Zeros of Whittaker Function with Accurate Error Estimation by Matrix Method

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Scope of Research

○ **Eigenvalue Problem for Infinite Matrices A**

⋆ Class of our Concern

- Complex, Symmetric, Tridiagonal Matrices
- $D(\mathbf{A}) \subset \ell^2, R(\mathbf{A}) \subset \ell^2$
- $\underline{\mathbf{A}}$ or $\mathbf{A^{-1}}$ is Compact

→ Relation with its Truncated Matrices

○ **Reformulate Special Function Problems in Matrix Language**

- Zeros of $J_\nu(z)$[4]
- Zeros of $zJ'_\nu(z) + HJ_\nu(z)$[8]
- Eigenvalues of Mathieu's Equation[11]
- Eigenvalues of Spheroidal Wave Equation[12]
- Zeros of Regular Coulomb Wave Function $F_L(\eta, \rho)$[5]
- Zeros of Whittaker Function $M_{k,\mu}(z)$ and $M'_{k,\mu}(z)$
- Eigenvalues of Lame Equation[9] (not proved)

Whittaker Equation

$$\frac{d^2w}{dz^2} + \left(-\frac{1}{4} + \frac{k}{z} + \frac{1/4 - \mu^2}{z^2} \right) w = 0 \qquad (1)$$

Two Independent Solutions:

$$\begin{cases} w = M_{k,\mu}(z) \\ \hline w = W_{k,\mu}(z) \end{cases}$$

Concrete form of $M_{k,\mu}(z)$ is

$$M_{k,\mu}(z) = e^{-z/2} z^{1/2+\mu} M(1/2 + \mu - k, 1 + 2\mu, z) \qquad (2)$$

([1, 13.1.32]), where $M(a, b, z)$ is Kummer's function

$$M(a, b, z) = 1 + \frac{az}{b} + \frac{(a)_2 z^2}{(b)_2 2!} + \cdots + \frac{(a)_n z^n}{(b)_n n!} + \cdots ,$$

with $(a)_n = a(a+1)(a+2)\cdots(a+n-1),\ (a)_0 = 1$

Literature

$$\left[\begin{array}{lll} \text{Numerical Computation of } M_{k,\mu}(z) & \Rightarrow & \text{Many} \\ \text{Zeros of } M_{k,\mu}(z) & \Rightarrow & \text{Few} \end{array} \right.$$

The Definition of the Problems

Given 2 parameters μ and k

$\Downarrow$

the rest parameter satisfying

$M_{k,\mu}(z) = 0$ or $M'_{k,\mu}(z) = 0$

What this research covers

$\star$ for $M_{k,\mu}(z) = 0$

1 compute $z \neq 0$, given μ, k

$\star$ for $M'_{k,\mu}(z) = 0$

2 compute $z \neq 0$, given μ, k

Three-Term Relations

By [2],

$$M_{k,\mu-1}(z) + \frac{2k}{(2\mu-1)(2\mu+1)}M_{k,\mu}(z) - \frac{(2\mu+1-2k)(2\mu+1+2k)}{8\mu(2\mu+1)^2(2\mu+2)}M_{k,\mu+1}(z) = \frac{1}{z}M_{k,\mu}(z) \tag{3}$$

The behavior of $M_{k,\mu}(z)$ (by [3])

$$\frac{M_{k,\mu+1}(z)}{M_{k,\mu}(z)} = -\frac{z}{4\mu}[1+o(1)]. \tag{4}$$

In analogy,

$$M'_{k,\mu}(z) = 2\mu M_{k,\mu-1}(z) - \left(\frac{2\mu-1}{2z} - \frac{k}{2\mu-1}\right) M_{k,\mu}(z) \tag{5}$$

with (3),

$$M'_{k,\mu}(z) = \left(\frac{2\mu+1}{2z} - \frac{k}{2\mu+1}\right) M_{k,\mu}(z) + \frac{(2\mu+1-2k)(2\mu+1+2k)}{8(\mu+1)(2\mu+1)^2}M_{k,\mu+1}(z) \tag{6}$$

Key Theorem on Infinite Matrices

[4, Theorem 1.1 & 1.4]

- $$\mathbf{A} = \begin{bmatrix} d_1 & f_2 & & \mathbf{0} \\ f_2 & d_2 & f_3 & \\ & f_3 & d_3 & \ddots \\ \mathbf{0} & & \ddots & \ddots \end{bmatrix}, \quad \begin{array}{l} d_n \to 0 \ (n \to \infty), \\ 0 \neq f_n \to 0 \ (n \to \infty) \end{array}$$
- $\mathbf{A}_n$: nth principal submatrix of $\mathbf{A}$
- $\lambda \neq 0$: a simple eigenvalue of $\mathbf{A}$
- λ_n : appropriate eigenvalue of $\mathbf{A}_n$
- $\mathbf{x} = [x^{(1)}, x^{(2)}, \ldots]^T \in \ell^2$: the eigenvector of $\mathbf{A}$ corresponding to λ and $\mathbf{x}^T\mathbf{x} \neq 0$
- $x^{(n+1)}/x^{(n)}$ is bounded for sufficiently large n

Key Theorem on Infinite Matrices

[4, Theorem 1.1 & 1.4] (continued)

$$\Downarrow$$

- There Exists $\{\lambda_n\}$ Such That $\lambda_n \to \lambda$
- $\lambda - \lambda_n = \dfrac{f_{n+1} x^{(n)} x^{(n+1)}}{\mathbf{x}^T \mathbf{x}} [1 + o(1)]$

$$(n \to \infty).$$

Problem **1**

1 Compute the Zero $z \neq 0$ of $M_{k,\mu}(z)$,
Given $k, 2\mu \neq -1, -2, \ldots$

$$\begin{bmatrix} M_{k,\mu}(z) \\ 0 \\ 0 \\ \vdots \end{bmatrix} + \mathbf{T}_{k,\mu}\mathbf{x} = \frac{1}{z}\mathbf{x},$$

$$\begin{aligned}
\mathbf{T}_{k,\mu} &= \begin{bmatrix} d_\mu & f_{\mu+1} & & \mathbf{0} \\ f_{\mu+1} & d_{\mu+1} & f_{\mu+2} & \\ & f_{\mu+2} & d_{\mu+2} & \ddots \\ \mathbf{0} & & \ddots & \ddots \end{bmatrix} : \ell^2 \to \ell^2, \text{ with} \\
d_\mu &= \frac{2k}{(2\mu+1)(2\mu+3)}, \\
f_\mu &= \sqrt{-\frac{(2\mu+1-2k)(2\mu+1+2k)}{16\mu(\mu+1)(2\mu+1)^2}}, \\
\mathbf{x} &= [\alpha_\mu M_{k,\mu+1}(z), \alpha_{\mu+1} M_{k,\mu+2}, \alpha_{\mu+2} M_{k,\mu+3}, \ldots]^T \\
\alpha_{\mu+n} &= \Pi_{i=1}^{n} f_{\mu+i} \ (n = 1, 2, \ldots), \ \alpha_\mu = 1
\end{aligned}$$

Zeros of $M_{k,\mu}(z) \Longleftrightarrow$ Compute z by the Eigenvalues of $\mathbf{T}_{k,\mu}$

Problem**1**

Theorem1 Computation of Zero of $M_{k,\mu}(z)$ is Equivalent to $z = 1/\lambda$ where λ is an Eigenvalue of $\mathbf{T}_{k,\mu}$

Theorem2 One can Choose each λ_n such that $1/\lambda_n = z_n \to z$. And the following Error Estimate is Valid:

$$z - z_n = -\frac{z^2 \alpha_{\mu+n}^2}{\mathbf{x}^T \mathbf{x}} M_{k,\mu+n}(z) M_{k,\mu+n+1}(z)[1 + o(1)]$$

$$\frac{z - z_{n+1}}{z - z_n} = -\frac{z^2}{(4n)^4}[1 + o(1)] \to 0 \ (n \to \infty)$$

λ_n : Appropriate Eigenvalue of $\mathbf{T}_{k,\mu}^{(n)}$

$\mathbf{T}_{k,\mu}^{(n)}$: nth principal submatrix of $\mathbf{T}_{k,\mu}$

Problem**2**

2 Compute the Zero $z \neq 0$ of $M'_{k,\mu}(z)$, Given $k, 2\mu \neq -1, -2, \ldots$

Recalling (6)

$$
\begin{aligned}
M'_{k,\mu}(z) &= \left(\frac{2\mu+1}{2z} - \frac{k}{2\mu+1}\right) M_{k,\mu}(z) \\
&\quad + \frac{(2\mu+1-2k)(2\mu+1+2k)}{8(\mu+1)(2\mu+1)^2} M_{k,\mu+1}(z),
\end{aligned}
$$

$$
\begin{bmatrix} \frac{2}{2\mu+1} M'_{k,\mu}(z) \\ 0 \\ \vdots \end{bmatrix} + \tilde{\mathbf{T}}_{k,\mu}\tilde{\mathbf{x}} = \frac{1}{z}\tilde{\mathbf{x}},
$$

$$
\tilde{\mathbf{T}}_{k,\mu} = \begin{bmatrix} \frac{2k}{(2\mu+1)^2} & \tilde{f}_\mu & & & \mathbf{0} \\ \tilde{f}_\mu & d_\mu & f_{\mu+1} & & \\ & f_{\mu+1} & d_{\mu+1} & f_{\mu+2} & \ddots \\ & & f_{\mu+2} & d_{\mu+2} & \ddots \\ \mathbf{0} & & & \ddots & \ddots \end{bmatrix} : \ell^2 \to \ell^2, \text{ with}
$$

$$
\begin{aligned}
\tilde{\mathbf{x}} &= [M_{k,\mu}(z), \tilde{f}_\mu \alpha_\mu M_{k,\mu+1}(z), \tilde{f}_\mu \alpha_{\mu+1} M_{k,\mu+2}, \ldots]^T \\
\tilde{f}_\mu &= \sqrt{-\frac{(2\mu+1-2k)(2\mu+1+2k)}{4(\mu+1)(2\mu+1)^3}},
\end{aligned}
$$

Problem **2**

Theorem3 Computation of Zero of $M'_{k,\mu}(z)$ is Equivalent to $z = 1/\lambda$ where λ is an Eigenvalue of $\tilde{\mathbf{T}}_{k,\mu}$

Theorem4 One can Choose each λ_n such that $1/\lambda_n = z_n \to z$. And the following Error Estimate is Valid:

$$\begin{aligned} z - z_n &= -\frac{z^2 \tilde{f}_\mu^2 \alpha_{\mu+n-1}^2}{\tilde{\mathbf{x}}^T \tilde{\mathbf{x}}} M_{k,\mu+n-1}(z) M_{k,\mu+n}(z) \\ \frac{z - z_{n+1}}{z - z_n} &= -\frac{z^2}{(4n)^4}[1 + o(1)] \to 0 \ (n \to \infty) \end{aligned}$$

λ_n : Appropriate Eigenvalue of $\tilde{\mathbf{T}}_{k,\mu}^{(n)}$

$\tilde{\mathbf{T}}_{k,\mu}^{(n)}$: nth principal submatrix of $\tilde{\mathbf{T}}_{k,\mu}$

New Relations

Relation1

$$
\begin{aligned}
&\left(M_{k,\mu}(z)^2 \left(\frac{M_{k,\mu+1}(z)}{M_{k,\mu}(z)} \right)' \right)' \\
= &\ \left(M'_{k,\mu+1}(z) M_{k,\mu}(z) - M'_{k,\mu}(z) M_{k,\mu+1}(z) \right)' \\
= &\ \frac{2\mu+1}{z^2} M_{k,\mu}(z) M_{k,\mu+1}(z). \qquad (7)
\end{aligned}
$$

Proof Substituting μ with $\mu+1$ in (1)

$$
\frac{d^2 M_{k,\mu+1}(z)}{dz^2} + \left(-\frac{1}{4} + \frac{k}{z} + \frac{1/4-(\mu+1)^2}{z^2} \right) M_{k,\mu+1}(z) = 0 \qquad (8)
$$

Computing (1) $\times M_{k,\mu+1}(z) -$ (8) $\times M_{k,\mu}(z)$

$$
\begin{aligned}
M''_{k,\mu}(z) M_{k,\mu+1}(z) \ - \ & M_{k,\mu}(z) M''_{k,\mu+1}(z) \\
& + \frac{2\mu+1}{z^2} M_{k,\mu}(z) M_{k,\mu+1}(z) = 0
\end{aligned}
$$

Relation2 Defining

$$y(z) \equiv \mathbf{x}^T\mathbf{x} = \sum_{i=0}^{\infty} \alpha_{\mu+i}^2 M_{k,\mu+i+1}^2(z),$$

$$\Downarrow$$

$$y(z) = z^2 \left(M'_{k,\mu+1}(z) M_{k,\mu}(z) - M'_{k,\mu}(z) M_{k,\mu+1}(z) \right) \quad (9)$$

Proof { (5)+(6) } × $M_{k,\mu}(z)$

$$\begin{aligned} M'_{k,\mu}(z)M_{k,\mu}(z) \; &= \; \frac{2\mu-1}{2} M_{k,\mu-1}(z) M_{k,\mu}(z) + \frac{1}{z} M_{k,\mu}^2(z) \\ &\quad - \frac{2\mu+1}{2} f_\mu^2 M_{k,\mu}(z) M_{k,\mu+1}(z). \end{aligned}$$

Replacing μ by $\mu+1, \mu+2, \ldots$ & adding both sides

$$\begin{aligned} &\sum_{i=0}^{\infty} \alpha_{\mu+i}^2 M'_{k,\mu}(z) M_{k,\mu+i+1}(z) \\ &= \frac{2\mu+1}{2} M_{k,\mu}(z) M_{k,\mu+1}(z) + \frac{1}{z} \sum_{i=0}^{\infty} \alpha_{\mu+i}^2 M_{k,\mu+i+1}^2(z) \end{aligned}$$

$$\Downarrow$$

Or

$$z^2\left(\frac{y(z)}{z^2}\right)' = y'(z) - \frac{2}{z}y(z) = (2\mu+1)M_{k,\mu}(z)M_{k,\mu+1}(z)$$

Recalling (7)

$$\left(M'_{k,\mu+1}(z)M_{k,\mu}(z) - M'_{k,\mu}(z)M_{k,\mu+1}(z)\right)' = \frac{2\mu+1}{z^2}M_{k,\mu}(z)M_{k,\mu+1}(z).$$

$$\Downarrow$$

$$\frac{y(z)}{z^2} - \left(M'_{k,\mu+1}(z)M_{k,\mu}(z) - M'_{k,\mu}(z)M_{k,\mu+1}(z)\right) = c$$

From the behavior of $M_{k,\mu}(z)$, $c=0$.

Error Formula→Closed Form

※Relation2 By (9)

$$y(z) = z^2 \left(M'_{k,\mu+1}(z) M_{k,\mu}(z) - M'_{k,\mu}(z) M_{k,\mu+1}(z) \right).$$

Problem**1**

$$\begin{aligned}
\mathbf{x}^T\mathbf{x} = y(z) &= z^2 \left(-M'_{k,\mu}(z) M_{k,\mu+1}(z) \right) \\
&\quad (\text{by } M_{k,\mu}(z) = 0) \\
&= \frac{2\mu+1}{2} \tilde{f}_\mu^2 z^2 M_{k,\mu+1}^2(z)
\end{aligned}$$

$$\left(\text{By (6) and } M_{k,\mu}(z) = 0,\ M'_{k,\mu}(z) = \frac{(2\mu+1-2k)(2\mu+1+2k)}{8(\mu+1)(2\mu+1)^2} M_{k,\mu+1}(z)\right)$$

Error Formula→Closed Form

※Relation2 By (9)

$$y(z) = z^2\left(M'_{k,\mu+1}(z)M_{k,\mu}(z) - M'_{k,\mu}(z)M_{k,\mu+1}(z)\right).$$

Problem**2**

$$\begin{aligned}\tilde{\mathbf{x}}^T\tilde{\mathbf{x}} &= M^2_{k,\mu}(z) + \tilde{f}^2_\mu y(z)\\ &= M^2_{k,\mu}(z) + \tilde{f}^2_\mu z^2 M'_{k,\mu+1}(z)M_{k,\mu}(z).\end{aligned}$$

By differentiating (6) and $M'_{k,\mu}(z) = 0$:

$$M'_{k,\mu+1}(z) = -\frac{1}{(2\mu+1)\tilde{f}^2_\mu}\left\{\frac{(2\mu+1)^2}{2z^2} - \frac{2k}{z} + \frac{1}{2}\right\} M_{k,\mu}(z)$$

$$\Downarrow$$

$$\begin{aligned}\tilde{\mathbf{x}}^T\tilde{\mathbf{x}} &= \frac{2}{2\mu+1}z^2\left(-\frac{1}{4} + \frac{k}{z} + \frac{1-4\mu^2}{4z^2}\right) M^2_{k,\mu}(z)\\ &= -\frac{2}{2\mu+1}z^2 M''_{k,\mu}(z)M_{k,\mu}(z) \text{ (by (1))}.\end{aligned}$$

Error Formula(Final Form)

Problem**1**

$$z - z_n = -\frac{2\alpha_{\mu+n}^2}{(2\mu+1)\tilde{f}_\mu^2} \times \frac{M_{k,\mu+n}(z)M_{k,\mu+n+1}(z)}{M_{k,\mu+1}^2(z)}[1+o(1)]. \tag{10}$$

Problem**2**

$$z - z_n = \frac{(2\mu+1)\tilde{f}_\mu^2\alpha_{\mu+n-1}^2}{2} \times \frac{M_{k,\mu+n-1}(z)M_{k,\mu+n}(z)}{M_{k,\mu}(z)M''_{k,\mu}(z)}[1+o(1)]. \tag{11}$$

Both Closed!

Concluding Remarks

- Zeros of $M_{k,\mu}(z)$
  $\rightarrow$ Reformulation into matrix language
- Zeros of $M'_{k,\mu}(z)$
  $\rightarrow$ Reformulation into matrix language
- Derived new formulas (e.g. (5), (9))
- Error formulas in a closed form
  ($M_{k,\mu}(z)$ and $M'_{k,\mu}(z)$)
- (Properties regarding the Zeros)

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