

# **Special Functions in Problem Solving Environments:** A personal view

ROBERT M. CORLESS, Editor-in-Chief, Maple Transactions, Canada

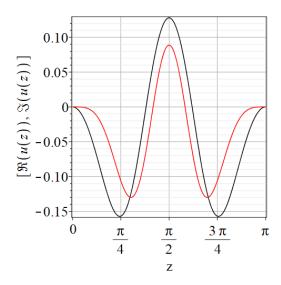


Fig. 1. This "teaser" figure shows the real (black) and imaginary (red) parts of a *generalized Mathieu* function, plotted using Maple.

**Abstract**. This paper discusses some of the philosophical and historical underpinnings of the talk "The Mathieu Functions: Computational and Historical Perspectives" given at the Maple Conference 2022. I also comment on the role Problem Solving Environments (PSEs) play in curating the computational knowledge of the 19th century, which is so necessary for us to think of special functions as *answers* rather than questions.

 ${\tt CCS\ Concepts: \bullet\ Computing\ methodologies} \rightarrow {\tt Representation\ of\ mathematical\ objects; Representation\ of\ mathematical\ functions.}$ 

Additional Key Words and Phrases: Special functions, 19th Century Mathematics, Computer Algebra, Symbolic Computation, Mathematical Knowledge Management

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Author's address: Robert M. Corless, rcorless@uwo.ca, Editor-in-Chief, Maple Transactions, London, Ontario, Canada, N6A 5B9.

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## 1 Introduction

Stigler's Law of Eponymy:

No scientific discovery is named after its original discoverer.

—Actually lots of people said this before Stigler (and he knew it: it's a joke).

The talk "The Mathieu Functions: Computational and Historical Perspectives" that I gave at the Maple Conference 2022 was based in large part on the paper [8], which is available open-access. I don't wish to repeat here the things that were written there, so I will examine a different perspective. The focus of this present paper will be on the notion of special function itself, with some eventual use of Mathieu functions as examples.

In some sense Mathieu functions are one of the "flowers" of the 19th century, being special functions that are *not* representable in terms of so-called hypergeometric functions (which I am not going to use, or even define, here<sup>1</sup>). Mathieu functions are still useful in modern engineering applications as well, so they will also serve to demonstrate the "why" of special functions. I do want to keep this paper reasonably short, however, and so I will omit—by far—more than I include. I will instead point out some further reading, some of which is delightful and useful, and some of which is merely useful.

I am writing for an audience of non-specialists<sup>2</sup>: the topic will be mathematical, certainly, and computational, certainly, but I will try to make sure that all definitions are given and that the presentation is self-contained enough to be read by anyone with an interest. In particular, I want teachers of mathematics at almost all levels to feel welcome reading this paper. There are a *lot* of barriers and gates in modern mathematics: long chains of definitions and theorems with obscure mathematicians' names on them, for instance; crazily complicated and conflicting notation, for another. I'll open as many gates and lower as many barriers as I can. I *will* assume a memory of calculus, however: the reader will need both derivatives and antiderivatives. Not how to *do* them, just what they *are* and how they are written.

Symbolic computation systems have helped with lowering barriers, quite remarkably. I once attended a talk on linear algebra where I was completely lost in the first half of the talk, until the speaker started putting Maple code up. At that point I said (quietly to myself) "Oh, so *that*'s all they meant!" I will use Maple syntax freely in this paper, not merely to demonstrate that Maple can do things (indeed I might show some places where it can't), but in order to make the material intelligible.

What I want this paper to do is to explain what special functions are, and why they are interesting, and what **Problem Solving Environments** (PSEs) like Maple do to help us to use them.

# 2 Why learn about special functions and their support in a modern PSE?

Modern computers can do *direct numerical simulation* of an amazing variety of physical, chemical, biological, and economic phenomena, using as basic elements only the operations of iteration [3], addition, subtraction, multiplication, and division. No special functions here, apparently! From one point of view, all you really need are polynomials and rational functions and iteration. And

<sup>&</sup>lt;sup>1</sup>I will mention "hypergeometric" functions four times in the text, and never define them. They are important, but I have to draw the line somewhere. Mathieu functions are *not* hypergeometric functions, although many other known functions *are*. The study of hypergeometric functions can thus systematize the study of a lot of special functions; but it wouldn't help us here.

<sup>&</sup>lt;sup>2</sup>who hopefully like formulas. There's going to be a few: 46 displayed in the text, to be precise.

linear algebra, of course. The resulting collection of tools are at the core of the discipline known as "Scientific Computing" or "Computational Science" or maybe "Computational Engineering".

Nowadays even this discipline, whatever it's called, is being challenged by certain Artificial Intelligence techniques which, it seems to me, just boil down to very large-scale linear algebra. Again, no special functions here<sup>3</sup>. So maybe we don't need special functions any more? Is the topic of "special functions" dead, or dying?

I remember overhearing three of my Numerical Analysis professors talking about this forty years ago: one of them expressed the opinion that, given the then-modern techniques for solving differential equations, the topic of "special functions" might be dying.

Well, special functions are *not* dead yet (ironically, and somewhat morbidly, all three of those professors *are*), and indeed it turns out that several serious recent advances in scientific computing depend directly on deep knowledge of special functions. I will give references and further readings at the end, but as one example of this for now, the paper [34] is just ten years old and has gathered close to two hundred citations. The main thing special functions are used for in this context is *speed*: by economizing the representation of the model solution, one can gain fantastic speedups.

As another example of the utility of special functions, the classic works on so-called *elliptic* functions continue to be among the most checked-out books in engineering libraries [28]. Not for speed so much, but rather for *understanding*. Elliptic functions are intelligible and astonishingly useful (and that book is one of my favourites). Elliptic functions are maybe the best thing that you could take away from this paper, out of all the special functions.

I claim that special functions have *instrumental value* and can be useful in computation for various practical purposes. I could back that claim up with citations and patents and actual physical devices.

I also claim, however, the more philosophical point that special functions are valuable in and of themselves, as pieces of the collective masterpiece that is mathematics, built up over the millennia in response to natural challenges and to human desires to explore. In my view, mathematics is comparable to language and to music as one of the greatest creations of the collective human mind. That view (which I really hold) itself has instrumental value as a motive for teaching mathematics to idealistic students (there are a lot of idealistic young people). The reason society *pays* for the teaching, though, is that mathematics is useful. Maybe we are lucky that these things go together for special functions.

Another point is that however mathematics is taught, and for whatever reasons, and to whomever it is taught, the body of knowledge that is mathematics must be carefully *curated*. It must be *organized*, conserved where needed or potentially needed, distributed to those who need or want it, and ruthlessly culled when no longer needed (this is harder than it looks: the good stuff must not be forgotten!). New works must be carefully considered.

Many people think that mathematical ideas are static. They think that the ideas originated at some time in the historical past and remain unchanged for all future times. There are good reasons for such a feeling. After all, the formula for the area of a circle was  $\pi r^2$  in Euclid's day and at the present time is still  $\pi r^2$ . But to one who knows mathematics from the inside, the subject has rather the feeling of a living thing. It grows daily by the accretion of new information, it changes daily by regarding itself and the world from new vantage points, it maintains a regulatory balance by consigning to the oblivion of irrelevancy a fraction of its past accomplishments.

-Philip J. Davis in [17]

<sup>&</sup>lt;sup>3</sup>Well, maybe a few, for smoothing things out between layers.

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I want to look, in this paper, at the role symbolic computation systems and other PSEs play in the curation of mathematical knowledge. What we'll go through is a personal view, and I would welcome discussion by submission of further papers to the Maple Transactions. Even if—no, *especially if*—you disagree with me. There's lots to think about, here.

My own view is based on my experience. I won't give a lengthy self-citation list, but I have published papers and book chapters on special functions since the early nineties, and similarly in some related areas such as approximation theory. I designed a poster for the Lambert *W* function, intended for public consumption, available for download at https://www.orcca.on.ca/LambertW.

I have also taught engineering calculus for many years, and various upper-year courses including courses on numerical analysis, symbolic computation, and, yes, on special functions. Let's see if I can make the story as interesting as it deserves. If I can't, that's on me.

Organization and System. Two of my colleagues (justly) criticized earlier drafts of this paper as not being systematic enough. Indeed, the facts in those drafts were presented more like items in a crowded candy store than in a library. I've tidied the paper up a little bit since then, but it's still a fair criticism. You see, I chose a historical approach at first, and the history actually *is* messy and disorganized, as history always is<sup>4</sup>. Nonetheless there are themes to choose from (for instance, some people like hypergeometric functions, although as I said Mathieu functions don't fit that theme) and I could certainly have done better than I did the first time. So, I have since edited the paper to bring out the theme of *computation*. There are at least two systematic aspects of computation that I could make use of, namely the importance of *iteration* and of what are now known as *Taylor polynomials*. These last are what you get when you truncate a Taylor series and can be useful for computing accurate values of various functions. Taylor series are properly a topic of differential calculus nowadays, and functions arose before differential calculus did, so this is ahistorical (but the importance of computation is not). The theme of computation does help to systematize the material, and so I'm grateful for the critical remarks that prompted this set of edits. The "candy store" impression might still linger a bit, though.

# 3 Elementary functions

The *elementary functions* of the calculus are not "elementary" in the sense of being simple, but instead they are "elementary" in a similar sense to the elementary particles of physics.

-James H. Davenport, footnote on p. 258 in [35].

The elementary functions are

- (1) polynomials,
- (2) rational functions,
- (3) radicals and other solutions of polynomial equations,
- (4)  $\ln z$ , and  $\exp z$  (which means  $e^z$  where e = 2.7182... is the base of the natural logarithm),
- (5) combinations thereof,

and that's it, that's all. By "combinations" I mean adding, subtracting, multiplying, dividing or functionally composing two elementary functions makes an elementary function: so  $\ln((1+x^2)/(2-x))$  is an elementary function, for instance. Anything that **cannot** be expressed as some combination of the basic elementary functions is considered **not** to be elementary.

Proving that something is *not* elementary turns out to require some rather advanced mathematics; we will touch only on the very simplest case, later. But first let's look over the elementary functions according to this system.

<sup>&</sup>lt;sup>4</sup>That's my excuse, anyway.

## 3.1 Polynomials

Polynomials are built from the fundamental operations of addition, subtraction, and multiplication. Humans are ok at addition and subtraction, or can be trained to be. My father told me once of an alcoholic accountant in Prince George in the early 1930s who could run his finger down a column of numbers, adding them mentally as he went; he would then run his finger back up the column, adding them in the opposite order as a check. Apparently, in spite of the alcohol, he was always correct. There are still people who can do this. Personally, I can only mentally add because I spent so many years marking papers. But I can do it<sup>5</sup>. It's useful when shopping.

Multiplication is not so straightforward, but with organization it can be done well by hand; and with tools like abaci it's even easy. So we can regard any combination of addition, subtraction, and multiplication as something that we can do if we have to. Thus, polynomial functions are the simplest part of our mathematical toolchest.

Notice that the ability to perform computation with them is of the essence. These are not just mathematical objects, but also involve *actions* that humans can do. Notice also that the computations are *finite*: we do something, and then we stop when we are satisfied with the result. This fact is so obvious that it sometimes gets forgotten, especially in calculus courses where so much time is spent on *infinite* processes and limits.

## 3.2 Rational Functions

Division—the action of undoing a multiplication—is harder for humans, but again with organization it can be done. In terms of mathematical functions, this gives us *rational* functions<sup>6</sup>. For instance, consider the curve named—in a curious fashion<sup>7</sup>—after Maria Gaetana Agnesi, who was the first woman to be recognized in Europe for her work in mathematics; this was in the 18th century. Her curve is called "The Witch of Agnesi" and was studied by Fermat and others before she did; score one for Stigler's law. The "Witch" has the equation

$$y = \frac{8a^3}{x^2 + 4a^2} \,. \tag{1}$$

Here a is the radius of a defining circle; for each value of a, one gets a different curve. Supposing x, y, and a all have the same units of length (say meters), this can be "nondimensionalized" by dividing both sides by a and rearranging the formula on the right to

$$Y = \frac{8}{X^2 + 4} \,, \tag{2}$$

where we have conveniently written Y for y/a and X for x/a. Now we can graph the nondimensional Y versus the nondimensional X, label the axes with x/a and y/a, and have all the (nonzero) Witches of Agnesi represented at once.

I won't explain any Maple commands here; they are considered as part of the explanation!

<sup>&</sup>lt;sup>5</sup>My favourite joke: there are three kinds of mathematicians, namely those who can count and those who can't. (ba-dump tsssh!). My daughter's favourite joke is similar: there are 10 kinds of people, namely those who understand binary and those who don't.

<sup>&</sup>lt;sup>6</sup>In my opinion, the main reason to teach children arithmetic with fractions is so that they can later handle the algebra of rational functions.

<sup>&</sup>lt;sup>7</sup>it seems to be a mistranslation of the Latin *versiera*, but I am not sure I believe that.

<sup>&</sup>lt;sup>8</sup>Nondimensionalization is one of the most useful things that I ever learned. I have found it hard to teach, though, and many students really don't like it. I don't know why not, but maybe it doesn't seem worth the mental effort nowadays.

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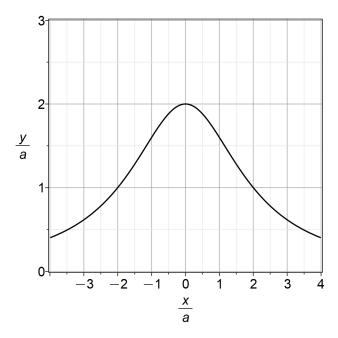


Fig. 2. The curve described by  $x^2y = 4a^2(2a - y)$ , named after Maria Gaetana Agnesi (1718–1799). Once it has been nondimensionalized, it is a single, simple, rational curve, which is certainly "elementary."

## 3.3 Radicals and Algebraic Functions

Writing something like  $\sqrt{2}$  is considered "elementary." The radical sign is familiar to all sufficiently advanced schoolchildren. But it is an interesting "step up" when  $\sqrt{x}$  is considered as a function. Square roots can be constructed using straightedge-and-compass<sup>9</sup>; something humans can do using only the simplest of tools. But *cube* roots *cannot* be constructed "exactly" with straightedge and compass! (This was the famous problem of doubling the cube, settled in 1837 by Wantzel.) But nonetheless *all n*th root radicals are considered to be *answers* and not questions. We will see an explanation of that once we have considered the logarithm function and the exponential function.

Algebraic functions are the next step up from polynomial and rational functions. These involve solving polynomial equations, such as quadratic equations, cubic equations, or quartic equations. For instance, if y solves the equation

$$y^3 + 3xy^2 + 2y + x^2 - 1 = 0 (3)$$

then y is an algebraic function of x. Since we have a formula in terms of radicals for solving a cubic equation, this is acceptable.

```
eq := y^3 + 3*x*y^2 + 2*y + x^2 - 1;
solve( eq, y ); # Not printed here, because it's daunting.
```

In a small enough neighbourhood of the point x = 1, y = 0 (for instance) the algebraic function represented by that equation is unique, and one can write down a Taylor polynomial for it using

<sup>&</sup>lt;sup>9</sup>Now *there* is a rabbit hole to go down. Some of my contemporaries at UBC when I was an undergraduate were among the last engineering class to be explicitly taught straightedge and compass constructions for approximate solution of engineering problems. Those methods were in use for thousands of years, therefore! Their influence on *proof* and on *mathematics* was profound. With their idealized construction of lines and circles, what could be done? And what *couldn't* be done?

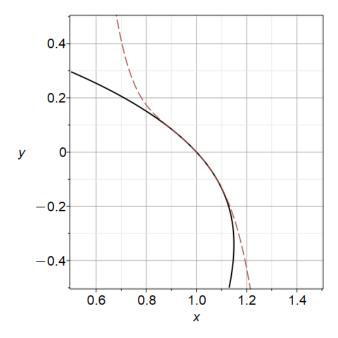


Fig. 3. The algebraic "function" from equation (3), together with a sixth order Taylor polynomial approximation (red dashed line) valid near the point x = 1, y = 0.

Maple in any of several ways, which I am not going to go into here (see ?solve, series for more details, if you want). The results of one method are graphed in Figure 3.

Exactly solving a *quintic* equation, which is degree 5, is more difficult, and was only proved *impossible* to solve in general *in terms of radicals* by Ruffini in 1814 and Abel in 1824. But one *can* exactly solve them in terms of *elliptic functions*. We therefore have the *contradictory* statement that "algebraic functions including the solutions of quintics are elementary functions" and "elliptic functions are not elementary functions."

This raises an important point: sometimes a function will fit more than one definition. We could impose a hierarchy, and say that being "elementary" has priority. But there are other instances where it goes the other way, notably with named families of polynomials. For instance, the functions  $T_n(x)$  defined by  $T_0(x) = 1$ ,  $T_1(x) = x$ , and  $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$  are all polynomials and thus elementary; but these particular polynomials are known as *Chebyshev* polynomials and they have some very special properties. For instance, when made monic by dividing each by  $2^{1-n}$  for n > 0, they give the polynomials with the smallest maxima on the interval  $-1 \le x \le 1$ . From a certain point of view, these can be considered to be *special* functions, and indeed many books on special functions have chapters on these and other "orthogonal" polynomial families. People seem to live with the ambiguity here. David Stoutemyer suggests the name "special polynomials!"

Let us return to considering algebraic functions, which are classified as being "elementary" as discussed above. In particular, let us return to the quintic.

Nowadays, in a stroke of sleight-of-hand so easy it seems facile to the point of imbecility, quintics can be exactly solved "in terms of themselves" the way Maple does it, with the **RootOf** function. What is the solution of  $y^5 + y^4 - 1 = 0$ ? Maple says,

$$RootOf(Z^5 + Z^4 - 1, index = 1)$$
(4)

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and four more, with index=2, 3, and so on. This seems the very definition of "begging the question"! But, if you have means to *compute* the solution to arbitrary accuracy, then don't you *have* a solution?

Note that one can do symbolic things with the **RootOf** form of the solution. Call the following root  $\alpha$ , say:

alias(alpha = 
$$RootOf(Z^5 + Z^4 + 1, Z)$$
);

Then the command

yields the rather nicer (in some sense) expression

$$\frac{1}{3}\alpha^4 + \frac{2}{3}\alpha^3 + \frac{2}{3}\alpha^2 + \frac{2}{3}\alpha + \frac{2}{3}.$$
 (5)

This is possible because any power of  $\alpha$  higher than 4 can be simplified using the original equation. So this is not begging the question, after all. To the contrary, it's a very powerful idea. The **RootOf** construct gives immediate access to *algebraic* functions in Maple, and supports the notion that roots of polynomials are elementary functions.

# 3.4 Exponentials and logarithms

I mentioned that humans are better at addition than they are at multiplication or division. This is why the invention of logarithms was greeted with so much acclaim:

$$a \cdot b = e^{\ln a + \ln b}$$

converts multiplication to addition, and division to subtraction. Common logarithms,  $\log_{10} x$  or simply  $\log x$  to everyone except snobbish mathematicians  $^{10}$ , are more convenient for human arithmetic than the natural logarithm is, because the size as a power of ten is instantly visible in the logarithm.

The base e was not invented<sup>11</sup> until Napier's time in the 1600s, although exponentiation is very old. According to the story at https://mathshistory.st-andrews.ac.uk/HistTopics/e/ the importance and the name e only gradually dawned on the mathematicians of that century.

The history of the computation of logarithm is astonishing, and Brigg's monumental work of hand computation of tens of thousands of entries to 14 decimal places just boggles my mind. That logarithms are available on dollar-store calculators nowadays is similarly boggling, but in a different way.

The logarithm and the exponential arrive together, as a pair. If you have the one, then you have the other: just interchange x and y. If  $y = \exp x$ , then  $x = \ln y$ . A table of exponentials is a table of logarithms. For me, though, I like to think of logarithm as being the most basic: I like the definition

$$\ln x := \int_{t-1}^{x} \frac{1}{t} dt \tag{6}$$

which depends on the integral calculus. Together with ancient rules for computing areas such as the trapezoidal rule or the midpoint rule, this gives a practical though tedious method to compute logarithms. One can do this in Maple:

 $<sup>^{10}</sup>$ The insistence on using  $\log x$  to mean  $\ln x$  is simply gatekeeping. Using  $\log$  for natural  $\log$  marks one as a "mathematician" as opposed to a physicist or engineer. It was Bill Gosper who pointed this cultural mistake on the part of mathematicians out in a way that I understood, and converted me. Maple uses both; Matlab (the snob) won't let you use  $\ln$ . This misses an important opportunity! David Jeffrey noticed that there was unused space for a subscript on  $\ln$ , and invented the notation  $\ln_k z$  to mean  $\ln z + 2\pi i k$ . I use this frequently! One couldn't use  $\log_k z$  for this, because that means " $\log$  to the base k."  $^{11}$ Invented? Discovered? I now prefer Mansi Bezbaruah's version, from Twitter: "Math wasn't invented or discovered, math was manifested."

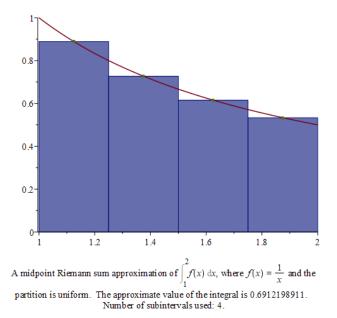


Fig. 4. An underestimate of  $\ln 2$  by the midpoint rule. To see that it's an underestimate, rotate each rectangle's top line about the point of contact until it's tangent. This preserves area. Because 1/x is convex upward, the curve will lie above the tangent.

```
ApproximateInt(1/x, x = 1 ... 2, method = trapezoid, partition = 4);
```

The midpoint rule *underestimates* this integral and the trapezoidal rule *overestimates* it. With just four panels, we get

$$M = \frac{4448}{6435} = 0.6912 \dots < \ln 2 < 0.6970 \dots = \frac{1171}{1680} = T$$

and taking the improving average<sup>12</sup> (2M + T)/3 we get 0.69315 which is in error by less than  $10^{-5}$ . The midpoint rule can be computed in Maple by

and the resulting plot is shown in Figure 4.

Perhaps just as importantly, this integral formula for logarithm connects to the work of Liouville, which we will talk about later, for *proving* certain functions are *not* elementary. How does this formula connect? Because one can use this definition of logarithm to *prove* that logarithm is neither a polynomial function, nor a rational function, nor an algebraic function. It's not so easy, though! Try it, and see!

Once one has a definition of logarithm, one can define the exponential function  $y = \exp x$  as the solution to the nonlinear equation  $x - \ln y = 0$ , and compute accurate values of  $\exp x$  by Newton's method or some other iteration. This choice is something of a matter of taste; one could instead

<sup>&</sup>lt;sup>12</sup>See for instance [12] for a discussion of why this particular average is the right one for combining an estimate from the midpoint rule with an estimate from the trapezoidal rule. In short, it's because the midpoint rule is usually twice as accurate as the trapezoidal rule, and its error is usually the opposite sign.

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start with a good method to compute  $\exp x$  and then compute logarithms by solving  $x = \exp y$  for y.

The other logarithms, namely log to base 10 written  $\log x$  or  $\log_{10} x$  for clarity, and  $\log$  to base 2 written as  $\log x$  (in computer science) or  $\log_2 x$  for clarity, are defined by an appropriate scaling:  $\log_b x = \ln x / \ln b$ . Maple uses  $\log_{\mathbb{C}}[b](x)$  and "simplifies" it immediately to that ratio.

$$x^a := e^{a \ln x} \tag{7}$$

and so all radicals (in that case, a = 1/n) can be written in this straightforward way as a composition of two elementary functions. This confirms our earlier classification of radicals as elementary.

## 3.5 Trig functions

What about the trig functions? Well, both trig functions and inverse trig functions can be defined in terms of exponentials and logs, if we allow complex numbers:

$$\sin z := \frac{e^{iz} - e^{-iz}}{2i} \tag{8}$$

$$\cos z := \frac{e^{iz} + e^{-iz}}{2} \ . \tag{9}$$

The hyperbolic functions are also elementary:

$$\sinh z := \frac{e^z - e^{-z}}{2} \tag{10}$$

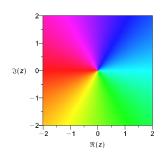
$$cosh z := \frac{e^z + e^{-z}}{2} .$$
(11)

Let's turn it up a notch and look at complex values. We plot  $\sin z$  in Figure 5b, in a way that might be new to you, by plotting its complex argument (also called the phase) by a particular colour scheme. One can learn to identify important features, such as zeros and singularities, simply by looking for where all the colours meet. This is done in Maple with the command

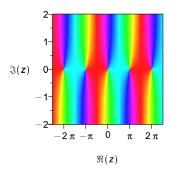
```
plots[complexplot3d]( sin(z),
  z = -2.5*Pi - 2*I .. 2.5*Pi + 2*I,
  style = surfacecontour, contours = [0],
  orientation = [-90, 0], lightmodel = none,
  font = ["Arial", 24], labelfont = ["Arial", 24],
  grid = [200, 200], tickmarks = [spacing(Pi), default, default]
  );
```

What this does is to relate the image f(z) to the phase of  $z = r \exp i\theta$ . One associates a particular colour with the phase angle  $\theta$  using the colorwheel in Figure 5a. Then everything with  $\theta = 0$  gets coloured (by the Maple command above) a light blue. Different  $\theta$  get the different colours that you can see in Figure 5a. Where all the colours meet must either be a zero f(z) = 0 or a pole 1/f(z) = 0. You can tell one from the other by the *direction* (clockwise or counterclockwise) compared to the graph of the phase of just z itself. In Figure 5b you can see zeros of  $\sin z$  this way; there are no poles. It's worth experimenting with.

The fact that one can plot four-dimensional functions by using colour [44] seems to have caught most mathematicians by surprise. The real surprise is that by using only *three* dimensions (two in directional space and one in colour space), we can get the complete picture: the fourth dimension is somehow irrelevant, or implied, or deducible from the other three. We can in fact plot complex functions using just three dimensions in several ways (and this is not new), but this new



(a) Phase plot of z, giving the colorwheel



(b) Phase plot of  $\sin z$ 

Fig. 5. One new technological development is that we can do *phase plots* of complex-valued functions. On the left, we have  $w = z = x + iy = re^{i\theta}$  pictured. Each ray with constant angle  $\theta$  has the same colour. If we plot  $\sin z$  using the same scheme, we can pick out places where all the colours meet. Those are the zeros of  $\sin z$ , namely multiples of  $\pi$ . This new visualization technique is remarkably powerful.

colour technique, also called *domain colouring*, is rather welcome. But complex numbers are full of surprises.

It is a surprise to most students to find that (for example) one can solve the equation  $y = \sin z$  for z in terms of y using logarithms. It's a bit easier for them to solve the related equation  $y = \sinh x$  for x in terms of y because there are no obvious complex numbers present. One uses the definition above:  $2y = \exp(x) - \exp(-x) = E - 1/E$  if  $E = \exp(x)$ ; then this quadratic equation can be solved for E. Indeed, multiply by E to get  $E^2 - 2yE - 1 = 0$ , and then

$$e^{x} = E = y \pm \sqrt{y^2 + 1} \tag{12}$$

and then for real y the choice of sign is determined by the fact that the exponential is always positive, and  $\sqrt{y^2+1} > |y|$ . So we get  $x = \ln(y+\sqrt{y^2+1})$  as an explicit expression for the functional inverse of sinh x. There's an analogous one for  $\arcsin(x)$ . Maple knows them both, of course.

convert(arcsin(z), ln);

$$-\operatorname{I}\ln\left(\operatorname{I}z+\sqrt{-z^2+1}\right) \tag{13}$$

Maple uses I for the square root of -1. I have never liked this notation, but one gets used to it.

REMARK 3.1. I strongly dislike the notation  $\sin^{-1} x$  for the functional inverse of the sine function. So many students are confused by it, and slip into thinking that this is the same thing as the reciprocal  $1/\sin x$ . My colleague David Jeffrey has invented a much superior and more general notation, which I hope will catch on: if y = f(x) then  $x = \inf f(y)$ . There's space for a subscript to indicate branches, if f(x) takes on the same value y for differing values of x.

Writing inverse functions in terms of branches gets tricky, and one has to be careful about what are called "branch cuts." I've written at length about that elsewhere, so I won't belabour the point here. David Jeffrey and I have also written about Riemann surfaces, which is a different way to deal with multivalued functions. That method is very popular with pure mathematicians, but doesn't

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really work computationally: one wants the computer to return just one single x for a given y. David has written about this with the intriguing suggestion of using something he calls "charisma" and that might work [23]. I hope that catches on, too.

## 3.6 Implicitly elementary functions, and the Lambert W function

There's a grey area: we allow functional inverses of all the functions discussed so far to be elementary, but not inverses of *combinations* of these, to be elementary. Instead they get a special name, to wit: *implicitly elementary*. For example, the Lambert W function [11] is not elementary, but it is implicitly elementary, being a distinguished solution of the equation

$$we^{w} - z = 0. (14)$$

The solution of this equation is w = W(z). Maple writes instead LambertW(z), because single-letter names are important user "real estate" in the name space. If all solutions are wanted, we say  $w = W_k(z)$ , while Maple says **solve**(w\***exp**(w)-z,w, allsolutions=**true**) is LambertW(\_Z2,z). Maple has introduced a symbol here, which we can interrogate: **about**(\_Z2); yields

```
Originally _Z2, renamed _Z2~:

is assumed to be: integer
```

It's more human to write  $W_k(z)$  and use the old FORTRAN convention (any variable starting with a letter I through N is an INteger) to indicate to the reader that k is an integer. W(z) without a subscript is shorthand for the principal branch,  $W_0(z)$ .

Written the other way around,  $z = w \exp w$  is an elementary function of w. This always happens for implicitly elementary functions.

The Lambert W function is well-known nowadays because it was implemented in Maple from the early days, and because its solution for the tower-of-exponentials problem<sup>13</sup> was listed on the Frequently Asked Question list of the USENET discussion group sci.math. Gaston Gonnet used it in one of his papers in the early 1980s, and made a nice connection to the Gamma function as well (which I rediscovered for myself in 2016 when I started writing a paper on the Gamma function with Jon Borwein). So Gaston implemented it in Maple, and the most frequent way people encounter W for the first time is as the result of a call to the solve command.

```
solve( y*exp(y) - z, y );
```

yields LambertW(z). The first question the surprised user asks is "what in the world is Lambert W?" and the help system in Maple is ready to answer that.

Here are two more facts about *W*. First is my favourite integral, for which Bill Gosper said in an email to me that the midpoint rule converged "slambangularly!"

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{(1 - v \cot v)^2 + v^2}{z + v \csc v e^{-v \cot v}} \, dv \,. \tag{15}$$

This is equal to W(z)/z for all  $z > -\exp(-1)$  and therefore for at least some complex z in a domain containing that line segment. Both the midpoint rule and the trapezoidal rule work *spectrally*<sup>14</sup> well to evaluate the integral. This provides a nice means to compute W(z), although there are better

 $<sup>^{13}</sup>$ If  $x^{x^{x^{\cdots}}} = 2$ , what is x? Now replace 2 with 4. Oops? What is this tower, in general? See the Lambert W poster linked earlier

<sup>&</sup>lt;sup>14</sup>This is a technical term which means that the error diminishes *exponentially* with the amount of effort expended. Put in a little more effort, you get a *lot* less error! The word "exponentially" has entered the public vocabulary in a sloppy way, but we all got a sharp reminder of what it actually means with the COVID-19 pandemic.

ways yet. In some sense this integral is analogous to

$$J_0(x) = \frac{1}{\pi} \int_0^{\pi} \cos(x \sin \theta) d\theta \tag{16}$$

for the Bessel function  $J_0(z)$ . This integral allows computing  $J_0(z)$  by numerically approximating the integral on the right hand side.

My second favourite W fact involves the denominator of the integrand in (15). That expression presents an interesting nonlinear equation to solve for v once z is given. After all, one would not want to integrate over a singularity! It turns out that all solutions to that equation are found in the following bi-infinite set (for a proof, see [13]):

$$v_{k,j} = \frac{W_k(z) - W_j(z)}{2i} \ . \tag{17}$$

That is, the solutions of this frighteningly complicated nonlinear equation can all be written as differences of various branches of Lambert W.

Solving nonlinear equations is very hard in general; this is one of the most complicated "naturally occurring" equations that I know that can actually be solved explicitly in terms of "known" (special!) functions.

I leave those two facts for you to ruminate on at your pleasure. You might try computing a few values of branch differences of Lambert W and verifying that those do provide solutions to the equation. For instance,

```
Digits := 30;
eq := z + v*csc(v)*exp(-v*cot(v));
eval(eq, v = (LambertW(2, z) - LambertW(5, z))/(2*I));
eval( %, z=0.12345 );
```

yields real and imaginary parts each on the order of  $10^{-28}$ . Using a higher value of **Digits** gets a smaller residual, and this is convincing evidence that we have it right.

You might also try proving that all solutions are of this form. It's not absurdly hard, once you know that it's possible, and it gives practice with Lambert *W*. It should be within reach for high school students who know about the exponential definitions of the trig functions (he says confidently).

## 3.7 Historical remarks

The trig functions, more-or-less contemporaneously to the solution of a quadratic equation, might go back to Babylonian times and ancient astronomy and may date as far back as 3700BCE (this is disputed, though). People wanted (and still want) to calculate trig functions in order to use them for astronomy and other purposes, and so the history of these functions is inevitably bound up in the history of how to compute them.

On solving quadratics, cubics, and quartics: the history of solving the cubic on Wikipedia is pretty interesting reading, and there is a more complicated formula for solving quartics in terms of radicals. Indeed it involves first solving a "resolvent cubic." We talk a little about these in Computational Discovery on Jupyter, my book with Neil Calkin and Eunice Chan. See in particular Mandelbrot Activity 6.

## 4 The role of computation and the search for better methods

Not everything is numerical analysis, you know, Rob.

-M.A.H. "Paddy" Nerenberg, to a younger RMC

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The modern definition of a function is as "a set of ordered pairs." That's nothing but a table. This suggests that if you have one element of an ordered pair, you ought to be able to access the other. If someone has already done the work for you, then indeed a table of values is a useful way to represent functions. If you don't have a table, then you need some way to accurately compute the values of the function. Indeed this is kind of a minimum requirement. But my late friend Paddy was right, too—there's more to it than that. Identities are useful (for instance, there seems to be a relation between Lambert W and inverse spherical Bessel functions which no-one had suspected [38]), and so are other properties such as convexity. PSEs provide access to those other things, too. I will contend that numerical evaluation of functions ranks pretty highly, though, and we need *methods* for that.

# 4.1 Taylor polynomials

One way to compute functions is by their Taylor polynomials. Some were known for trig functions already by Mahadva of Sangamagrama (c. 1340–c. 1425). The formula for Taylor series in general is

$$f(x) = f(a) + f'(a)(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \cdots$$
 (18)

and beginning students really have trouble keeping all those symbols in their precise places. Part of the issue is that they don't see f(a) or f'(a) as constants (how could they be? There's a function in there! And if x is a variable, why isn't a?). Practice, practice. Another really big issue is that they do not see the right-hand side as being the slightest bit simpler than the left. After all, their calculator usually has a button for f(x) and why would you want to use a more complicated formula? One can sometimes say that the calculator uses Taylor polynomials to evaluate the function (which is a "lie to children" because most calculators use better methods), and that they are learning (something about) how it works internally.

One could use the "binomial theorem"

$$(1+x)^n = \sum_{k\geq 0} \binom{n}{k} x^k$$

to approximate cube roots, for instance (although one has to be able to compute binomial coefficients for fractional n), as I mentioned: but once one has Taylor polynomials, one really has everything. This was one of Newton's greatest achievements, by the way, to realize that these polynomials could be used for basically everything.

The "Taylor" in the name "Taylor series" and "Taylor polynomials" was *Brook* Taylor, who published on them in 1715, almost four hundred years after Mahadva. And as just mentioned, Newton certainly knew what they were previously in the 1600s, as well. Then there is Colin Maclaurin who later used them, specialized to expansion about zero, so in that case they are then called Maclaurin series, which also hardly seems fair. Stigler's law is really ticking up its score.

series( 
$$sin(x)$$
,  $x=Pi/4$ , 4 );

vields

$$\frac{\sqrt{2}}{2} + \frac{1}{2}\sqrt{2}\left(x - \frac{\pi}{4}\right) - \frac{1}{4}\sqrt{2}\left(x - \frac{\pi}{4}\right)^2 - \frac{1}{12}\sqrt{2}\left(x - \frac{\pi}{4}\right)^3 + O\left(\left(x - \frac{\pi}{4}\right)^4\right). \tag{19}$$

This is first few terms of the Taylor series for  $\sin(x)$  about the expansion point  $x = \pi/4$ , as computed by **series**, one of the oldest Maple commands. One converts to a Taylor *polynomial* by the command **convert**(%, **polynom**); and this removes the big-Oh term, and, more importantly, converts from the internal **series** data structure to something more appropriate for a polynomial.

It is relatively new in Maple that one can ask for *infinite* power series [39, 19]:

convert(sin(x), FormalPowerSeries, x = Pi/4);

yields

$$\left(\sum_{n=0}^{\infty} \frac{\sqrt{2} (-1)^n \left(x - \frac{\pi}{4}\right)^{2n}}{2 (2n)!}\right) + \left(\sum_{n=0}^{\infty} \frac{\sqrt{2} (-1)^n \left(x - \frac{\pi}{4}\right)^{2n+1}}{2 (2n+1)!}\right). \tag{20}$$

I have always thought of this kind of thing as "putting the skills of an Euler, or of a Ramanujan, at the fingertips of the students (or researchers)". This is an example of curation of mathematical knowledge, because the knowledge is put in a form where it can be retrieved or applied to the situation at hand. You can see that quite a bit of knowledge of the sin function has been included in the system: evaluation for complex z, the knowledge of exact special values, and how to compute infinite series and finite polynomials.

Maple knows Taylor series for many special functions.

#### 4.2 Iteration

It turns out that the idea of *iteration* is also remarkably old, perhaps going back as far as 1700BCE [3]. Archimedes used it (in essence) in his method of exhaustion for computing  $\pi$  by approximating a circle first by a polygon with N sides and then by another with 2N sides, but it first appears unequivocally in the literature by 75AD in the writings of Heron of Alexandria. We have already given a link to the famous iteration of Newton.

The idea itself is so simple as to almost disappear on examination: if something worked once, do it again and make the result even better! For square roots, the Babylonian iteration runs as follows. To compute  $\sqrt{2}$  (say), start with an initial estimate, say  $x_0 = 1$ . Then one can improve this estimate by using the estimate in the rule

$$x_{n+1} = \frac{1}{2} \left( x_n + \frac{2}{x_n} \right) .$$

That is, we take the average of our estimate  $x_n$  and its cofactor  $2/x_n$ ; if  $x_n < \sqrt{2}$  then the cofactor  $2/x_n > \sqrt{2}$  and vice-versa and so either way the average *ought* to be better than the previous estimate.

The idea of iteration is hidden in this explanation by the conceptual leap in using the index n (meant to be the sequence of integers  $0, 1, 2, \ldots$  until we got tired or were satisfied) to indicate repetition.

This particular iteration was later generalized, as we have noted and linked, by Newton (and others—some people call the method "the Newton–Raphson–Kantorovich method") to give a method for solving any algebraic equation, given a good enough initial estimate. The method can also solve nonlinear differential equations or even harder equations; it's a workhorse of modern scientific computing.

This idea can be combined with Taylor series, and the use of Taylor series "reversion" to solve equations approximately in fewer iterations than Newton's method uses. This was first done by Schroeder, who gave two infinite families of iteration schemes of arbitrarily high order for solving equations. His schemes keep getting reinvented [37].

Iteration can be used in the following way to evaluate the exponential function. Suppose that we have a good method to evaluate  $\exp x$  if x is small, say  $|x| \le 0.1$ . One candidate would be the approximation (which comes from Taylor polynomials, but with a further idea due to the French mathematician Henri Padé, namely to use rational functions, not just polynomials):

$$\exp x \approx \frac{1 + x/2 + x^2/10 + x^3/120}{1 - x/2 + x^2/10 - x^3/120} \ .$$

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This is accurate to about  $10^{-12}$  on  $-0.1 \le x \le 0.1$ .

But perhaps you want to compute exp 2. The argument  $x_0 = 2$  is not small enough to use the rational function above directly. So, instead, compute  $\exp x_1$  where  $x_1 = x_0/2$  which is 1, and once you have that then square the result. Here  $x_1$  is still not small enough, so divide by 2 again; and again, and again, until one arrives at  $x_5 = 2/2^5 = 1/16$  which is smaller than 0.1. Using the rational approximation above gives  $\exp 1/16 \approx 1.06449445891790$ . Squaring that five times gives  $\exp 2 \approx 7.38905609893927$  which is in error by less than  $2 \cdot 10^{-12}$ . This particular kind of iteration goes by the name of "argument reduction." This idea (not the specific Padé rational above) is very much used today to evaluate *matrix* exponentials, and so qualifies as a "modern method."

## 4.3 Modern methods

Methods for the computation of trig functions and of logarithm were worked out over significant time spans, but Taylor polynomial methods were of very substantial help. All through the 19th century and even in the early 20th century Taylor polynomial methods remained a "serious" contender for the best way to compute a function. Indeed, special functions were regarded as "solved" if one had a convergent Taylor series for them. Gauss heavily used series for the hypergeometric functions in the early 19th century.

In principle, one can truncate series to get polynomials and use them to compute values for any smooth function. In practice, it's not always so easy, because Taylor polynomials can be (and frequently are) what is known as "ill-conditioned" and using them in a brute force way needs high-precision arithmetic, which is costly in terms of computer time. Something better is needed, usually.

Maple has quite sophisticated methods, often much better than just using Taylor polynomials, and if Maple knows *anything* about a function, it knows how to evaluate it at a given point, to a given accuracy. That's basically the first thing that gets written. For some functions this is easier than it is for others.

Some of these better methods were already being developed in the 19th century, including Fourier series—which expanded functions not in terms of polynomials, but in terms of the "elementary" trig functions, which themselves were computed by Taylor polynomial methods and refinements, but were now considered as *answers* rather than as questions.

This shift, from question to answer, occurs repeatedly in the history of mathematics, and is worthy of note. Once something can be computed "sufficiently easily," it can become an answer, I think; although that's not the whole story. But, methods of computation play a significant role in defining what the elementary objects of mathematics are.

Another interesting *new* method of computation was the Arithmetic-Geometric Mean (AGM) iteration, invented by Gauss in the early 19th century. We will see this in action when we look at elliptic functions. The iteration, which uses square roots, is superficially similar to Archimedes' method of computing  $\pi$  by inscribed polygons and circumscribed polygons (itself a lot of fun to think about and I wish I could take the time, here), but is subtly different. "Timing" turns out to be everything, and the AGM iteration converges astonishingly quickly. This method allows one to compute the so-called *Jacobian elliptic functions*, also invented in the 19th century, extraordinarily rapidly. From that, one gets the fastest known way to compute ordinary trig functions!

Mathieu's 1868 paper comes right in the middle of all of this explosion of the theory and practice of functions. What he invented in order to understand the "nodal lines" of a vibrating drum with a fixed elliptical rim, are now called Mathieu functions. He used series extensively in his computations; not just Taylor series, but also Fourier series (he didn't call them that) and perturbation series. Indeed he invented a new perturbation series method (now known as the Lindstedt–Poincaré method, Stigler wins again) as well.

At about the same time, Pafnuty Chebyshev, Charles Hermite, Henri Padé and others were refining the approximation methods of Newton, Cauchy, and others, to start the body of work known today as Approximation Theory. The results of this body of work are in heavy use, behind the scenes, in symbolic computation systems and other PSEs (and even in hardware), to support accurate evaluation of both elementary and special functions.

# 5 Symbolic computational support for functions

In a modern symbolic computation system, as we have seen already, one wants to be able to manipulate expressions that define functions to make new expressions; one wants to compute series; one wants to differentiate these objects; to integrate them (in finite terms as elementary functions, or to prove that they are not elementary); **to evaluate them at a given point or at many given points**; and to plot them. One might wish to prove that the functions being considered have certain properties (such as always being positive, or being convex). A modern symbolic computation system has to anticipate the needs of most users. But probably the most fundamental need is to evaluate the function accurately wherever the user wishes, and do it at lightning speed.

We're not there yet, and in fact there are some thorny hidden difficulties (one is known as the Table Maker's Dilemma). But there has been a lot of progress.

## 5.1 Historical remarks

Perhaps the history of symbolic computation systems begins with the work of Jean Sammet (1928–2017), who was the first Chair of the Special Interest Group on Symbolic and Algebraic Manipulation. She was the principal designer of FORMAC (FORmula MAnipulation Compiler). This was a preprocessor for FORTRAN which allowed what we call symbolic computation today. Another important piece of history is the famous 1972 HAKMEM by Beeler, Gosper, and Schroeppel which contains an amazing number of special function facts. It can be found at <a href="https://w3.pppl.gov/~hammett/work/2009/AIM-239-ocr.pdf">https://w3.pppl.gov/~hammett/work/2009/AIM-239-ocr.pdf</a>. Then there was ALTRAN (which was the language Keith Geddes first used in order to teach computer algebra to Waterloo grad students, including me, before we switched to the brand-new system Maple in the middle of the term; this was 1981 I believe). Of course there was REDUCE and Macsyma in there as well.

Mathematica arrived on the scene in 1988. Nowadays there are several systems, including SymPy and SAGE Math. Some systems have come and gone, such as Theorist, which was quite interesting in its attempt to do automatic case analysis, and Derive which survives now only in ghost form on some kinds of calculators, I believe.

All of these systems—all—had some kind of implementation of elementary functions. All of them could evaluate elementary functions; most could differentiate them, and some could integrate them (or could prove that the resulting integrals would not be elementary). The implementation of special functions varied widely. Macsyma had quite a lot, as I recall. The Hewlett-Packard calculator series could do complex arithmetic, knew a lot of special functions including the Gamma function, could integrate and differentiate and compute Taylor polynomials; I miss that calculator. Although there are nice emulators available free these days.

# 5.2 Real arithmetic

The "real number system" has an unfortunate name. It should have been called the "continuum number system" or some such, because the word "real" has the decidedly hard-to-ignore connotation of "actual." If something is not a "continuum number" then it would be quite easy to believe that it might be some other kind of number. If it's not a "real number" then there's this connotation that it's like Pinocchio, who is not a "real boy." Indeed to the contrary one can wonder if "real numbers"

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are actually objects that really exist; some of them do, certainly, but others? It gets iffy, out on the borders. But there's no changing the name now. Almost every symbolic computation system has some kind of implementation of something that is intended to act like "real numbers," even though this is technically impossible. We only ever have finite representations and we can only work with numbers that can be constructed or represented somehow; and we don't have enough alphabet to do otherwise. Most real numbers, in fact, are not computable. Nonetheless, we do what we can and everyone pretends it's enough. When the computer fails to come back from a computation because of one of the impossibility problems (recognizing zero) we shrug. When floating-point approximate numbers give us grief, we do our best to compensate.

# 5.3 Complex arithmetic

For me, complex floating-point arithmetic is the natural setting for elementary and special functions. Complex numbers are perfectly "real" meaning actual. Here is the square root of minus one: (0, 1). Complex numbers are just pairs of "continuum" numbers. And functions of complex numbers are some of the simplest functions.

There are lots of discrete functions of course, that is, functions of integers taking integer values, and they are very useful; but for me  $\mathbb C$  is where it's at. And with computers to take the tedium out, there's no reason to fear the complex plane. So I expect all symbolic computation system implementations of all elementary functions and special functions to work, and work well, over  $\mathbb C$ . Unfortunately, this is not at all the case (even for Maple). Most users just want "real" numbers, so the complex numbers get second billing; and moreover complex-valued functions *are* harder to implement, so the developers have to work harder. But when we get to the Mathieu functions, we will certainly want complex values.

## 5.4 Polynomials and Rational Functions as Workhorses

Once one has a solid foundation of complex floating-point numbers, one can quickly implement *polynomials* and *rational functions* on top of them. And then one can implement the *square root function*, and the *absolute value* function. This one is ridiculously hard: overflow is a real problem for it. But the details were worked out in the 1970s already. My favourite method is contained in [33], but it's not as practical as the scaling methods Maple uses.

There is a *huge* body of theory, called Approximation Theory, of how best to allocate the effort amongst these elementary operations so as to compute the value of the function you want. Chebyshev approximation is widely considered to be the *best*; everyone wants the best. I used a bit of jargon there: Chebyshev approximation means approximating by simpler functions so that the *maximum error* in the approximation is *minimized*. There is also expansion in what are known as *Chebyshev polynomials* (which are maybe my runner-up favourite set of functions), which provide "near" best approximation.

For the Mathieu function code that I implemented and described in my talk for the Maple Conference, I chose something else, namely what Erik Postma and I called a "blend." A blend is a combination of two Taylor polynomials expanded at either end of an interval. It was invented by Charles Hermite, and its proper name is "two point Hermite interpolational polynomial." Here is

the formula: the "grade<sup>15</sup>" m + n + 1 polynomial

$$H_{m,n}(s) = \sum_{j=0}^{m} \left[ \sum_{k=0}^{m-j} \binom{n+k}{k} s^{k+j} (1-s)^{n+1} \right] p_j$$

$$+ \sum_{j=0}^{n} \left[ \sum_{k=0}^{n-j} \binom{m+k}{k} s^{m+1} (1-s)^{k+j} \right] (-1)^j q_j$$
(21)

has a Taylor series matching the given m + 1 values  $p_j = f^{(j)}(0)/j!$  at s = 0 and another Taylor series matching the given n + 1 values  $q_j = f^{(j)}(1)/j!$  at s = 1. Putting this in symbolic terms and using a superscript (j) to mean the jth derivative with respect to s gives

$$\frac{H_{m,n}^{(j)}(0)}{j!} = p_j$$
 and  $\frac{H_{m,n}^{(j)}(1)}{j!} = q_j$ 

for  $0 \le j \le m$  on the left and for  $0 \le j \le n$  on the right. Blends turn out to have decent numerical properties: they can be rapidly (enough) evaluated, and differentiated, and integrated (this was a very nice bonus), and combined with each other. They can be connected pairwise using Taylor polynomials known at the knots of a polygonal path in the complex plane (in which case I call it a "blendstring"—it's really a special kind of piecewise polynomial). The real reason I chose to do this is that if you have a nice differential equation to solve, then you can find Taylor polynomials easily, pretty much everywhere you land. So it is easy to build up a precise, accurate, and convenient representation for the solution of the differential equation. It works well for the Mathieu equation.

Earlier I complained that Taylor series were hard to teach to students, and that they did not like the complicated formula. One facetious benefit of teaching students about blends might be that they would appreciate the simplicity of Taylor polynomials more! The formula involves *binomial coefficients* instead of just factorials, as with Taylor series. And a blend has two Taylor polynomials hidden in it (one at one end, and one at the other). So, yes, blends are more complicated than Taylor polynomials. But they can be a million times more accurate than Taylor polynomials, even when the grade at each end is just 10. So maybe they are worth the pain.

Computer algebra systems don't generally use blends, but choose from other, classical, methods. They might choose piecewise combinations of Chebyshev polynomials; or rational functions. Most of Maple's accurate evaluations of special functions are ad-hoc and special-purpose, although there is a significant interest nowadays at Maplesoft in uniformizing the relevant methods. But perhaps if one has a function that has special properties, one should take advantage of them; so I suspect that there will always be room for special-purpose methods.

## 6 Special Functions

Here's a vague definition for you: A special function is a useful function that is not elementary. Clearly there's some room for argument! Bessel functions (invented by Daniel Bernoulli (1700–1782) before the astronomer Bessel (1784–1846) worked on them, go Stigler) are very frequently used, and no-one would dispute their utility. Similarly with the error function, or the  $\Gamma$  function. But there are "special" functions, even some with famous names attached, that are nothing but curiosities today<sup>16</sup>. Let's give some examples of the survivors.

 $<sup>^{15}</sup>$ The word "grade" means "degree at most." A polynomial of grade 5 might be degree 0, or 1, or 2, or 3, or 4, or even 5, but not 6 or higher.

<sup>&</sup>lt;sup>16</sup>This turned out to be a dangerous statement. Every example that I thought of turned out to have *some* use and someone advocating for it. The best example I came up with was the "versine" function—but that's an elementary function!

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## 6.1 The Gamma function

The grandparent of all special functions, manifested in the 1700s, is Euler's  $\Gamma$  function, which *interpolates* the factorial function. The factorial function, of course, is nowadays written n! and means  $1 \cdot 2 \cdot 3 \cdots (n-1) \cdot n$ ; we have already used it above in the formula for Taylor series. The question Euler wondered about was what could it mean to take (1/2)! or the factorial of any other non-integer. He solved the problem completely.

Euler's definition was as an infinite product, but he also came up with the following integral, valid for x > 0:

$$x! := \int_{t=0}^{1} \ln^{x} \left(\frac{1}{t}\right) dt . \tag{22}$$

Maybe you were expecting a different integral? Sure and this one (also due to Euler) is better known!

$$x! := \int_{t=0}^{\infty} e^{-t} t^x dt .$$
(23)

Stirling came up with a lovely (but divergent) asymptotic series for the factorial, which begins as

$$\ln(x!) = \left(x + \frac{1}{2}\right)\ln(x + \frac{1}{2}) - \left(x + \frac{1}{2}\right) + \ln\sqrt{2\pi} + O\left(\frac{1}{x + \frac{1}{2}}\right) \tag{24}$$

Since  $\Gamma(x) = (x - 1)!$  we have the similar formula

$$\ln \Gamma(x) = (x - \frac{1}{2})\ln(x - \frac{1}{2}) - (x - \frac{1}{2}) + \ln\sqrt{2\pi} + O\left(\frac{1}{x - \frac{1}{2}}\right). \tag{25}$$

This is astonishingly accurate for large enough x, even though divergent, and moreover may be "reverted" to get an approximation for the functional inverse of the  $\Gamma$  function (or, equivalently, of the factorial function). In an entirely unexpected <sup>17</sup> way, the Lambert W function makes another appearance: to solve  $x = \Gamma(y)$ , put  $v = x/\sqrt{2\pi}$  and u = y - 1/2. The solution process using Lambert W is then clearer (try it!) and the end result is

$$y \approx \frac{1}{2} + \frac{\ln(x/\sqrt{2\pi})}{W\left(\frac{1}{e}\ln(x/\sqrt{2\pi})\right)}.$$
 (26)

Let's try that out and try to find a y so that  $\Gamma(y) = 100$ .

yields 5.888, and  $\Gamma(5.888) = 99.24$ . Not bad!

One of the benefits of extending one's vocabulary of functions is that you have greater power of expression. You can say more things, with greater concision. Sometimes you can say things that you did not even know were expressible, before you learned the vocabulary.

## 6.2 Elliptic functions

One of the integrals that students have a hard time with in calculus is the following:

$$I(x) = \int_{t=0}^{x} \frac{1}{\sqrt{1-t^2}} dt . {27}$$

<sup>&</sup>lt;sup>17</sup>Well, maybe not that unexpected.

Maple says, uh, that's inv sin(x) (actually it uses the notation arcsin(x), of course). Of course this is right. That means I(x) = y where sin y = x. So this integral gives the functional inverse of something interesting.

Now let's look at a mildly more complicated integral, namely

$$A(x) = \int_{t=0}^{x} \frac{1}{\sqrt{(1-t^2)(1-k^2t^2)}} dt.$$
 (28)

Here  $0 \le k \le 1$  is a parameter, called the elliptic modulus. This integral (studied by the great Legendre, and by Abel whom the Abel prize is named for) is *not an elementary function*.

It was Liouville who first *proved* in 1835 that this function cannot be expressed in terms of elementary functions [43, p. 126]. It is here that the distinction between "computer algebra systems" and "symbolic computation systems" starts to bite, with Liouville's theory, which began as analysis but was later developed by algebraists such as Ritt into the field of differential algebra that we have today. A modern computer algebra system can *prove* that a given integral is not elementary, by using the Risch algorithm or its refinements. But this proof is essentially algebraic, and ignores some rather important analytical things in the theory of special functions, such as branch cuts. But we will not dwell on this divide, and instead return to the nonelementary integral for A(x) above.

The integral A(x) can, however, be expressed as <sup>18</sup>

$$inv sn(x, k) (29)$$

the functional inverse of the Jacobian elliptic function  $\operatorname{sn}(x,k)$ . The integral is therefore what is termed an "elliptic integral." Many researchers have worked on these. For instance, Sofya Kovalevskaya wrote a paper on elliptic integrals in 1874 which she presented to the University of Göttingen as part of her doctoral dissertation; she was the first woman awarded a PhD in mathematics in Europe.

The value of this particular elliptic integral depends on the elliptic modulus k, as well as on x. There are three main Jacobian elliptic functions, sn, cn, and dn. They correspond as  $k \to 0$  to sine, cosine, and the very simple function which is identically 1. In fact, with just one more function, namely the Jacobian *amplitude* function am(u, k), then

$$\operatorname{sn}(u,k) = \sin(\operatorname{am}(u,k)) \tag{30}$$

$$cn(u,k) = cos(am(u,k))$$
(31)

and

$$\frac{d}{du}\operatorname{am}(u,k) = \operatorname{dn}(u,k) \tag{32}$$

```
K := EllipticK(1/sqrt(2));
plot([JacobiSN(u, 1/sqrt(2)), JacobiCN(u, 1/sqrt(2)), JacobiDN(u, 1/sqrt(2))],
        colour = ["Executive_Blue", "Executive_Red", black],
        thickness = [1, 1, 1], view = [-4*K .. 4*K, -2 .. 2],
        axes = boxed, font = ["Arial", 16],
        labelfont = ["Arial", 16],
        labels = [u, y], gridlines = true );
```

produces the plot in Figure 6. These are modestly more complicated than trigonometric functions, but *once you get used to them* they are almost indispensable. You do, however, have to get used to them. Maybe that's the real definition of a special function: a non-elementary function that *you are used to*.

 $<sup>^{18}</sup>$ Maple does not do it this way, however. It gives instead **EllipticF**(x,k), which is much the same thing.

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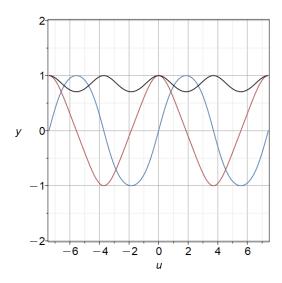


Fig. 6. The Jacobian elliptic functions  $\operatorname{sn}(u,k)$  (in blue),  $\operatorname{cn}(u,k)$  (in red), and  $\operatorname{dn}(u,k)$  (in black) for  $k=1/\sqrt{2}$  and two periods. One sees that sn is like sine (it *is* a sine, just with different argument), cn is like cosine (likewise), and dn is like 1.

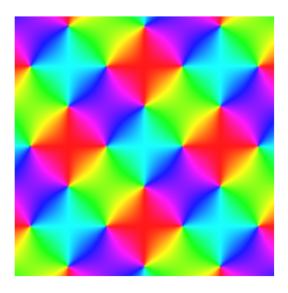


Fig. 7. A phase plot of **JacobiCN**(z,k) for k = 0.2. Can you see the zeros and poles?

I said "modestly more complicated," and that's true. We find [28, p. 27] that they are *doubly periodic* with not only a real period but also a complex period. Moreover, they not only have zeros like the trig functions, they also have poles. See if you can pick out the zeros and poles of cn(z, k) in Figure 7.

Elliptic functions are also incredibly fast to compute to high precision. The key<sup>19</sup> is the AGM iteration: start with two numbers, call them  $a_0 > 0$  and  $b_0 > 0$ . Then compute, for n = 1, 2, and so on until  $a_n = b_n$  to your desired precision,

$$a_n = \frac{1}{2} (a_{n-1} + b_{n-1})$$

$$b_n = \sqrt{a_{n-1}b_{n-1}}.$$
(33)

This works for complex numbers, too, but let's "keep it real" for the example. Choosing two numbers more or less at random just to show the iteration, take  $a_0 = 1$  and, say,  $b_0 = 10$ . Then convergence in double precision happens in five iterations.

> Digits := 15;

$$Digits := 15$$
 (34)

> AGM :=  $(a,b) \rightarrow (\frac{(a+b)}{2}, \operatorname{sqrt}(a \cdot b));$ 

$$AGM := (a, b) \mapsto \left(\frac{a}{2} + \frac{b}{2}, \sqrt{b \cdot a}\right)$$
 (35)

> AGM(1.0, 10.0)

> AGM(%);

> AGM(%);

$$4.25078685759612, 4.25002734923307$$
 (38)

> AGM(%);

$$4.25040710341460, 4.25040708644996$$
 (39)

> AGM(%);

$$4.25040709493228, 4.25040709493228$$
 (40)

I want to go on to tell you about *Landen transformations* which are just a different way to organize that iteration, and how Gauss used a very non-intuitive change of variables on an elliptic integral to prove that what the AGM iteration converges to is expressible as an elliptic integral, but this is already too much detail. All I want you to retain from this sketch is that (a) elliptic functions are like trig functions and nearly as useful once you get used to them, and (b) they can be computed quickly.

Therefore, they should be thought of as *answers* and not as *questions*. It is this thought that truly answers the question "what is a special function."

<sup>&</sup>lt;sup>19</sup>Well, one key. Another way to do it is by what are called theta function series, which are "lacunary" meaning very sparse. A typical theta function series is  $\sum_{k\geq 0} z^{k^2}$  which looks rather like a Taylor series; but the square in the power means that the terms are 1, z,  $z^4$ ,  $z^9$ , and so on, and *most* of the terms that would be present in an ordinary power series are missing. This means that computation with these is much more rapid than they are with ordinary series.

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## 6.3 The Mathieu functions

Twenty-four pages in, and I am finally getting to the Mathieu functions. Good gravy. Well, I hope that you are still with me. We'll start by reminding you about the trig functions and their connection to a differential equation. They satisfy

$$\frac{\ddot{y}(\theta)}{y(\theta)} = -n^2 \tag{41}$$

where *n* is an integer. Wait, what?

If we rearrange that we get  $\ddot{y}(\theta) + n^2y(\theta) = 0$  which looks more familiar (where Newton's dot notation is being abused here to mean differentiation with respect to  $\theta$ , and two dots means do it twice), and the solutions are  $y(\theta) = A\cos n\theta + B\sin n\theta$ , which are periodic with period  $2\pi$ . This particular way of approaching the trig functions comes from solving the partial differential equation (PDE) known as Laplace's equation on a disk by the technique known as "separation of variables<sup>20</sup>", leading naturally to the *eigenvalues*  $-n^2$  which have to be the negatives of squares of integers if the solutions  $y(\theta)$  are to be periodic with period  $2\pi$ . Separation of variables is a topic of one's second differential equations course, normally; or it might happen in first year physics.

Now let's complicate the differential equation *just* a bit:

$$\frac{\ddot{y}(\theta) - 2q\cos 2\theta \, y(\theta)}{y(\theta)} = -a \tag{42}$$

where now the eigenvalue (this time called a) again has to be chosen so that  $y(\theta)$  is periodic with period  $2\pi$ . We also have a new parameter in the problem, q. This has to do with the geometry, which (as in the previous collection) is that of an ellipse. Here q is proportional to the distance between the foci of the ellipse. If the ellipse is actually just a circle, then q=0 and we reduce to trig functions. So we somehow feel that the Mathieu functions must be (as the Jacobian elliptic functions were) analogous to trig functions.

And, they are. But the eigenvalues are, sadly, more complicated. For small values of q, they are like  $a = n^2$ , but for larger values they can do different things. This complicates the vocabulary. But, at its most basic, we will have

$$\operatorname{ce}_n(\theta;q)$$
 (43)

which will be *like*  $\cos n\theta$  when q is small. It is *even*, and periodic with period  $2\pi$ . If moreover the integer n=2m is itself an even integer, then the function  $ce_{2m}(\theta;q)$  is periodic with period  $\pi$ , just like  $\cos(2m\theta)$  is. Similarly,

$$\operatorname{se}_n(\theta;q)$$
 (44)

is like  $\sin n\theta$ . Maple knows quite a bit about these functions. It calls them **MathieuCE**(n,q,theta) and **MathieuSE**(n,q,theta).

This use of capital letters is a bit of an unfortunate clash of notation because the *modified* Mathieu functions are frequently denoted with capital letters, e.g.  $Ce_k(\theta;q)$ . Well, Maple's implementation of *modified* Mathieu functions (also called *radial* Mathieu functions) is hidden away, anyway: they are simply the ordinary Mathieu functions (also called the *angular* Mathieu functions), but with purely imaginary argument.

```
plot([seq(MathieuCE(k, 1.0, theta), k = 0 .. 3)], theta = 0 .. 2*Pi,
    axes = boxed, gridlines = true,
    font = ["Arial", 16], labelfont = ["Arial", 16],
    labels = [theta, typeset(ce[k](theta))],
    tickmarks = [spacing(Pi/2), default] );
```

<sup>&</sup>lt;sup>20</sup>This technique is probably the first one taught for solving PDE. It's quite an old technique, and Mathieu used it explicitly, and credited the physicist Lamé. In fact the history goes back to Johann Bernoulli and to Leibniz. Stigler wins another round.

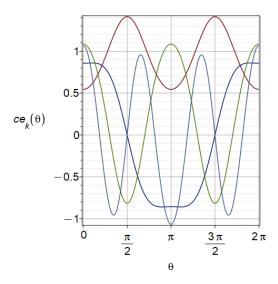


Fig. 8. The first four even Mathieu functions. You can figure out which is which by looking to see which ones have period  $\pi$ , which then must be k=0 and k=2, and the simpler one is k=0; then the other two must be k=1 and k=3 and again the simpler one has k=1.

produces the graph in Figure 8.

Acquiring the vocabulary of the Mathieu functions and internalizing it means learning how the eigenvalues work (sadly, it's complicated) and how to compute them. This is where one of the great achievements of Gertrude Blanch was: She was the first to compute the *double* eigenvalues systematically.

Once one can compute the eigenvalues reliably, one has to learn how to compute the eigenfunctions, that is, the ce and the se functions. That's not as hard. In particular, it is not as hard because one can compute Taylor polynomials for the eigenfunctions remarkably quickly, because the differential equation for the Mathieu function can be rewritten as a D-finite or *holonomic* equation: if  $v = \cos \theta$  then in terms of the new variable v, the Mathieu equation can be written as

$$(1 - v^2)\frac{d^2y}{dv^2} - v\frac{dy}{dv} + (a + 2q(1 - 2v^2))y = 0.$$
 (45)

This formulation is due to Mathieu himself, who noted that series computation (by hand!) was simpler with it because instead of a cosine term, the differential equation has *polynomial* coefficients. This class of equations is attracting current attention for precisely this feature, which means its solutions may be computed rapidly [42, 32].

You can use gfun[diffeqtorec] to find the following recurrence relation for the Taylor coefficients  $u_k$  of the solution  $y(v) = \sum_{k \ge 0} u_k (v - \alpha)^k$  to that form of the Mathieu equation:  $(\alpha^2 - 1)u_{k+4} = 0$ 

$$-\frac{4qu_k}{(k+4)(k+3)} - \frac{8\alpha qu_{k+1}}{(k+4)(k+3)} + \frac{\left(-4\alpha^2 q - k^2 + a - 4k + 2q - 4\right)u_{k+2}}{(k+4)(k+3)} - \frac{(2k+5)\alpha u_{k+3}}{(k+4)(k+3)}.$$
 (46)

Once you can compute the eigenfunctions, then answering PDE questions with elliptic geometry in terms of Mathieu functions becomes natural. And that, in a nutshell, is what the paper [8] is about.

I will end with a picture. In 2020 I wrote a paper which I put on the arXiv but have never submitted anywhere else [15]. I might try to improve it for Maple Transactions, because what it

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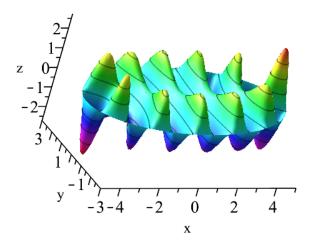


Fig. 9. The opening picture from my talk: the "Whispering" modes in an elliptical gallery. If you stand at one focus, and speak, the sound waves will travel along the edges of the gallery and collect at the other focus, so you can speak one to the other without being overheard. In the picture you can see the larger amplitude waves near the edges.

does is use my Mathieu function code to draw the "nodal lines" for elliptic drums, which was the subject of Mathieu's 1868 paper [30] (translated to English in [31]). Using that code and Maple's graphical capabilities it's easy to draw the pictures that Mathieu predicted would occur if one sprinkled sand on an elliptical drum and vibrated it at various frequencies. The sand collects on the motionless loci. In Figure 9 we go one step farther and plot it in 3d and in colour. For my talk, which everyone remembers perfectly of course, I started with an animation of a figure like this one, showing the membrane vibrating in that mode.

As a final remark on Mathieu functions, they were named by Sir Edmund Whittaker at an International Congress of Mathematicians, from "elliptic cylinder functions" to "Mathieu functions" specifically in honour of Mathieu's pioneering 1868 paper [30]. They may, indeed, be one of the very few exceptions to Stigler's Law of Eponymy.

## 7 Notes and further references

If you are only going to read one work on the  $\Gamma$  function, then it must be the Chauvenet prize-winning paper "Leonhard Euler's Integral" by Philip J. Davis [17]. The paper is approximately as old as I am, and it reads like a lucid dream. It's in JSTOR, and everyone gets one hundred free papers from JSTOR every month, so you should use one of those free papers up on this one. I cited this paper in my own paper [6] on  $\Gamma$ , written with the late Jon Borwein, and maybe it was my favourite of all we read. But now there is the lovely paper [25], as well. So don't stop with just one!

I very much enjoyed Eli Maor's historical book *Trigonometric Delights* [29]. Ed Barbeau's book [4] is an excellent reference for advanced high school students or beginning university students on polynomials. To find out how elementary functions are described in modern computer algebra, see the monumental [18] by von zur Gathen and Gerhard, and in particular see Chapter 22.

On elliptic functions, the book *Elliptic Functions and Applications* by D. F. Lawden, which I have cited already [28], is one of my favourite math books of all. It is pellucidly written, with lean dry prose that is *always* on point. You find page after page after page of formulas, sometimes taking up

the whole page almost, which looks intimidating until you realize that there is *not a single error* or misprint. Then you fall in love with the book. I have been reading and re-reading this book for more than thirty years now, and I have never found a single mistake. I have implemented many of those said formulas and they have *always* been reliable. What a book! I collect autographs by authors of math books, and I wish I had the author's autograph for this one.

One of the best things about that book is its collection of classic applications, such as the harmonic oscillator  $y'' + \sin(y) = 0$ . Many people are under the impression that this "cannot be solved" analytically, and of course if they mean (under their breath) "in terms of elementary functions" they are right; but the solution is extremely simple in terms of elliptic functions. There is also a direct solution of the general relativity equations for the precession of the orbit of Mercury! And the book *begins* with the theta series solution of the heat equation. Elliptic functions are, and always have been, applied mathematics!

Another of my favourite books is the Nobel Prize-Winner Subrahmanyan Chandresekhar's wonderful *Ellipsoidal Figures of Equilibrium* which studies the shape of planets, using elliptic functions [10]. In looking for the BibTeX entry for that, I just found this minute a "2010" paper<sup>21</sup> by him giving a historical account, which I will read *right now*<sup>22</sup> [9].

The classic paper [7] shows how to compute elementary functions quickly in high precision by using elliptic functions as an intermediate step. See also [16]. My friend Jacques Carette recommends the papers [26, 46, 24] for more details on D-finite functions.

General works on special functions include the encyclopedic [1] (Gertrude Blanch wrote the chapter on Mathieu functions). This has been superseded by the online Digital Library of Mathematical Functions, dlmf.nist.gov. Probably the best textbook is [45], although it's old-fashioned in the extreme. It's still *absolutely* worth reading. Then there is the gigantic [2], and hundreds more. For computation of special functions, see the SIAM book by Gil, Segura, and Temme [20]. The classic book [5] uses a lot of special functions, and teaches quite a bit about them through that use. A very modern take (although based on classical 19th century mathematics) can be found in [41].

Orthogonal polynomials are special functions, too (as previously noted, the definitions are not sharp-edged). Another one of my "top few" books is *Chebyshev Polynomials* by Rivlin [36]. That was the first of my "autographed" books—I met Ted Rivlin at IBM T.J. Watson Research Center in Yorktown Heights, New York, on my first sabbatical in 1994. Chebyshev polynomials are interesting for their own sake, but they have remarkable instrumental power for computing. That brings us to the next major reference, which is another of my "top few" favourite books: Nick Trefethen's amazing book *Approximation Theory and Approximation Practice* [40], which I reviewed in [14].

Then there is Nick Higham's amazing book, *Functions of Matrices* [22]. It turns out that one needs to apply special functions to matrix arguments, as well, in many applications.

Finally, maybe my favourite book of all: Concrete Mathematics by Graham, Knuth, and Patashnik [21] (autographed only by Donald Knuth—I have sadly missed my chance with the late Ron Graham, and have not met Oren Patashnik). The special functions covered in that book are mostly discrete, such as the binomials and Stirling numbers and the like, but it also treats the hypergeometric functions starting on p. 204. So if you have been frustrated waiting to learn about them, start there! The book was used as an undergraduate textbook, and contains many marginalia contributed by students, some of which are very funny indeed. Readable, beautiful, and useful. If you only choose one book to actually read out of the list I have given you so far, make it this one.

<sup>&</sup>lt;sup>21</sup>The normally reliable website doi2bib.org got the date wrong! It's 1967, not 2010! I have reported this via Twitter. Let's see if it gets fixed.

<sup>&</sup>lt;sup>22</sup>Or maybe not. The UWO library is missing that exact volume online. Maybe they have it in print.

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# 8 Concluding remarks

It is a profoundly erroneous truism, repeated by all copy-books and by eminent people when they are making speeches, that we should cultivate the habit of thinking of what we are doing. The precise opposite is the case. Civilization advances by extending the number of important operations which we can perform without thinking about them. Operations of thought are like cavalry charges in a battle—they are strictly limited in number, they require fresh horses, and must only be made at decisive moments.

—Alfred North Whitehead, Introduction to Mathematics, Chapter 5

The central point of this paper, which I hope is clear now, is that special functions are pieces of mathematical vocabulary. Once you get used to them (and being able to compute them, perhaps by Taylor polynomials or by iteration or something more advanced, is part of that), and regard them as *answers* rather than as *questions*, then you can use them to *think* with. As per Whitehead's famous remark quoted above, this will increase the effectiveness of your thoughts.

The purpose of computing is insight, not numbers.

—Richard W. Hamming

Formulas can give insight, but only if the terms in the formula are familiar.

One really important new factor nowadays is that we have computers to help. One of the best ways that they can help mathematical thinking is by encoding knowledge of special functions: how to evaluate them, how to differentiate or integrate them, how to combine them with other functions. Even just giving us unambiguous notation to work with<sup>23</sup> would be a huge advantage.

It is this curation of 19th century special functions in symbolic computation systems and other PSEs—starting with the work of Gertrude Blanch and the others on the fantastic project which became Abramowitz and Stegun and then the DLMF—which has led to significant revival of interest in special functions. The modern research field of *Mathematical Knowledge Management* starts from here, but then so does a lot of modern, ongoing research into special functions.

Looking forward, there are two new books using an old approach that has been revitalized in a serious way: first, Riemann Problems and Jupyter Solutions, an online (free!) book by David I. Ketcheson, Randall J. LeVeque, and Mauricio J. del Razo. If you prefer a printed version, you may purchase one from SIAM [27]. Second, the book [41] (which I had previously mentioned) shows how to use that old technique, plus the Fast Fourier Transform, to compute special functions accurately and quickly throughout the complex plane. The journey continues.

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This paper is dedicated to the memory of my colleague Henning Rasmussen, who taught me about Airy functions.

<sup>&</sup>lt;sup>23</sup>Hoo, boy. Don't we wish.

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