ 的对称性, 得

$$\tilde{\sigma}_{a2}+\tilde{\sigma}_{b2}=\delta^{k+1}\left(\left(\binom{n}{k-1}+\binom{n+1}{k-1}-\binom{n-1}{k-1}-\binom{n-2}{k-1}\right)n(n+1)\right)=0,$$
$$\tilde{\sigma}_{a1}+\tilde{\sigma}_{b1}=0.$$

因此

$$\langle\sigma^{k+1}\boldsymbol{a}_n,\tilde{\boldsymbol{e}}^{[k]}\rangle=\tilde{\sigma}_0=(k+1)\tilde{\epsilon}\ ((N+2)-(k+2)(n+1)+(k+1)^2).$$

定理 7 (3.10)–(3.11) 中五对角线矩阵可以分别经左、右杨辉下三角阵相似变换化简为上三角阵的充分必要条件是

$$\epsilon:=2+2\alpha_{20}-\alpha_{11}-2\beta_{10}+2\beta_{11}=0,\tag{3.15}$$

或

$$\tilde{\epsilon}:=2+2\alpha_{20}-\alpha_{11}+2\beta_{10}-2\beta_{11}=0.\tag{3.16}$$

推论 1 对于 (3.10)–(3.11) 中五对角线矩阵 A,

- 若 $2+2\alpha_{20}-\alpha_{11}=2(\beta_{10}-\beta_{11})$, 则

$$\begin{aligned}\lambda_{mn}(A)&=(\alpha_{20}-\beta_{10}+1)n^2+2(\alpha_{20}-1)mn+(\alpha_{20}+\beta_{11}+1)m^2\\&\quad+(\alpha_{10}-\beta_{00}+\beta_{10}-\beta_{11}-1)n+(\alpha_{10}+\beta_{00}-1)m+\alpha_{00};\end{aligned}\tag{3.17}$$

- 若 $2+2\alpha_{20}-\alpha_{11}=-2(\beta_{10}-\beta_{11})$, 则

$$\begin{aligned}\lambda_{mn}(A)&=(\alpha_{20}+\beta_{10}+1)n^2+2(\alpha_{20}-1)mn+(\alpha_{20}-\beta_{11}+1)m^2\\&\quad+(\alpha_{10}+\beta_{00}-\beta_{10}+\beta_{11}-1)n+(\alpha_{10}-\beta_{00}-1)m+\alpha_{00}.\end{aligned}\tag{3.18}$$

证明 由于 $n+m=N$, 如果 $\epsilon=0$, 则有

$$\begin{aligned}\lambda_{N0}&=\langle\boldsymbol{a}_0,\boldsymbol{e}^{[0]}\rangle=\alpha_{00}+(\alpha_{10}+\beta_{00}-1)N+(\alpha_{20}+\beta_{11}+1)N^2,\\\lambda_{N-1,1}&=\langle\delta\boldsymbol{a}_1,\boldsymbol{e}^{[1]}\rangle=\alpha_{00}-2\beta_{00}+4+(\alpha_{10}+\beta_{00}-2\beta_{11}-5)N+(\alpha_{20}+\beta_{11}+1)N^2,\\\lambda_{N-2,2}&=\langle\delta^2\boldsymbol{a}_2,\boldsymbol{e}^{[2]}\rangle=(\alpha_{00}-4\beta_{00}+2\beta_{11}-2\beta_{10}+16)+(\alpha_{10}+\beta_{00}-4\beta_{11}-9)N\\&\quad+(\alpha_{20}+\beta_{11}+1)N^2,\end{aligned}$$

从而

$$\begin{aligned}\lambda_{mn}(A)&=\frac{(n-1)(n-2)}{2}\lambda_{N0}-n(n-2)\lambda_{N-1,1}+\frac{n(n-1)}{2}\lambda_{N-2,2}\\&=\alpha_{00}+(\alpha_{10}+\beta_{00}-1)N+(\alpha_{20}+\beta_{11}+1)N^2+(\beta_{11}-\beta_{10}-4)n^2\\&\quad-(2\beta_{00}-\beta_{10}+\beta_{11}+2N(\beta_{11}+2)n.\end{aligned}$$

证毕. □

进而,

推论 2 当 $\epsilon=0$ 时,

$$\lambda_{mn}=\frac{1}{2}(n-1)(n-2)\langle \boldsymbol{a}_n,\boldsymbol{e}^{[0]}\rangle-n(n-2)\langle\delta\boldsymbol{a}_n,\boldsymbol{e}^{[1]}\rangle+n(n-1)\langle\delta^2\boldsymbol{a}_n,\boldsymbol{e}^{[2]}\rangle; \tag{3.19}$$

而当 $\tilde{\epsilon}=0$ 时,

$$\lambda_{mn}=\frac{1}{2}(n-1)(n-2)\langle \boldsymbol{a}_n,\tilde{\boldsymbol{e}}^{[0]}\rangle-n(n-2)\langle\sigma\boldsymbol{a}_n,\tilde{\boldsymbol{e}}^{[1]}\rangle+n(n-1)\langle\sigma^2\boldsymbol{a}_n,\tilde{\boldsymbol{e}}^{[2]}\rangle. \tag{3.20}$$

4 在二维二阶自共轭 PDE 特征多项式问题中的应用

考虑复平面 $(z,\bar{z})$ 上的二阶自共轭 PDE 特征问题[15, 18, 20]

$$\boldsymbol{L}[u(z,\bar{z})]:=\left(\frac{\partial}{\partial z},\frac{\partial}{\partial \bar{z}}\right)\begin{pmatrix}A_{20} & A_{11}\\ \bar{A}_{11} & \bar{A}_{20}\end{pmatrix}\begin{pmatrix}\frac{\partial}{\partial z}\\ \frac{\partial}{\partial \bar{z}}\end{pmatrix}u(z,\bar{z})=\lambda\, u(z,\bar{z}),\qquad \forall (z,\bar{z})\in\Omega, \tag{4.1}$$

这里系数 A_{20},A_{11} 是复变量 $(z,\bar{z})$ 的二次多项式. 由

$$\Omega:=\{(z,\bar{z})|-(A_{20}\bar{A}_{20}-A_{11}\bar{A}_{11})\geqslant 0\} \tag{4.2}$$

定义的区域为单连通有界闭区域, 内积的定义为

$$\langle f,g\rangle:=\int_{\Omega}f(z,\bar{z})\,\bar{g}(z,\bar{z})\,dz\,d\bar{z}. \tag{4.3}$$

如同一维的正交多项式常考虑 $[-1,1]$ 区间, 两个端点是 $x^2=1$ 的两个根. 二维正交多项式的一个常考虑的区域是过复平面上 $z^3=1$ 三个根 ($z=1,\omega=-\frac{1}{2}+i\frac{\sqrt{3}}{2},\bar{\omega}=-\frac{1}{2}-i\frac{\sqrt{3}}{2}$) 的曲边三角域. 容易看出,

$$g_{20}:=z^2-\bar{z},\quad g_{11}:=z\bar{z}-1,\quad g_{02}:=\bar{z}^2-z=\bar{g}_{20} \tag{4.4}$$

是过 $z^3=1$ 三个根 $(1,\omega,\bar{\omega})$ 的仅有的三个独立的二次复多项式.

现在我们应用前两节的结论进而研究若干较广区域上本征问题 (4.1) 多项式解的存在性. 当系数 A_{20},A_{11},A_{02} 均为二次复多项式时, 所对应的边界曲线

$$J=A_{11}\bar{A}_{11}-A_{20}\bar{A}_{20}=0$$

是条四次多项式曲线.

本节考虑过三个点 $(1,\omega,\bar{\omega})$、带五个实参数、且区域关于 x 轴对称的一般系数如下,

$$\begin{aligned}A_{20}&=ag_{20}+cg_{11}+bg_{02},\\ A_{11}&=dg_{20}+eg_{11}+dg_{02},\\ A_{02}&=bg_{20}+cg_{11}+ag_{02}.\end{aligned} \tag{4.5}$$

这里二元四次曲线区域族通式为

$$J(z,\bar{z}):=A_{20}A_{02}-A_{11}^2=0. \tag{4.6}$$

将 (4.5) 代人二阶自共轭 PDE 特征方程 (4.1),

$$L[z^m\bar{z}^n] = bn(n-1)z^{m+2}\bar{z}^{n-2} + n(2d\ m + c\ n + 2d)z^{m+1}\bar{z}^{n-1} + (a(m^2+n^2) + 2e\ m\ n + (a+e)(m+n))z^m\bar{z}^n + m(2d\ n + c\ m + 2d)z^{m-1}\bar{z}^{n+1} + bm(m-1)z^{m-2}\bar{z}^{n+2} + \Pi_{m+n-1}.$$

相应于五对角线矩阵 (3.11) 的形式,

$$\begin{aligned} &a_2(m,n) = bn(n-1), \quad a_1(m,n) = n(2dm + cn + 2d), \\ &cc(m,n) = a(m^2+n^2) + 2emn + (a+e)(m+n), \\ &b_2(m,n) = bm(m-1), \quad b_1(m,n) = m(cm + 2dn + 2d). \end{aligned}$$

当 $b=0$ 时, 所对应的矩阵为形如 (3.1)–(3.2) 三对角线, 将诸系数

$$\beta_{10} = 2d, \quad \beta_{11} = c, \quad \beta_{00} = 2d, \quad \alpha_{20} = a, \quad \alpha_{11} = 2e, \quad \alpha_{10} = a+e$$

代入判别式 (3.3) 可表示为

$$\delta_\Delta := (2\alpha_{20} - \alpha_{11})^2 - 4(\beta_{10} - \beta_{11})^2 = 4((a-e)^2 - (2d-c)^2),$$

而当 $b \neq 0$ 时, 令诸系数

$$\beta_{10} = \frac{2d}{b}, \quad \beta_{11} = \frac{c}{b}, \quad \beta_{00} = \frac{2d}{b}, \quad \alpha_{20} = \frac{a}{b}, \quad \alpha_{11} = \frac{2e}{b}, \quad \alpha_{10} = \frac{a+e}{b}.$$

此时判别式 (3.12) 归结为

$$\delta_\Delta := (2 + 2\alpha_{20} - \alpha_{11})^2 - 4(\beta_{10} - \beta_{11})^2 = \frac{4}{b^2}((a+b-e)^2 - (2d-c)^2).$$

根据定理 7 及其推论可得

定理 8 以 (4.5) 为系数的二阶自共轭 PDE 特征方程 (4.1) 有多项式解的充分必要条件是 $J(z,\bar{z}) = 0$ 为单连通有界闭区域以及如下判别式为零两个事实同时成立,

$$\delta_\Delta := (a+b-e)^2 - (2d-c)^2. \tag{4.7}$$

进而, 当 $a+b+c = e+2d$ 时, 由杨辉三角左预变换子, 相应特征值当 $b \neq 0$ 时及 $b=0$ 时分别等于

$$\begin{aligned} \lambda_{mn} &= \frac{1}{b}((a+b+c)m^2 + 2(a-b)mn + (a+b-2d)n^2 + (a-b+2d+e)m + (a-b-c+e)n), \\ \lambda_{mn} &= (a+c)m^2 + 2amn + (a-2d)n^2 + (a+2d+e)m + (a-c+e)n. \end{aligned} \tag{4.8}$$

而当 $a+b-c = e-2d$ 时, 由杨辉三角右预变换子, 相应特征值当 $b \neq 0$ 时及 $b=0$ 时分别等于

$$\begin{aligned} \lambda_{mn} &= \frac{1}{b}\big((a+b-c)m^2 + 2(a-b)mn + (a+b+2d)n^2 + (a-b-2d+e)m + (a-b+c+e)n\big), \\ \lambda_{mn} &= (a-c)m^2 + 2amn + (a+2d)n^2 + (a-2d+e)m + (a+c+e)n. \end{aligned} \tag{4.9}$$

推论 3 二阶自共轭 PDE 特征方程 (4.1) 在单条二元二次曲线域上具有多项式解的区域只能是圆域.

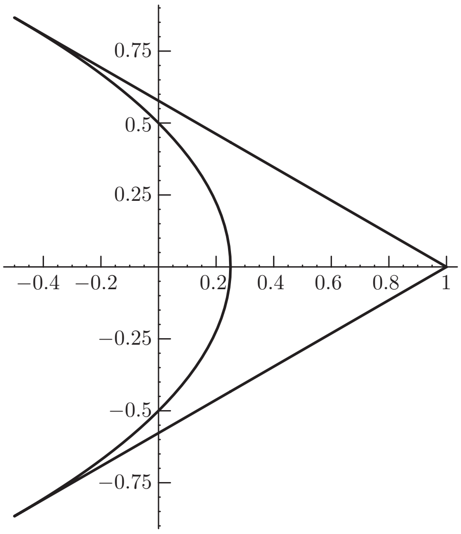

图 1 两直线与抛物线相交曲三角域

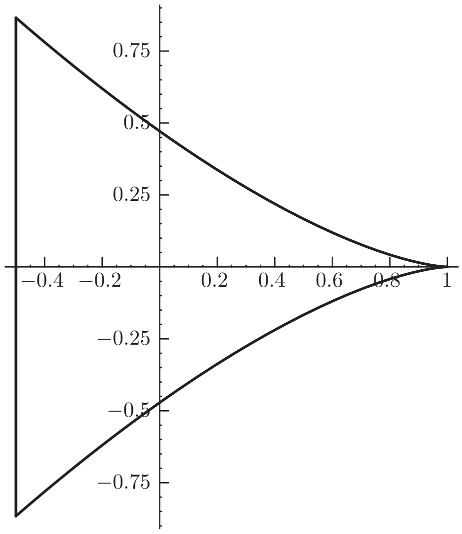

图 2 直线与三次曲线相交曲三角域

事实上, 首先, 在所有的单条二次曲线中, 双曲线与抛物线均为开曲线, 只有椭圆是有界闭曲线. 而由系数 (4.5), 二元四次曲线区域退化为椭圆只有以下两种可能: $a=b=c=0, d=\beta_0, e=-2\beta_1$ 及 $a=b=\beta_0, c=-2\beta_1, d=e=0$, 这时相应的判别式 δ_Δ 均非零, 除非是圆域 $\beta_0^2=\beta_1^2$.

作者在专著 [15] 已证明, 当且仅当 $\gamma=0,1,2$ 时,

$$\begin{aligned} &A_{20}=\gamma\, g_{20}=\gamma(z^2-\bar{z}), \quad A_{11}=g_{11}=z\bar{z}-1, \\ &J(z,\bar{z})=(z\bar{z}-1)^2-\gamma^2(z^2-\bar{z})(\bar{z}^2-z) \end{aligned} \tag{4.10}$$

的特征值问题 (4.1) 在闭区域上有多项式解, 其对应的区域分别为圆域、三角域与三向对称的二元四次曲线域, 即所谓的 Stener 区域 (如图 4). 下面列出二元四次多项式闭区域 (4.5)–(4.6) 上有多项式解的其他三个区域.

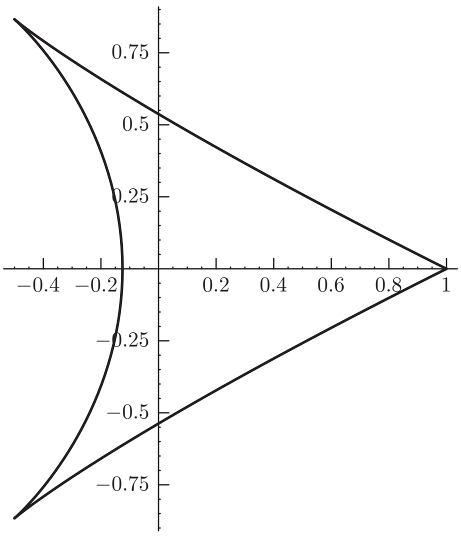

图 3 轴对称四次曲三角

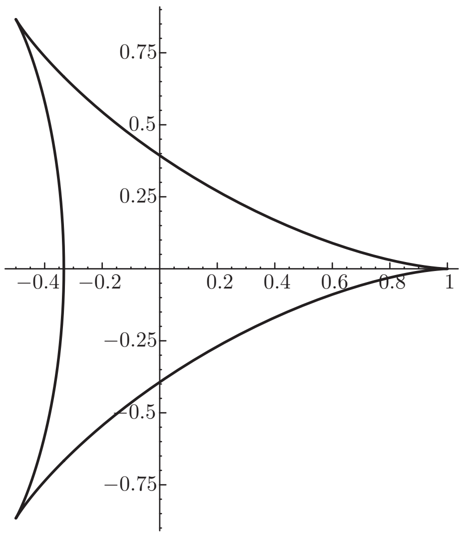

图 4 三向对称曲三角

- **两直线与抛物线相交曲三角域** (Koorwinder 正交多项式域) (如图 1 所示)

$$
\begin{aligned}
&A_{20} = 2g_{20} - g_{11} + g_{02} = 2z^2 + \bar{z}^2 - z\bar{z} - z - 2\bar{z} + 1, \\
&A_{11} = g_{20} + g_{02} = z^2 + \bar{z}^2 - z - \bar{z}, \qquad (4.11) \\
&J(z,\bar{z}) = (1 - 2(z+\bar{z}) + (z-\bar{z})^2)(1 - (z+\bar{z}) + (z^2 - z\bar{z} + \bar{z}^2)). \qquad (4.12)
\end{aligned}
$$

特征值所对应五对角线矩阵是

$$
\begin{aligned}
M_{n+m+1} = \mathrm{FiveDiagonal}\{&m(m-1), 2m - m^2 + 2mn, \\
&2(m^2+n^2) + 2(m+n), 2n - n^2 + 2mn, n(n-1)\}. \qquad (4.13)
\end{aligned}
$$

将诸系数

$$a = 2, \quad b = 1, \quad c = -1, \quad d = 1, \quad e = 0$$

代入判别式 (4.7) 为零. 由此可知, 相应的特征值确为二次多项式. 进而, 由 $a + b + c = e + 2d$, 根据定理 4 中公式 (4.8) 可知: 对于 $n = 0, 1, \ldots, N$,

$$\lambda_n(A) = 2m^2 + 2mn + n^2 + (3m + 2n). \qquad (4.14)$$

这个多项式在文献上称为 Koornwinder 多项式[18,21].

- **一直线与二元三次曲线相交之曲三角域** (如图 2 所示)

$$
\begin{aligned}
&A_{20} = 7g_{20} - g_{11} + g_{02} = 7z^2 - z\bar{z} + \bar{z}^2 - z - 7\bar{z} + 1, \\
&A_{11} = -2g_{20} + 5g_{11} - 2g_{02} = -2(z^2 + \bar{z}^2) + 5z\bar{z} + 2(z\bar{z}) - 5, \qquad (4.15) \\
&J(z,\bar{z}) = 3(z + \bar{z} + 1)(z^3 + 3z\bar{z}(z+\bar{z}) + \bar{z}^3 - 15(z^2 + \bar{z}^2 + 6z\bar{z} + 12(z+\bar{z}) - 8).
\end{aligned}
$$

将诸系数

$$a = 7, \quad b = 1, \quad c = -1, \quad d = -2, \quad e = 5$$

代入判别式 (4.7) 也为零. 由此可知, 相应的特征值确为二次多项式. 但此时 $a + b + c \neq e + 2d$ 而 $a + b - c = e - 2d$, 根据定理 4 中公式 (4.9), 由杨辉三角右预变换子可知: 对于 $n = 0, 1, \ldots, N$,

$$\lambda_{mn}(A) = \langle \sigma^n \boldsymbol{a}_n^{[n]},\ \tilde{\boldsymbol{e}}^{[n]} \rangle = 9m^2 + 12nm + 4n^2 + 15m + 10n. \qquad (4.16)$$

- **轴对称、且非三向对称的二元四次曲线曲三角域** (如图 3 所示)

$$
\begin{aligned}
&A_{20} = 61g_{20} - 10g_{11} + 13g_{02} = 61z^2 - 10z\bar{z} + 13\bar{z}^2 - 13z - 61\bar{z} + 10, \\
&A_{11} = 19g_{20} + 26g_{11} + 19g_{02} = 19(z^2 + \bar{z}^2 z - \bar{z}) + 26(z\bar{z} - 1), \qquad (4.17) \\
&\frac{1}{144} J(z,\bar{z}) = 3(z^4 + \bar{z}^4) - 12z\bar{z}(z^2 + \bar{z}^2) + 18z^2\bar{z}^2 - 22(z^3 + \bar{z}^3) \\
&\qquad + 6z\bar{z}(z+\bar{z}) + 15(z^2 + \bar{z}^2) + 30z\bar{z} - 12(z+\bar{z}) - 4. \qquad (4.18)
\end{aligned}
$$

这时, 特征值所对应五对角线矩阵是

$$
\begin{aligned}
M_{n+m+1} = \mathrm{FiveDiagonal}\{&13(m-1)m, m(-10m + 38n + 38), \\
&61m^2 + 52nm + 87m + 61n^2 + 87n, (38m - 10n + 38)n, 13(n-1)n\}. \qquad (4.19)
\end{aligned}
$$

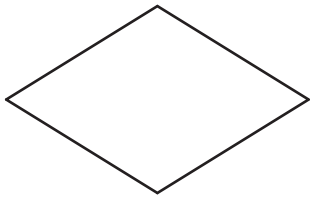

图 5 菱形域

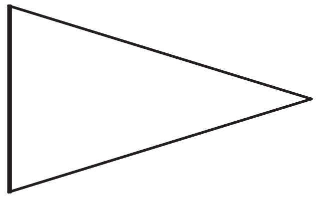

图 6 带一条二重边界的三角形域

将诸系数

$$a = 61, \quad b = 13, \quad c = -10, \quad d = 19, \quad e = 26$$

代入判别式 (4.7) 为零. 由此可知, 相应的特征值确为二次多项式. 进而, 由 $a + b + c = e + 2d$, 根据定理 4 中公式 (4.8) 由杨辉三角左预变换子可知: 对于 $n = 0, 1, \dots, N$,

$$\lambda_{mn}(A) = \langle \delta^n \boldsymbol{a}_n^{[n]}, \ \boldsymbol{e}^{[n]} \rangle = 2(32m^2 + 48nm + 18n^2 + 56m + 42n). \tag{4.20}$$

容易验明, 当二元本征多项式的总次数 $m + n = N$ 固定时, (4.14), (4.16), (4.20) 中的 $N + 1$ 个特征值都没有重特征值, 所以相应的自共轭偏微分方程 (4.1) 的本征多项式在该区域内按内积 (4.3) 正交.

终上所述, 我们可以证明

命题 1 考虑以 (4.5) 为系数的二阶自共轭 PDE 特征方程 (4.1), 与 x 轴对称的二元四次闭曲线区域族中存在二元正交多项式解的区域在几何可归结为以下的八种形状: 即

- 1) 圆域 (二次曲线);
- 2) 三角形上域 (Appell 多项式);
- 3) 三向对称曲三角域 (Stener 多项式) (图 4);
- 4) 两直线与抛物线相交曲三角形域 (Koorwinder 多项式) (图 1);
- 5) 菱形域 (非张量积型) (图 5);
- 6) 带一条二重边界的三角形域 (图 6);
- 7) 直线与二元三次曲线相交之曲三角形域 (图 2);
- 8) 轴对称、且非三向对称的二元四次曲线曲三角形 (图 3).

当判别式 (4.7) 不为零时, 以 (4.5) 为系数的二阶自共轭 PDE 特征方程 (4.1) 在相应的二元四次闭区域内部没有正交多项式解, 其解为二元特殊函数. 这时的特征值与特征向量计算也可应用本文提出的预变换方法迭代, 其结果将有待今后发表.

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On pre-transformed methods for eigen-problems, I: Yanghui-triangle transform and 2nd order PDE eigen-problems

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Abstract A so-called pre-transformed method for solving eigen-problems is proposed in this paper. The aim is to reduce the total sum of off-diagonal entries in lower triangular of $T^{-1}AT$ much smaller than the original one. Finding a good pre-transformer, just like a good pre-conditioner in solving linear system, may accelerate the eigen-solver iteration. In this paper, we take the pre-transformer T as a special elementary unit triangular, which is called Yanghui matrix.

Yanghui triangle was found in China much earlier than Pascal triangle in abroad. Some sufficient and necessary conditions, with which a matrix can be reduced to an upper triangular form through similar transforming with Yanghui matrix, are given. As an application, the existence of a class of 2-D second order PDE eigen-polynomial problems is proved.

Keywords: pre-transformed methods for eigen-problems, 2nd order PDE polynomials, Yanghui triangle matrix
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