Guidelines for Domain Errors in Mathematical Special Functions

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1 Introduction

In 2003, the C++ committee accepted for TR-1 a proposal [Bro03a] to substantially enhance the mathematical facilities of the standard C++ library. Several discussions on the committee mail reflector and several follow-up documents [Pla03, Bro03b, Bro03c, Pla04] further addressed this issue. While the substantive content of the proposal has not been changed, nor have substantive changes been proposed, one set of details remain to be addressed: where shall domain errors be produced?

In the discussions which have attempted to resolve these details, we have seemed to "go around in circles" several times—addressing the same issue differently in different contexts. As we now see it, we lack a clearly defined set of guiding principles, or philosophy, according to which such decisions should be made. This paper is our attempt to define a set of guiding principles which the committee can use to guide its decisions on these matters, and to determine where these guidelines affect the previous proposal.

We first summarize the open questions about this proposal. We then consider several philosophies which could be adopted for the specification of the behavior of all the mathematical functions in the standard C++ library. We propose the choice of a single philosophy to guide our specifications, and analyze the specifications in light of that philosophy.

We do not propose, herein, any changes to the TR-1. However, if the Committee accepts our recommendation, we will propose specific wording changes in time for disposition at the next meeting.

2 The Open Issues

The open issues regarding the mathematical special functions library have a single subject: the specification of domain errors for the functions.

In [Pla04], Bill Plauger raises questions about several functions. We summarize those questions here.

assoc_legendre $P_\ell^m(x)$

There are two questions raised. The first concerns the domain of the index m; specifically, the question is about whether or not a domain error should occur for $m > \ell$.

The second question concerns the domain of x; specifically, the question is whether a domain error must occur for $x > 1$.

beta $B(x, y)$

The question raised here concerns whether domain errors occur for all integral (x, y) such that both $x \le 0$ and $y \le 0$, or only for some such values.

legendre $P_\ell(x)$

The question concerns whether a domain error occurs for $x > 1$.

bessel $J_\nu(x)$, $N_\nu(x)$, $I_\nu(x)$, $K_\nu(x)$, $j_\nu(x)$, $n_\nu(x)$

The question concerns whether a domain error occurs for $x < 0$.

We believe there are other issues, similar to these, to be settled. In order to discover them, and to find their resolutions, it is useful to find the categories which they comprise. That is the purpose of the next section.

3 Two Examples

To describe more clearly the kinds of problems which need to be addressed, let us consider as examples two of the functions listed in [Bro03c]: the beta function $B(x, y)$, and the (cylindrical) Bessel functions, *i.e.*, $J_\nu(x)$. To discuss the beta function, we must also discuss the gamma function, to which it is related. We consider these functions first.

3.1 Euler's Gamma and Beta Functions

The beta function $B(x, y)$ may be defined in several ways. Perhaps the simplest is the definition chosen in [Bro03c], which relates the beta function directly to the gamma function:

$$B(x, y) = \frac{\Gamma(x)\,\Gamma(y)}{\Gamma(x + y)}. \tag{1}$$

The gamma function $\Gamma(x)$ has poles of order 1 at all integral $x \le 0$. The reason can be seen easily in Figure 1; the limiting value of the function as we approach these points is not defined,

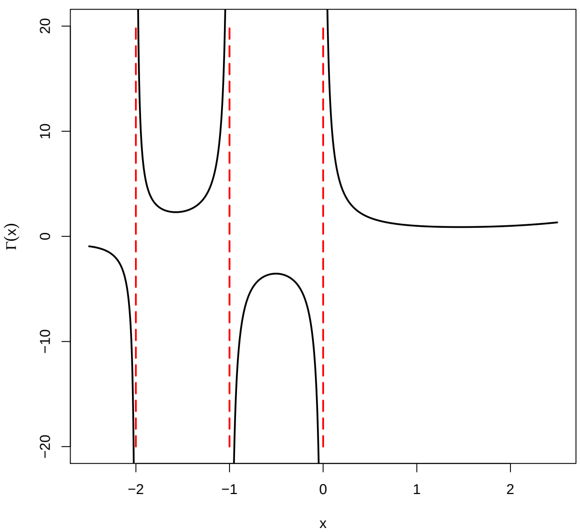

Figure 1: The gamma function, $\Gamma(x)$. Dashed lines indicate values of x for which the function is undefined.

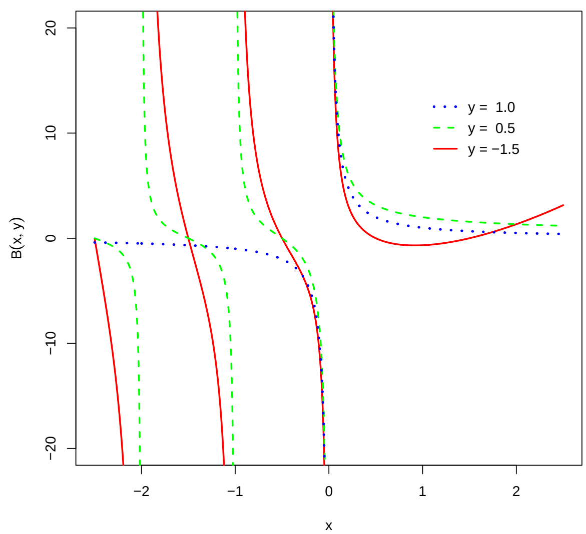

Figure 2: The beta function, $B(x, y_i)$, for selected values of y_i. Note that $B(x, y) = B(y, x)$, so one can also read this $B(x_i, y)$ for selected x_i.

because approaching from above and approaching from below yield different limits. The mathematical function is clearly undefined at these poles, and so the library function must return a domain error. In fact, the C99 library functions which approximate the gamma function do report domain errors for integral values of $x \le 0$.

This illustrates our first guiding rule, which is the same rule used elsewhere in the math library:

Guideline 1 *A mathematical function is said to be defined at a point* $a = (a_1, a_2, \ldots)$ *if the limits as* $x = (x_1, x_2, \ldots)$ *approaches* a *from all directions agree. The defined value may be any number, or* $+\infty$*, or* $-\infty$*.*

The library function which approximates a mathematical function shall signal a domain error whenever evaluated with argument values for which the mathematical function is undefined.

It is important to note this guideline is specified more precisely than it may at first seem to be. While it is true that not every real number can be represented as a floating-point quantity within a finite number of bits, it is also true that every floating-point value[1] corresponds *exactly* to one real value.

Returning to the beta function, analysis shows that it has poles, but *not* for all integral non-positive x and y. Although the Γ function in terms of which it is defined has poles at all these values, it is mathematically possible for poles to "cancel," leaving a finite quotient. For example, if we consider $x = -2$ and $y = 1$, we find the numerator contains a pole ($\Gamma(-2)$) as does the denominator ($\Gamma(-1)$); the resulting quotient, however, is finite. Details are shown in the

[1]Except, of course, for floating-point representations of special values such as signed infinities, NaNs, and signed zeros.

appendix. Figure 2 shows the beta function as a function of x for three fixed values of y. As can be seen in the plot, $B(x, y)$ has poles at *some*, but not all, negative integral values of x; the behavior of the function at negative integral x depends on the value of y. For example, at $y = 1$, there are no poles at negative integral values of x; the only pole is at $x = 0$.

Thus the beta function is defined "almost everywhere" in the (x, y) plane, and is undefined at only precisely identifiable points. It seems reasonable, therefore, for the library function that approximates the beta function to be *not* limited to positive x and y; instead, it should be defined everywhere the mathematical function is defined, and to indicate a *domain error* for those and only those argument values for which the mathematical function is undefined.

Closely related to Guideline 1 is another clear guideline that results from our choice to limit the mathematical special functions library to real-valued functions of real arguments. This rule has also been applied elsewhere in the math library:

Guideline 2 *The library function which approximates a mathematical function shall signal a domain error whenever evaluated with argument values for which the mathematical function obtains a non-real value.*

In the next example, we consider a function for which the answer seems less clear.

3.2 Cylindrical Bessel Functions

The cylindrical Bessel functions $J_\nu(x)$, $N_\nu(x)$, $I_\nu(x)$ and $K_\nu(x)$ appear in the solutions to Bessel's equation:

$$x^2 \frac{d^2 f}{dx^2} + x \frac{df}{dx} + (x^2 - \nu^2)\, f = 0, \tag{2}$$

a differential equation that appears in many physical contexts[2]. An important feature of this equation is that it appears in physical problems possessing circular symmetry.

In such problems, the part of the equation that corresponds to Equation 2 is a *radial* equation; that is, the variable x corresponds to the radial coordinate of a system with circular symmetry. Since the radial coordinate measures the distance from the origin of the circle, it can not be negative. This would seem to give us a reason to decree that all the cylindrical Bessel functions should yield domain errors when evaluated with $x < 0$.

However, the Bessel functions are defined not only as solutions to Bessel's equation; each may also be defined by a particular convergent infinite sum which solves Equation 2, as is done in [Bro03c]. We can demonstrate that *some* of the sums converge and yield real-valued results for $x < 0$.

For example, the definition of $J_\nu(x)$ given in [Bro03c] is:

$$J_\nu(x) = \sum_{k=0}^{\infty} \frac{(-1)^k\, (x/2)^{\nu+2k}}{k!\, \Gamma(\nu + k + 1)}. \tag{3}$$

When $\nu = 0$:

$$J_0(x) = \sum_{k=0}^{\infty} \frac{(-1)^k\, (x/2)^{2k}}{(k!)^2} \tag{4}$$

where we have used the identity $k! = \Gamma(k + 1)$ for non-negative integral k. We see that $J_0(x)$ is an *even* function, *i.e.*, $J_0(x) = J_0(-x)$, because the sum involves only even powers of x. Clearly then

[2] This equation appears in many problems involving waves constrained to circular boundaries. Such problems arise in such fields as elasticity, fluid flow, electrical field theory, and aerodynamics.

$J_0(x)$ is defined, according to Equation 3, for $x < 0$. In fact, $J_\nu(x)$ is well-defined (by Equation 3) for negative values of x wherever ν is integral.

This would seem to give us a reason to allow at least some of the cylindrical Bessel functions to be defined for $x < 0$.

We note that [Bro03c] states, for each of the cylindrical Bessel functions, "A domain error may occur if x is less than zero." This statement was chosen to allow the implementer freedom to choose a solution to this problem according to the implementor's best estimate of the client's needs.

After several discussions with committee members and other colleagues on this issue, we no longer believe it benefits the users to permit such latitude. Thus we believe the committee must resolve such issues. There are thirteen instances of "domain error may occur" in [Bro03c], which is also the language in the current draft of TR1. In order to remove these, we need to evaluate each one. But before we can evaluate each function, we must first have a guiding principle by which we will make the decisions.

In the next section, we discuss the several options which seem possible.

4 Three Philosophies

We see three broadly different sets of guidelines, or philosophies, according to which the decisions regarding the definition of domain errors could be made. These three philosophies may be characterized as:

- follow the specifications in [ISO92];
- define the functions broadly, *i.e.*, wherever *mathematically possible*;
- define the functions where *natural*.

Let us consider each of these possibilities.

4.1 Follow ISO 31:1992(E)

The accepted proposal [Bro03c] refers to [ISO92] as the defining source for the set of functions to be included in the Standard. It may seem reasonable, therefore, also to rely on [ISO92] for the actual definitions of the functions. We believe this to be untenable, as the following examples demonstrate.

The special functions are listed in Table 14 of [ISO92]. The first function listed is the cylindrical Bessel function of the first kind, denoted there as $J_\ell(x)$, with the definition:

$$J_\ell(x) = \sum_{k=0}^{\infty} \frac{(-1)^k \, (x/2)^{\ell+2k}}{k! \, \Gamma(\ell+k+1)} \qquad \ell \geq 0. \tag{5}$$

Note especially the explicit domain of the index, $\ell \geq 0$.

There is already a fatal flaw in this definition; the general solution to Bessel's equation (Equation 2, where we use ℓ rather than ν as the index), for non-integral values of ℓ, is[3]:

$$y(x) = AJ_\ell(x) + BJ_{-\ell}(x), \tag{6}$$

where A and B are constants to be determined by the boundary conditions of the problem being solved. This solution shows the immediate, and critical, problem with the definition of $J_\ell(x)$ in

[3]Consult almost any text on differential equations for the solution of Bessel's equation, *e.g.*, [Hil76].

[ISO92]: the specified domain of the index excludes the negative values of ℓ which are *necessary* for evaluation of the solution of the very equation the Bessel functions solve!

The problems continue with the very next definition in [ISO92]:

$$N_\ell(x) = \lim_{k\to\ell} \frac{J_k(x)\,\cos(k\pi) - J_{-k}(x)}{\sin(k\pi)}. \tag{7}$$

We note that either k or $-k$ must be negative when $k \neq 0$, and so either $J_k(x)$ or $J_{-k}(x)$ is undefined, according to Equation 5.

Other definitions in [ISO92] exhibit similar, and additional, problems. It seems clear that we can not make use of the formulations given for these functions in [ISO92].

4.2 Maximally Broad Definitions

Choosing the maximally general definition of each function has the advantage of providing the greatest degree of support for the users. This seems a considerable advantage. However, we believe this philosophy is also untenable.

The mathematical literature often deals with these functions as complex-valued functions of complex arguments. [Bro03c] was intentionally limited to deal only with real-valued functions of real arguments, and so much of the generality found in the mathematical literature is inapplicable.

Furthermore, different authors define extensions of the various functions included in [Bro03c] in different manners. Were we to accept this as our guiding philosophy, we would still need guidelines for choosing among the available extensions for several functions.

Finally, we believe that choosing the maximally general formulation for each function significantly increases the difficulty of implementation. It is not clear there is much, if any, concrete gain to the users from this extra work.

4.3 Natural Definitions

We prefer to define the functions where *natural*. Perhaps this seems to beg the question—who defines what is natural?

To answer this question, it is important to note that all of the functions described in [Bro03c] arise from the solution of some differential or integral equation, *e.g.*, the cylindrical Bessel functions appear in the solutions of Equation 2. In these cases, it is often possible to identify, from the equation itself, what is the natural domain of the function.

Since each function appears in the context of the solution of a differential or integral equation, we believe that *most* of the user community will have *most* of their needs for these functions met if we define the domains of the functions according to this guideline:

Guideline 3 *The definition of each special function, including its domain, should be determined by the natural areas of application of that function. In most cases, this is determined by the differential or integral equation to which the function is a solution, and the physical context in which the equation appears.*

5 A Review of All Special Functions

In this section, we review each of the special functions in [Aus04] in light of our recommended Guideline 3. The headings of the subsections below give the function names and the section number in [Aus04] where the function synopsis is given.

5.1 associated Laguerre polynomials (5.2.1.1)

[Aus04] states:

> **Effects**: These functions compute the associated Laguerre functions of their respective arguments n, m, and x.
>
> **Returns**: The associated Laguerre functions return
>
> $$L_n^m(x) = e^x \frac{d^m}{dx^m} L_n(x). \tag{8}$$

As will be discussed in Section 5.18, n must be a non-negative integer and $x \geq 0$. Further, m must also be a non-negative integer since it corresponds to the order of the derivative in Equation 8.

5.2 associated Legendre functions (5.2.1.2)

[Aus04] states:

> **Effects**: These functions compute the associated Legendre functions of their respective arguments l, m, and x. A domain error occurs if m is greater than l. A domain error may occur if the magnitude of x is greater than one.
>
> **Returns**: The assoc_legendre functions return
>
> $$P_\ell^m(x) = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x). \tag{9}$$

As will be discussed in Section 5.19, ℓ must be a non-negative integer and $x \geq 0$. Further, m must also be a non-negative integer since it corresponds to the order of the derivative in Equation 9.

5.3 beta function (5.2.1.3)

[Aus04] states:

> **Effects**: These functions compute the beta function of their respective arguments x and y. A domain error may occur (a) if either x or y is a negative integer, or (b) if either x or y is zero.
>
> **Returns**: The beta functions return
>
> $$B(x,y) = \frac{\Gamma(x)\,\Gamma(y)}{\Gamma(x+y)}.$$

§3.1 and §A describe the domain of the beta function. The specification of the domain in [Aus04] is unnecessary. We believe there is no reason to mandate that the library function signal a domain error for any argument for which the mathematical function is defined and is real-valued, so we believe that *no* explicit specification of domain errors is needed.

5.4 (complete) elliptic integral of the first kind (5.2.1.4)

[Aus04] states:

> **Effects**; These functions compute the complete elliptic integral of the first kind of their respective arguments k. A domain error occurs if the magnitude of k is greater than one.
>
> **Returns**: The complete elliptic integrals of the first kind return
>
> $$K(k) = F(k, \pi/2) = \int_0^{\pi/2} \frac{d\vartheta}{\sqrt{1 - k^2 \sin^2 \vartheta}}.$$

We note that if $|k| > 1$ the value of the integral is complex. Thus, according to Guideline 2, for $|k| > 1$ a domain error must occur. Because this is implicit in the equation, there is no need to specify a domain error in the **Effects** clause.

5.5 (complete) elliptic integral of the second kind (5.2.1.5)

[Aus04] states:

> **Effects**; These functions compute the complete elliptic integral of the second kind of their respective arguments k. A domain error occurs if the magnitude of k is greater than one.
>
> **Returns**: The complete elliptic integrals of the second kind return
>
> $$E(k, \pi/2) = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2 \vartheta}\, d\vartheta.$$

We note that if $|k| > 1$, the value of the integral is complex. Thus, according to Guideline 2, for $|k| > 1$ a domain error must occur. Because this is implicit in the equation, there is no need to specify a domain error in the **Effects** clause.

5.6 (complete) elliptic integral of the third kind (5.2.1.6)

[Aus04] states:

> **Effects**; These functions compute the complete elliptic integral of the third kind of their respective arguments k and ν. A domain error occurs if the magnitude of k is greater than one.
>
> **Returns**: The complete elliptic integrals of the third kind return
>
> $$\Pi(\nu, k, \pi/2) = \int_0^{\pi/2} \frac{d\vartheta}{(1 - \nu \sin^2 \vartheta)\sqrt{1 - k^2 \sin^2 \vartheta}}.$$

We note that if $|k| > 1$ the value of the integral is complex. Thus, according to Guideline 2, for $|k| > 1$ a domain error must occur. Because this is implicit in the equation, there is no need to specify a domain error in the **Effects** clause.

5.7 confluent hypergeometric functions (5.2.1.7)

[Aus04] states:

> **Effects**: These functions compute the confluent hypergeometric functions of their respective arguments a, c, and x. A domain error occurs (a) if c is a negative integer, or (b) if c is zero.
>
> **Returns**: The confluent hypergeometric functions return
>
> $$F(a;c;x) = \frac{\Gamma(c)}{\Gamma(a)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(c+n)} \frac{x^n}{n!}.$$

The specification of the domain in [Aus04] is unnecessary. We believe there is no reason to mandate that the library function signal a domain error for any argument for which the mathematical function is defined and is real-valued, so we believe that *no* explicit specification of domain errors is needed.

5.8 regular modified cylindrical Bessel functions (5.2.1.8)

[Aus04] states:

> **Effects**: These functions compute the regular modified cylindrical Bessel functions of their respective arguments nu and x. A domain error may occur if x is less than zero.
> **Returns**: The regular modified cylindrical Bessel functions return
>
> $$I_\nu(x) = i^{-\nu} J_\nu(ix) = \sum_{k=0}^{\infty} \frac{(x/2)^{\nu+2k}}{k!\Gamma(\nu+k+1)}.$$

As was discussed in some detail in Section , these functions are mathematically defined when $x < 0$ but little is gained by implementing them there since doing so is unnatural in the sense of Guideline 3. In that spirit, we propose that their implementation be explicitly restricted to the domain $x \geq 0$. We note here that this same logic applies to all of the cylindrical Bessel functions since they are all variations on solutions of the same differential equation. Indeed, the same may be said of the spherical Bessel functions as well after realizing that the x argument for them corresponds to the radius variable in spherical coordinates rather than in cylindrical coordinates. Negative radii are equally unnatural in both cases. We further note that all of this is independent of ν in both the cylindrical and spherical case.

5.9 cylindrical Bessel functions (of the first kind) (5.2.1.9)

[Aus04] states:

> **Effects**: These functions compute the cylindrical Bessel functions (of the first kind) of their respective arguments nu and x. A domain error may occur if x is less than zero.

> **Returns**: The cylindrical Bessel functions (of the first kind) return
>
> $$J_\nu(x) = \sum_{k=0}^{\infty} \frac{(-1)^k (x/2)^{\nu+2k}}{k!\Gamma(\nu+k+1)}.$$

Implementing these functions for $x < 0$ is unnatural in the sense of Guideline 3. Hence, we propose that x be explicitly restricted to the domain $x \geq 0$.

5.10 irregular modified cylindrical Bessel functions (5.2.1.10)

[Aus04] states:

> **Effects**: These functions compute the irregular modified cylindrical Bessel functions of their respective arguments nu and x. A domain error may occur if x is less than zero.
>
> **Returns**: The irregular modified cylindrical Bessel functions return
>
> $$K_\nu(x) = (\pi/2)i^{\nu+1}(J_\nu(ix) + iN_n u(ix))$$
>
> or, equivalently
>
> $$K_\nu(x) = \begin{cases} \frac{\pi}{2} \frac{I_{-\nu}(x) - I_\nu(x)}{\sin \nu\pi} & \text{for non-integral } \nu \\ \frac{\pi}{2} \lim_{\mu\to\nu} \frac{I_{-\mu}(x) - I_\mu(x)}{\sin \mu\pi} & \text{for integral } \nu \end{cases}.$$

Implementing these functions for $x < 0$ is unnatural in the sense of Guideline 3. Hence, we propose that x be explicitly restricted to the domain $x \geq 0$.

5.11 cylindrical Neumann functions (5.2.1.11)

[Aus04] states:

> **Effects**: These functions compute the cylindrical Neumann functions, also known as the cylindrical Bessel functions of the second kind, of their respective arguments nu, and x. A domain error may occur if x is less than zero.
>
> **Returns**: The cylindrical Neumann functions return
>
> $$N_\nu(x) = \begin{cases} \frac{J_{-\nu}(x)\cos\nu\pi - J_\nu(x)}{\sin\nu\pi} & \text{for non-integral } \nu \\ \lim_{\mu\to\nu} \frac{J_{-\mu}(x)\cos\mu\pi - J_\mu(x)}{\sin\mu\pi} & \text{for integral } \nu \end{cases}.$$

Implementing these functions for $x < 0$ is unnatural in the sense of Guideline 3. Hence, we propose that x be explicitly restricted to the domain $x \geq 0$.

5.12 (incomplete) elliptic integral of the first kind (5.2.1.12)

[Aus04] states:

> **Effects**; These functions compute the incomplete elliptic integral of the first kind of their respective arguments k and φ. A domain error occurs if the magnitude of k is greater than one.
>
> **Returns**: The incomplete elliptic integrals of the first kind return
>
> $$F(k, \varphi) = \int_0^{\varphi} \frac{d\vartheta}{\sqrt{1 - k^2 \sin^2 \vartheta}}.$$

In the discussion (Section 5.4) of the complete elliptic integral of the first kind, we noted that if $|k| > 1$, the value of the function is complex. For the *incomplete* elliptic integral of the first kind, the situation is more complicated. While the incomplete elliptic integral is complex for non-zero φ and $|k| > 1$, the incomplete elliptic integral is 0 when $\varphi = 0$, regardless of the value of k. Nonetheless, we believe it is *natural* to restrict the domain of this function to $|k| \leq 1$.

We note that one generally first encounters this integral in the study of the simple pendulum in elementary physics. There, the parameter k has a physical interpretation as $\sin \vartheta_0/2$, where ϑ_0 is the magnitude of the initial displacement of the pendulum. With that understanding, it is entirely reasonable to limit $|k| \leq 1$.

5.13 (incomplete) elliptic integral of the second kind (5.2.1.13)

[Aus04] states:

> **Effects**; These functions compute the incomplete elliptic integral of the second kind of their respective arguments k and φ. A domain error occurs if the magnitude of k is greater than one.
>
> **Returns**: The incomplete elliptic integrals of the second kind return
>
> $$E(k, \varphi) = \int_0^{\varphi} \sqrt{1 - k^2 \sin^2 \vartheta} d\vartheta.$$

In the discussion (Section 5.5) of the complete elliptic integral of the second kind, we noted that if $|k| > 1$, the value of the function is complex. For the *incomplete* elliptic integral of the second kind, the situation is more complicated. While the incomplete elliptic integral is complex for non-zero φ and $|k| > 1$, the incomplete elliptic integral is 0 when $\varphi = 0$, regardless of the value of k. Nonetheless, we believe it is *natural* to restrict the domain of this function to $|k| \leq 1$.

Similar to Section 5.12, the parameter k has a physical interpretation as the $\sin$ of a real angle. Consequently, it is still reasonable to limit $|k|$ to be less than or equal to 1.

5.14 (incomplete) elliptic integral of the third kind (5.2.1.14)

[Aus04] states:

> **Effects**; These functions compute the incomplete elliptic integral of the third kind of their respective arguments k, ν and φ. A domain error occurs if the magnitude of k is greater than one.
>
> **Returns**: The complete elliptic integrals of the third kind return
>
> $$\Pi(\nu, k, \varphi) = \int_0^{\varphi} \frac{d\vartheta}{(1 - \nu \sin^2 \vartheta)\sqrt{1 - k^2 \sin^2 \vartheta}}.$$

In the discussion (Section 5.6) of the complete elliptic integral of the third kind, we noted that if $|k| > 1$, the value of the function is complex. For the *incomplete* elliptic integral of the third kind, the situation is more complicated. While the incomplete elliptic integral is complex for non-zero φ and $|k| > 1$, the incomplete elliptic integral is 0 when $\varphi = 0$, regardless of the value of k. Nonetheless, we believe it is *natural* to restrict the domain of this function to $|k| \le 1$.

Similar to Section 5.12, the parameter k has a physical interpretation as the $\sin$ of a real angle. Consequently, it is still reasonable to limit $|k|$ to be less than or equal to 1.

5.15 exponential integral (5.2.1.15)

[Aus04] states:

> **Effects**: These functions compute the exponential integral of their respective arguments x.
>
> **Returns**: The exponential integral functions return
>
> $$Ei(x) = \int_{-x}^{\infty} \frac{e^{-t}}{t} dt.$$

Since this function is well behaved for all x, nothing more needs to be said.

5.16 Hermite polynomials (5.2.1.16)

[Aus04] states:

> **Effects**: These functions compute the Hermite polynomials of their respective arguments n and x.
>
> **Returns**: The Hermite functions return
>
> $$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{10}$$

n must be a non-negative integer since it corresponds to the order of the derivative in Equation 10. Since these functions are well behaved for all x, nothing more needs to be said.

5.17 hypergeometric functions (5.2.1.17)

[Aus04] states:

> **Effects**: These functions compute the hypergeometric functions of their respective arguments, a, b, c, and x. A domain error may occur if the magnitude of x is greater than or equal to one.
>
> **Returns**: The hypergeometric functions return
>
> $$F(a, b; c; x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{x^n}{n!}$$

The specification of the domain in [Aus04] is unnecessary. We believe there is no reason to mandate that the library function signal a domain error for any argument for which the mathematical function is defined and is real-valued, so we believe that *no* explicit specification of domain errors is needed.

5.18 Laguerre polynomials (5.2.1.18)

[Aus04] states:

> **Effects**: These functions compute the Laguerre polynomials of their respective arguments n and x.
>
> **Returns**; The Laguerre functions return
>
> $$L_n(x) = e^x \frac{d^n}{dx^n}(x^n e^{-x}).$$

The Laguerre functions are the solutions to Laguerre's equation:

$$x\frac{d^2y}{dx^2} + (1-x)\frac{dy}{dx} + ny = 0. \tag{11}$$

Laguerre polynomials are Laguerre functions for which n is a non-negative integer.

Equation 11 appears in the solution of problems expressed in spherical coordinates, in which x represents the radius. Implementing these functions for $x < 0$ is unnatural in the sense of Guideline 3. Hence, we propose that x be explicitly restricted to the domain $x \geq 0$.

5.19 Legendre polynomials (5.2.1.19)

[Aus04] states:

> **Effects**: These functions compute the Legendre polynomials of their respective arguments l and x. A domain error may occur if the magnitude of x is greater than one.
>
> **Returns**; The Legendre functions return
>
> $$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l.$$

The Legendre functions, $P_\ell(x)$, appear in the solution of the potential equation (Laplace's equation) in spherical coordinates, in cases with azimuthal symmetry. There we encounter the differential equation

$$\frac{d}{dx}\left[(1-x^2)\frac{dF}{dx}\right] + \ell(\ell+1)\,F = 0 \qquad x = \cos\vartheta \text{ and } 0 \leq \vartheta \leq \pi, \tag{12}$$

where ϑ represents the polar angle of the spherical coordinate system, which ranges from 0 at the "north pole" to π at the "south pole." Thus in common use, we find x limited to the interval $-1 \leq x \leq 1$.

Legendre polynomials are Legendre functions for which ℓ is a non-negative integer. A feature that sets these particular polynomials apart from most others is that they form a complete set of orthonormal functions over the interval $[-1, 1]$.

5.20 Riemann zeta function (5.2.1.20)

[Aus04] states:

Effects: These functions compute the Riemann zeta function of their respective arguments x. A domain error occurs if x is equal to one.

Returns; The Riemann zeta functions return

$$\zeta(x) = \begin{cases} \sum_{k=1}^{\infty} k^{-x} & \text{for } x > 1 \\ 2^x \pi^{x-1} \sin(\frac{\pi x}{2}) \Gamma(1-x) \zeta(1-x) & \text{for } x < 1 \end{cases} .$$

The value of the Riemann zeta function at $x = 1$ is undefined because the limits from the two directions do not agree. Thus the library function should signal a domain error at that value of x, by our Guideline 1. We believe there is no reason to mandate that the library function signal a domain error for any argument for which the mathematical function is defined and is real-valued, so we believe that *no* explicit specification of domain errors is needed.

5.21 spherical Bessel functions (of the first kind) (5.2.1.21)

[Aus04] states:

Effects: These functions compute the spherical Bessel functions of the first kind of their respective arguments n and x. A domain error may occur if x is less than zero.

Returns: The spherical Bessel functions return

$$j_n(x) = (\pi/2x)^{1/2} J_{n+1/2}(x).$$

Implementing these functions for $x < 0$ is unnatural in the sense of Guideline 3. Hence, we propose that x be explicitly restricted to the domain $x \geq 0$.

5.22 spherical associated Legendre functions (5.2.1.22)

[Aus04] states:

Effects: These functions compute the spherical associated Legendre functions of their respective arguments l, m and ϑ. A domain error may occur if the magnitude of m is greater than l.

Returns: The associated spherical Legendre functions return

$$Y_l^m(\vartheta, 0)$$

where

$$Y_l^m(\vartheta, \varphi) = (-1)^m \left[\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_l^m(\cos\vartheta) e^{im\varphi}.$$

These functions appear in the solution of Laplace's equation in problems involving spherical symmetries. In such problems, the solutions require $|m| \leq \ell$; hence, by Guideline 3, we propose m be explicitly restricted to $|m| \leq \ell$.

5.23 spherical Neumann functions (5.2.1.23)

[Aus04] states:

Effects: These functions compute the spherical Neumann functions, also known as the spherical Bessel functions of the second kind, of their respective arguments n and x. A domain error may occur if x is less than zero.

Returns; The spherical Neumann functions return

$$n_n(x) = (\pi/2x)^{1/2} N_{n+1/2}(x).$$

Implementing these functions for $x < 0$ is unnatural in the sense of Guideline 3. Hence, we propose that x be explicitly restricted to the domain $x \geq 0$.

6 Consideration of C99

One of our goals in revising §5.2 of TR-1 is to retain, or improve if possible, the degree of compatibility with the C language that was an explicit goal of the original proposals. The C99 standard [ISO99] includes a description of error handling that differs significantly from that of C89 [ISO90]. The published rationale describes the reasons for these changes. We believe that the liaison group should provide a recommendation for how domain errors should be signaled by functions in this library.

7 Impact on Notation

Guideline 1 states when a library function shall signal a domain error. In this section, we take up the question of how to express the domain of the mathematical functions.

We have also chosen, in Guideline 3, the rule by which we will select the formulation of the mathematical functions. What is still left to be specified is the expository form for the presentation of the domain.

Because of the language in Guideline 1, we believe the clearest exposition is to specify the domain of the function explicitly, *in the definition of the function itself*, as a qualification on the values of the arguments of the mathematical function. For example, we propose that the definition of the cylindrical Bessel function of the first kind be:

$$J_\nu(x) = \sum_{k=0}^{\infty} \frac{(-1)^k \, (x/2)^{\nu+2k}}{k! \, \Gamma(\nu+k+1)} \qquad \text{where} \qquad 0 \leq x \leq \infty \ . \tag{13}$$

We note that, because the allowed values of ν are not restricted, that all values obtainable by the corresponding `double` parameter are implicitly allowed.

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A A Brief Analysis of Euler's Gamma and Beta Functions

In this Appendix, we present a few facts about the gamma and beta functions which are useful in reasoning about their behaviors.

The gamma function $\Gamma(x)$ has poles at $x = -n$, for $n = 0, 1, 2, \ldots$. [AS74, §6.1.3]. The function is discontinuous at these points; it approaches $+\infty$ as one approaches the pole from one direction, and $-\infty$ as one approaches the pole from the other direction. Thus $\Gamma(x)$ is *undefined* for these values of x.

A few features of the gamma function will turn out to be useful in analyzing related functions. The most important are the recurrence relationship:

$$\Gamma(x+1) = x\Gamma(x), \tag{14}$$

and the Taylor expansion around zero, showing the structure of the pole at zero [SO87, §43:6:1]:

$$\lim_{x\to 0} \Gamma(x) = \frac{1}{x} + \gamma + \frac{6\gamma^2 + \pi^2}{12}\, x + \mathcal{O}(x^2), \tag{15}$$

where the symbol γ represents *Euler's constant*, $\gamma \approx 0.577215665$.

Using Equations 14 and 15, we can derive the expansion for the $\Gamma(x)$ near one of the poles, *e.g.*, $x = -5$, yielding:

$$\Gamma(-5+\varepsilon) \approx -\frac{1}{120\varepsilon} + \frac{60\gamma - 137}{7200} + \frac{(1800\gamma^2 - 8220\gamma + 300\pi^2 + 12019)\,\varepsilon}{432000} + \mathcal{O}(x^2), \tag{16}$$

where $|\varepsilon| \ll 1$. For ε near 0 (and thus for x near -5), the first term dominates. And so we see that $\Gamma(x)$ has a pole at $x = -5$, with the the function approaching a different limit as one approaches -5 from above than the limiting value when $x = -5$ is approached from below.

To investigate the pathologies of the beta function, we have to consider all the locations in the (x, y) plane where any of $\Gamma(x)$, $\Gamma(y)$ or $\Gamma(x+y)$ has a pole, and we have to note the structure of the pole. Since $\Gamma(x)$ has poles only for integral $x \leq 0$, the only possible problems is when one or both of x and y is a non-positive integer. The behavior is most easily summarized by noting whether or not the sum $x + y$ is also positive, negative, or zero.[4]

Table 1 describes the behavior of $B(x, y)$ for the "suspicious" values of x, y, and $x + y$. In this table, the notation $-$ indicates that the quantity in that column is 0 or a negative integer; a $+$ indicates that the quantity is *not* one of these values—it may be non-integral, or a positive integer. Also provided is an example (x, y) point that falls in each category; where the value of the function is defined, the value for the example point is also given.

Table 1: Behavior of $B(x, y)$; see the text for explanation of notations.

x	y	$x+y$	example	$B(x,y)$
$+$	$+$	$+$	(2,1)	defined (0.5)
$+$	$+$	$-$	(-0.4, -0.6)	0
$+$	$-$	$+$	(3,-1)	undefined
$+$	$-$	$-$	(1,-2)	defined (-1/2)
$-$	$+$	$+$	(-1,3)	undefined
$-$	$+$	$-$	(-2,1)	defined (-1/2)
$-$	$-$	$+$	can not happen	NA
$-$	$-$	$-$	(-1,-1)	undefined

[4] Determination of this behavior requires study of the Taylor expansion of the beta function, which can be determined from Equations 1 and 15. The details are beyond the scope of this note. We present only the results of such analysis.

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