Not-Quite-Transcendental Functions and their Applications

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ABSTRACT

Transcendental functions, such as exponentials and logarithms, appear in a broad array of computational domains: from simulations in curvilinear coordinates, to interpolation, to machine learning. Unfortunately they are typically expensive to compute accurately. In this note, we argue that in many cases, the properties of the function matters more than the exact functional form. We present new functions, which are not transcendental, that can be used as drop-in replacements for the exponential and logarithm in many settings for a significant performance boost. We show that for certain applications using these functions result in no drop in the accuracy at all, as they are perfectly accurate representations of themselves, if not the original transcendental functions.

1. Introduction

A transcendental function cannot be expressed as a finite series of algebraic operations—in other words, it transcends algebra (Townsend, 1915). The implementation of a transcendental function on a computer, thus, typically relies on a computationally expensive finite truncation of an infinite series, with sufficiently many terms chosen to satisfy a required precision (Cody and Waite, 1980). Unfortunately, transcendental functions, such as exponentials, logarithms, and trigonometric functions, are ubiquitous in mathematics, science, and engineering, making them a necessary evil in computational science. This ubiquity has lead to a plethora of approaches in both hardware and software for accelerating the approximate calculation of transcendental functions stretching back decades (Marino, 1972; Perini and Reitz, 2018). Approximations carry with them a cost in accuracy, which must be accounted for.

However, there are several settings where transcendental functions are used where what matters is the properties of the function, rather than its precise, transcendental nature. We therefore propose that, in these settings, one may replace certain transcendental functions with non-transcendental functions that look like the original functions but are easier to compute. We call these functions not-quite transcendental (NQT). NQT functions are not necessarily approximations to transcendental functions, although they may be (and have broadly been) applied that way. Rather they are exact functional representations of themselves that share desirable properties of a given transcendental function.

In the remainder of this note, we cover several case studies where NQT functions may be applied with no loss of accuracy instead of the traditionally used transcendental function: coordinate transformations, logarithmic interpolation, activation functions in neural networks; and maximum likelihood estimation. We use the first case study to introduce the NQT functions we will study—exponentials, logarithms, and hyperbolic functions. After the case studies we present performance and accuracy results, before offering a few concluding thoughts.

2. First Case Study: Coordinate Transformations

Consider a problem with large dynamic range. For example, in simulations of the in-spiral and merger of two neutron stars, as observed by the LIGO-VIRGO gravitational wave interferometers (Abbott et al., 2017), dynamics occur at a length scale of a few tens of kilometers, but gravitational waves must be extracted from a simulation in the far zone, perhaps thousands of kilometers away from the binary. Models of the accretion disk around the supermassive black hole at the center of our galaxy—as recently dramatically observed by the Event Horizon Telescope (Akiyama et al., 2022)—suffer a similar difficulty. Dynamics happens on relatively short length scales, near the event horizon, but boundary conditions are only known far from the black hole. This difficulty appears commonly in astrophysics but extends to applications as far ranging as quantum chemistry; The primary modes of the radial component of electron
wavefunctions in an atom occur at roughly a Bohr radius, however, the wavefunctions are normalized via an integral extending over all space (Grant, 2007).

One way of capturing this dynamic range is through adaptive mesh refinement (Berger and Oliger, 1984) or a non-uniform grid. Another approach, however, is to apply a coordinate transformation. A spherical simulation grid with grid spacing growing exponentially in radius may be implemented by defining a new coordinate,

\[ \tilde{r} = \ln(r) \]  

(1)

and writing the governing equations in terms of \( \tilde{r} \) rather than \( r \). This is exactly the approach taken in the vast majority of simulation codes used by the Event Horizon Telescope team (McKinney and Gammie, 2004). One may even bring the entire real number line to finite grid coordinates by using a transformation such as \( \tilde{x} = \tanh(x) \) so that a physically infinite distance has a coordinate value of \( \pm 1 \). Such was the approach taken by the first simulation of a full orbit of a binary black hole system (Pretorius, 2005). However, what matters in equation (1) is not that a logarithm is used. Rather the important property of the transformation is that it is \emph{approximately} logarithmic—that derivatives of the transformation scale roughly inversely with \( r \), so that the physical grid spacing roughly scales with \( r \). We now introduce the NQT function that meets these needs.

3. The Not-Quite-Transcendental Functions for Logarithms and Exponentials

We begin with the well-known exploit of the construction of a floating point number. A positive floating point number \( n \) is internally represented as \( n = m \times 2^p \), where \( m \in (0, 1/2) \) is the mantissa and the integer \( p \) is the exponent. Most programming languages and hardware vendors provide the ability to pull apart \( n \) into its components, \( m \) and \( p \). This implies that

\[ \lg(n) = \lg(m) + p \]  

(2)

which reduces the standard problem of computing a logarithm to computing \( \lg(m) \) on the interval \([0, 1/2)\). Change of basis formulae can then move from \( \lg \) to whatever logarithmic basis is appropriate.

We define the NQT function

\[ \lg_{\text{NQT}}(n) = 2(m-1) + p, \]  

(3)

which is both continuous and differentiable (i.e., \( C^1 \)). As observed in Hall, Lynch and Dwyer (1970), this function can be interpreted as a piecewise-linear interpolation of \( \lg(x) \), however we treat it as an independent function in its own right. Moreover, it is exactly invertible by simply finding \( m \) and \( p \) and computing \( m \times 2^p \). We define this inverse function as \( \text{pow}_{\text{NQT}}(x) \). Multiplication by a constant value is all that is required to convert these functions to NQT versions of \( \log_{10}(x) \) and \( 10^x \). One can further optimize the implementation of these NQT functions via so-called \emph{integer aliasing}, as described in, e.g., Blinn (1997).

Hyperbolic functions and their inverses are composed of sums and products of exponentials and logarithms, and so NQT hyperbolic functions can be constructed by sums and products of NQT logs and exponents. NQT hyperbolic tangent, for example, is given by \( \tanh_{\text{NQT}}(x) = \left( e^{2x_{\text{NQT}}} - 1 \right) / \left( e^{2x_{\text{NQT}}} + 1 \right) \), where \( e^{x_{\text{NQT}}} \) is the NQT counterpart of the natural exponential function.

\( \lg_{\text{NQT}} \) and \( \text{pow}_{\text{NQT}} \) are \emph{compatible} with commonly used low-accuracy approximations of \( \lg(x) \) and \( 2^x \)—indeed they coincide with their transcendental counterparts to a few percent. However we emphasize that they are not approximations in this context. If we deliberately define a coordinate transformation given by \( \tilde{r} = \lg_{\text{NQT}}(r) \), that transformation is exact and exactly invertible. No accuracy is lost in a simulation that uses NQT log coordinates compared to a simulation that uses truly logarithmic coordinates.\(^1\)

4. Second Case Study: Logarithmic Interpolation

Tabulated data often spans many orders of magnitude. Nuclear reaction rates used in astrophysics are infamous in this regard (Meisel, 2008). Equations of state for real materials such as iron and steel are another common example

\(^1\)We note that because these functions are only \( C^1 \) they may not be appropriate for coordinate transformations if a very high-order numerical method, such as a spectral method is used, as smoother (in the formal sense) functions may be required for good convergence.
A common approach is to apply a logarithmic coordinate transformation, as described in Section 2, to the independent and/or dependent variable. This results in log-log or log-linear interpolation. As with Section 2 above, the key is not that the interpolation grid be exactly logarithmic. Rather the defining trait is that the transformed interpolation grid can cover many orders of magnitude such that the relative interpolation error remains roughly constant. And as with Section 2 the NQT counterparts to the logarithm and exponential functions satisfy these criteria exactly—often better than their transcendental counterparts.

5. Third Case Study: Activation Functions

A neural network is built on two core components: a linear operation typically implemented as matrix multiplication, and a nonlinear operation, called an activation function (Goodfellow, Bengio and Courville, 2016). Common activation functions include the rectified linear unit (RELU) and the hyperbolic tangent. The important properties of an activation function are that it is: (a) nonlinear and (b) differentiable.

In the case of the hyperbolic tangent activation function, the exact functional form matters less than the above key points, as well as the ability to span the range $(-1, 1)$ with a non-vanishing derivative. Activation functions are also ideally easy to implement and cheap to compute. The NQT tangent function meets these criteria.

6. Fourth Case Study: Maximum Likelihood Estimation

In probability theory one often wishes to compute the outcome that is most probable. This procedure is called maximum likelihood estimation. For some set of $N$ independent random variables $x_1, \ldots, x_N$ with probability density functions $p_1(x_1) \ldots p_N(x_N)$, this procedure amounts to finding the vector $(x_1, \ldots, x_N)$ that maximizes the product $\prod_{i=1}^N p_i(x_i)$. Most probability density functions are logarithmically concave, making it convenient to transform this optimization problem to maximize (Millar, 2011) $\ln(\prod_{i=1}^N p_i(x_i))$. Here the important property of $\ln$ is that it is monotone and approximately logarithmic, which the NQT log is.

Traditionally these calculations leverage the transitive property of logs that $\ln(xy) = \ln(x) + \ln(y)$. Unfortunately, our NQT functions are only approximately transitive, and so this transformation can not necessarily be applied. That said, for MLE estimation, if the argmax of $\sum_i \ln_{NQT} p(x_i)$ is the same as the argmax of $\ln_{NQT}(\prod p(x_i))$, then one can leverage transitivity.

7. Performance Experiments

To investigate the performance of our NQT functions, we compare them to the standard library (STL) implementations of their transcendental counterparts in Table 1. We examine three relevant functions: $f(x) = 10^x$, $f(x) = \log_{10}(x)$, and $f(x) = \tanh(x)$. Timings in Table 1 are shown in nanoseconds per point, where we use a sufficiently large grid to saturate the target hardware. We run on an Nvidia V100 GPU as well as an Intel Xeon Gold 6254 CPU. In the latter case, we ran our tests with both GNU and Intel compilers.

Broadly we find significant speedups across the board, with the largest speedup being more than a factor of 8x for the exponential on Cascade lake with the intel compiler. We find the least impressive speedups for $\tanh(x)$, perhaps because it has received vendor attention due to application in machine learning. Nevertheless, speedups are at least 1.2x on the V100 and much larger on the Skylake.

8. Concluding Thoughts

In this short note, we introduce the not-quite-transcendental counterparts to exponential, logarithmic, and hyperbolic transcendental functions. We show that for several common problems in computational science, transcendental functions are used because of several desirable properties, but the exact form of the function does not matter. Therefore, using the not-quite-transcendental counterpart offers a performance improvement for no accuracy cost. In our numerical experiments we find perfect invertability of our NQT functions and a speedup over their transcendental counterparts as high as 8.2x.

In future work, it would be interesting to find not-quite-transcendental counterparts to trigonometric functions. However, we expect that trigonometric functions are more often required exactly and thus fewer applications for not-quite-transcendental versions would be available.
Table 1
Performance Comparison Between standard library (STL) implementations of transcendental functions and our implementations of their not-quite-transcendental (NQT) counterparts. Timings are in nanoseconds per point, while speedups are the performance improvement of the NQT implementation over the STL implementation. Calculation was performed on a sufficiently large vector to saturate the hardware. The V100 calculation was performed with cuda 11.4.2 with the GCC backend using GCC 9.4.0. The cascade lake calculation was performed with either GCC 9.4.0 or with the Intel 19.0.5 compiler as annotated. The CPU was an Intel Xeon Gold 6254.

| Architecture     | STL | NQT | Speedup | STL | NQT | Speedup | STL | NQT | Speedup |
|------------------|-----|-----|---------|-----|-----|---------|-----|-----|---------|
| Volta V100       | 2.7e-2 | 5.7e-3 | 4.7   | 1.2e-2 | 5.7e-3 | 2.0   | 7.8e-3 | 6.3e-3 | 1.2     |
| Cascade Lake (gnu) | 5.8e+1 | 1.1e+1 | 5.1   | 3.1e+1 | 1.1e+4 | 2.7   | 3.4e+1 | 1.4e+1 | 2.2     |
| Cascade Lake (int) | 1.2e+1 | 1.4e+0 | 8.2   | 6.5e+0 | 1.3e+0 | 4.8   | 8.2e+0 | 1.9e+1 | 4.2     |

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