Computation of Generalized Mathieu Functions

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We are looking for expositions on topics of interest to the Maple community. Use of Maple is not required. Listed in DBLP and CORR. Journal launched in 2021. Have a look; for instance at my paper Special functions in Maple, a personal view.

Our first issue featured a paper by Peter Baddoo and Nick Trefethen on Log-lightning computation of capacity and Green's functions. A later issue featured Fredrik Johansson's Arbitrary precision computation of the Gamma function.

The Mathieu equation

$$\frac{d^2y}{dx^2} + [a - 2q\cos(2x)]\,y = 0\,. \tag{1}$$

The parameter q is given by the physics or the geometry of the specific problem at hand; the eigenvalue a must be calculated in order to ensure periodicity of y, given q. There are an infinite number of eigenvalues a for any particular value of q, and these are numbered in a conventional order.

The so-called *modified* Mathieu equation is related to equation (1) by the transformation $z = \pm ix$ (the sign makes no difference):

$$\frac{d^2y}{dz^2} - [a - 2q\cosh(2z)]\,y = 0\,. \tag{2}$$

Mathieu functions

The Mathieu *functions* are defined to be the 2π periodic solutions of the Mathieu equations. Other solutions to the Mathieu equation are not, technically, Mathieu functions.

The Mathieu functions are commonly written as $\mathrm{ce}_m(z;q)$ and $\mathrm{se}_m(z;q)$. Modified Mathieu functions are not periodic and are written $\mathrm{Ce}_m(z;q)$ and $\mathrm{Se}_m(z;q)$.

[Other names: *angular* and *radial* Mathieu functions].

Because

$$\frac{y''}{y} = -n^2 \tag{3}$$

and

$$\frac{y''}{y} = -a + 2q\cos 2x \tag{4}$$

are not so different for small q, we expect that the eigenvalues a will be close to the squares of integers, for small q.

$\mathrm{ce}_m(z;q)$ is like $\cos mz$ and $\mathrm{se}_m(z;q)$ is like $\sin mz$, at least for small q.

Fourier series and Ince's matrix formulation

Postulating a Fourier series expansion for a Mathieu function gets (by the trig identities for $\cos 2x \cos kx$ and for $\cos 2x \sin kx$) an infinite tridiagonal matrix for the Fourier coefficients, after separating out the even and odd m.

$$2\cos 2x\ \cos kx = \cos(k+2)x + \cos(k-2)x \tag{5}$$

$$2\cos 2x\ \sin kx = \sin(k+2)x + \sin(k-2)x \tag{6}$$

Eigenvalues and Eigenfunctions: for $\mathrm{ce}_{2j}(z;q)$

$$\begin{bmatrix} 0 & \sqrt{2}q & 0 & 0 & 0 & \cdots \\ \sqrt{2}q & 4 & q & 0 & 0 & \cdots \\ 0 & q & 16 & q & 0 & \cdots \\ 0 & 0 & q & 36 & q & \cdots \\ 0 & 0 & 0 & q & 64 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \sqrt{2}A_0 \\ A_2 \\ A_4 \\ A_6 \\ A_8 \\ \vdots \end{bmatrix} = a \begin{bmatrix} \sqrt{2}A_0 \\ A_2 \\ A_4 \\ A_6 \\ A_8 \\ \vdots \end{bmatrix}. \tag{7}$$

The eigenvalues of this matrix are denoted $a_0(q)$, $a_2(q)$, $a_4(q)$, ... and indeed for real q these occur in increasing order:
$a_0(q) < a_2(q) < a_4(q) < \cdots$.

Eigenvalues and Eigenfunctions: for $\mathrm{ce}_{2j+1}(z;q)$

$$\begin{bmatrix} 1+q & q & 0 & 0 & \cdots \\ q & 9 & q & 0 & \cdots \\ 0 & q & 25 & q & \cdots \\ 0 & 0 & q & 49 & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} A_1 \\ A_3 \\ A_5 \\ A_7 \\ \vdots \end{bmatrix} = a \begin{bmatrix} A_1 \\ A_3 \\ A_5 \\ A_7 \\ \vdots \end{bmatrix} \tag{8}$$

The eigenvalues of equation (8) are denoted $a_{2j+1}(q)$.

The eigenvectors give the Fourier coefficients of the corresponding eigenfunction $\mathrm{ce}_{2j+1}(z;q)$. Indexing becomes perplexing.

Eigenvalues and Eigenfunctions: for $\mathrm{se}_{2j}(z;q)$

$$\begin{bmatrix} 4 & q & 0 & 0 & \cdots \\ q & 16 & q & 0 & \cdots \\ 0 & q & 36 & q & \ddots \\ 0 & 0 & q & 64 & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} B_2 \\ B_4 \\ B_6 \\ B_8 \\ \vdots \end{bmatrix} = a \begin{bmatrix} B_2 \\ B_4 \\ B_6 \\ B_8 \\ \vdots \end{bmatrix} \tag{9}$$

The eigenvalues of equation (9) are denoted $b_{2j}(q)$.

$$\begin{bmatrix} 1-q & q & 0 & 0 & \cdots \\ q & 9 & q & 0 & \cdots \\ 0 & q & 25 & q & \cdots \\ 0 & 0 & q & 49 & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} B_1 \\ B_3 \\ B_5 \\ B_7 \\ \vdots \end{bmatrix} = a \begin{bmatrix} B_1 \\ B_3 \\ B_5 \\ B_7 \\ \vdots \end{bmatrix} \tag{10}$$

The eigenvalues of equation (10) are denoted $b_{2j+1}(q)$.

Normalization

In appendix B of [1] we find a derivation of the bilinear form $(f,g) = \int_0^{2\pi} f(x)g(x)dx$ under which eigenfunctions are orthogonal, and a proof that the inner product $< f,g >= \int_0^{2\pi} f(x)\overline{g(x)}dx$ does *not* work when q is nonreal.

This allows the possibility that Mathieu functions might have zero "norm" and indeed, for values of q for which there are *double eigenvalues*, they do.

So instead we normalize in the same way as the DLMF in equations 28.2.38 and 28.2.39 by insisting that either $y(0) = 1$ and $y'(0) = 0$ (like cosine) or $y(0) = 0$ and $y'(0) = 1$ (like sine).

The conventional ordering of eigenvalues

For $q = 0$ the eigenvalues are all m^2 for $m = 0, 1, 2, \ldots$. But they are (technically) double eigenvalues at $q = 0$, denoted $a_m(q)$ and $b_m(q)$ because at $q = 0$ the $a_m(0) = b_m(0)$.

Conventionally, as real q increases from 0 we smoothly follow the numbering, and the eigenvalues interlace.

If q is complex we imagine a smooth path, say θq for $0 \leq \theta \leq 1$, and assign the index m for the eigenvalue that ensures that $a_m(0) = m^2$. This doesn't always work, though, because *at a double eigenvalue the numbering becomes ambiguous*.

Gertrude Blanch and Double Eigenvalues

In the 1930s Mulholland & Goldstein computed the first few digits of the smallest norm value of q for which a double eigenvalue exists: $\mathrm{ce}_0(z;q)$ and $\mathrm{ce}_2(z;q)$ coalesce when $q \approx 1.469i$. In the 1960s Gertrude Blanch and her coauthors were the first to systematically compute the double eigenvalues. Their work was confirmed and extended by Hunter and Guerrieri in 1981.

Double eigenvalues were studied theoretically in the 1950s by Meixner and Schäfke and, later, Wolf. They were proved to be isolated, and triple eigenvalues and higher were ruled out.

But I could find no studies or software for the generalized eigenfunctions that seem to be needed for completeness of expansions. Even the numbering of the eigenvalues becomes problematic at double points (the Digital Library of Mathematical Functions has a convention that works in some circumstances)

Do we really need generalized eigenvectors/eigenfunctions?

The first and simplest way [to deal with double eigenvalues] is undoubtedly what people actually use: one pretends that the eigenvalue is not actually a double one—typically because of rounding error it would have split anyway into $a^* + d\sqrt{q - q^*} + \cdots$ and $a^* - d\sqrt{q - q^*} + \cdots$ where q is a floating-point approximation to q^* anyway—and then use the computed eigenfunctions from the matrix method, each with norm $O((q - q^*)^{1/2})$ and simply live with the errors. That does not sound like professional practice, but if it is done knowingly then we suspect that it will usually give perfectly reasonable answers. If done unknowingly then we disapprove, but the criminals will likely get away with it.

Can frequently avoid them

If one is solving a Helmholtz equation and the parameter q is purely imaginary and one needs a *range* of q that includes a double eigenvalue, then strictly speaking one needs to examine the generalized eigenfunctions.

BUT the solution to the underlying PDE is continuous with respect to q so if one samples just below the double point and just above the double point the solutions one gets will actually be close together and appear to vary smoothly: it's only the representation as a sum of eigenfunctions that has a representational discontinuity. If you don't get too close, the numerical difficulties (cancellation) aren't that bad.

If you did get too close to the double point, then computation of the eigenvalue (on some systems) slows down drastically because Newton's method fails to converge quickly.

Brutally truncating one of our matrices (for illustration purposes)

$$\begin{bmatrix} 0 & \sqrt{2}\,q & 0 & 0 \\ \sqrt{2}\,q & 4 & q & 0 \\ 0 & q & 16 & q \\ 0 & 0 & q & 36 \end{bmatrix} \tag{11}$$

has a characteristic polynomial $p(\lambda,q)$ that depends on q. The *discriminant* of $p(\lambda,q)$ with respect to λ is

$$\begin{aligned} &2048q^{12} + 606208q^{10} + 401883136q^{8} + 55523147776q^{6} \\ &+ 1115022163968q^{4} + 147288924094464q^{2} + 313103115878400\,. \end{aligned} \tag{12}$$

The smallest magnitude roots of this are approximately $\pm 1.46876833683659i$ which gives the Mulholland–Goldstein value to accuracy about 10^{-7}. At this value of q the matrix has a double eigenvalue. That double eigenvalue is a good approximation to a double eigenvalue of the Mathieu equation.

Blanch & Clemm Double Points

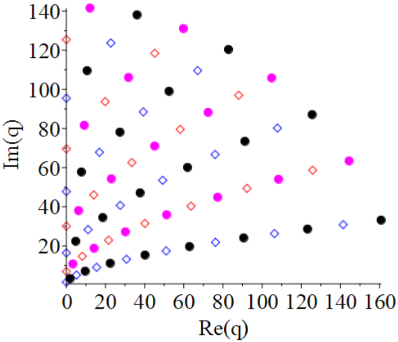


Figure 1: The double points known to Blanch & Clemm. I do not know any asymptotic formula, but such would clearly be useful.

The Jordan form

The Jordan form of that brutally truncated matrix is

$$\begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & a & 1 \\ 0 & 0 & 0 & a \end{bmatrix} \tag{13}$$

There is an eigenvector, giving the Fourier coefficients of the coalesced Mathieu functions $\mathrm{ce}_0(z,q) \approx \mathrm{ce}_2(z,q)$. The generalized eigenvector of the matrix gives the Fourier coefficients of the generalized Mathieu function. These can also be used in the Fourier–Bessel series for the modified Mathieu equation (I called those series preposterous).

Why that works

The Mathieu equation is

$$y'' + (a - 2q\cos 2x)y = 0\ . \tag{14}$$

The generalized function is $u = \partial y/\partial a$ and so satisfies

$$u'' + (a - 2q\cos 2x)u + y = 0\ . \tag{15}$$

In operator form this is

$$\left(\mathsf{D}^2 + a - 2q\cos 2x\right) u = -y \tag{16}$$

and if we replace D by the differentiation matrix and u and y by their vectors of Fourier coefficients we get the generalized eigenvector equation from the Jordan form. This might be obvious to people who teach linear algebra for a living but I had to painfully reconstruct the connection.

This works, in spite of the notorious ill-conditioning of the Jordan form, but is not what I used.

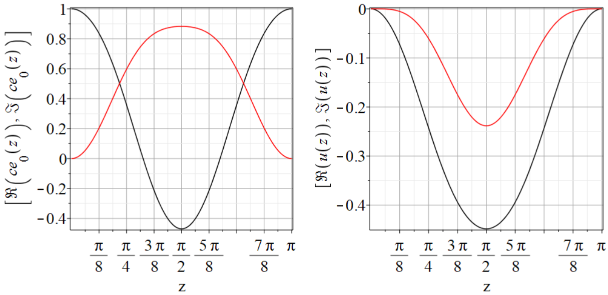
What I really did

I computed the double eigenvalues accurately by two-dimensional Newton's method refining estimates in the literature (Blanch & Clemm, Hunter & Guerrieri) (but simple averaging works fine, once you have identified the nearly-equal eigenvalues). I then solved the Mathieu differential equation using a Hermite–Obreshkov numerical method on a *blendstring* (see [2]). Then I computed the Green's function and directly solved the generalized eigenfunction equation:

$$u'' - (a - 2q\cos 2x)u = -y \tag{17}$$

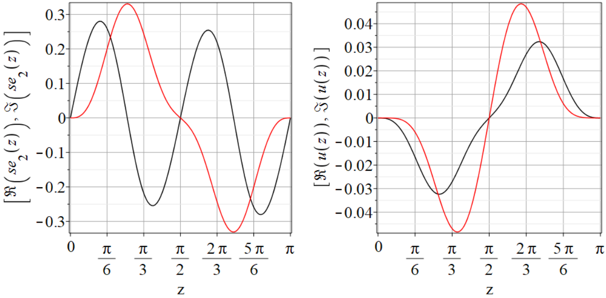
subject to zero initial conditions, by integration (integration of blends is easy).

I tested the residual and found it zero apart from rounding error.



(a) coalesced eigenfunctions (b) generalized eigenfunction

Figure 2: left: Real and imaginary parts of the coalesced eigenfunctions $v_1(z) = \mathrm{ce}_0(z; q) = \mathrm{ce}_2(z; q)$ corresponding to the Mulholland-Goldstein double point $q \approx 1.4688\, i$ (real part in black, imaginary part in red). On the right, we have the corresponding generalized eigenfunction obtained by solving $y'' + (a - 2q\cos 2z)y + v_1 = 0$.



(a) coalesced eigenfunctions (b) generalized eigenfunction

Figure 3: left: Real and imaginary parts of the coalesced eigenfunctions $v_1(z) = \mathrm{se}_2(z;q) = \mathrm{se}_4(z;q)$ corresponding to the next-largest pure imaginary double point $q = 6.92895\ldots i$ with eigenvalue approximately 11.1905. On the right, we have the corresponding generalized eigenfunction obtained by solving $y'' + (a - 2q\cos 2z)y + v_1 = 0$.

Why did I do it that way?

The Fourier and Fourier–Bessel methods seem to be the methods of choice for Mathieu functions. But I wanted something that I could independently assess for accuracy, and which might be useful in nonperiodic contexts (I am aiming at D-finite or *holonomic* functions, which have cheaply-available Taylor coefficients). This is ongoing work.

For Future Work

Desiderata:

- Sensible notation
- Bulletproof code (to use as Blanch says, “in a robot-like manner”)
- Asymptotic formulae for the double points

Stay tuned.

Acknowledgments

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Thank you for listening.

References

[1] Chris Brimacombe, Robert M. Corless, and Mair Zamir. **"Computation and Applications of Mathieu Functions: A Historical Perspective".** In: *SIAM Review* 63.4 (Nov. 2021), pp. 653–720. URL: `https://doi.org/10.1137/20m135786x`.

[2] Robert Corless. **"Blendstrings: an environment for computing with smooth functions".** In: *Proceedings of the 2023 International Symposium on Symbolic and Algebraic Computation*. 2023, pp. 199–207.