COMPUTING ACCURATE HORNER FORM APPROXIMATIONS TO SPECIAL FUNCTIONS IN FINITE PRECISION ARITHMETIC

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Abstract. In various applications, computers are required to compute approximations to univariate elementary and special functions such as exp and arctan to modest accuracy. This paper proposes a new heuristic for automating the design of such implementations. This heuristic takes a certain restricted specification of program structure and the desired error properties as input and takes explicit account of roundoff error during evaluation.

1. Introduction

Various programming language standards, such as the Java Language Specification [2] require that a certain set of elementary and special functions (in this paper simply “mathematical functions”) be provided for their native floating-point types and that their implementations are faithfully-rounded—that is, that they produce one of the two machine-representable numbers bracketing the exact, real-number value.

Projects such as LIBULTIM [20] and CRlibm [6] provide a wide array of correctly-rounded functions—that is, they always produce the closest machine-representable number to the exact function value. CRlibm provides correctly-rounded functions in all four rounding modes specified by the IEEE 754 floating-point arithmetic standard. The fdlibm library, developed by Sun, is a portable, widely-used math library that delivers faithfully-rounded results for a number of important functions.

LIBULTIM and CRlibm make extensive use of both of table lookups and of conditional branches in their function implementations. For most functions, the fdlibm library splits the function’s domain into several intervals and uses a different approximation on each interval.

If one wishes to compute the same mathematical function on several different inputs at once, it is natural to consider using the fast vector units that are widespread in modern computers. It is often difficult to achieve a significant speedup using a vector unit with code that is rich in table lookups and conditional branches since different entries of the vector can result in different table accesses or different code paths. In several models of processor power consumption, using a vector instruction in the place of a sequence of scalar instructions can also confer a significant power savings [18] [10].

Furthermore, mathematical function evaluation is responsible for a substantial fraction of execution time and power use in some applications. [10] gives a brief computational study of two applications in high-energy physics where faster but less accurate mathematical functions lead to physically acceptable results within a substantially shorter timeframe.

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Recent projects such as SLEEF [19] and Yeppp [7] provide general-purpose, fast, and reasonably accurate mathematical function implementations. These libraries allow a programmer to compute the same function applied to a vector of floating-point numbers considerably faster than by applying a traditional implementation to each element in sequence. The mathematical function implementations in these libraries consist of a simple argument reduction that is easy to vectorise, then a polynomial evaluation, then a reconstruction step that is also easy to vectorise. Both of these libraries focus on delivering results very quickly at the expense of a significantly weaker guarantee on the error between the delivered result and the mathematical result.

The work in this paper is motivated by a desire to improve the error bounds achievable within the algorithmic framework represented by SLEEF and Yeppp without sacrificing the speed of the resulting implementation.

Fundamental work on the problem of computing good machine approximations to functions has been done previously. I mention only the following two recent papers.

Brisebarre, Muller, and Tisserand [4] give an algorithm based on enumerating lattice points inside a polyhedron for finding the polynomial with machine-representable coefficients that best approximates, when evaluated in real arithmetic, a given function.

Brisebarre and Chevillard [3] give a heuristic based on lattice basis reduction for computing a polynomial with machine-representable coefficients that approximates a given function well when evaluated in real arithmetic.

2. Overview

This paper gives a heuristic that tries to find polynomials with machine-representable coefficients that approximate a given function well when evaluated in machine arithmetic. It takes as input a partially-specified straight-line program of fused multiply-adds (in a certain Horner-like form), an interval of interest, and a function that gives, for each machine-representable number in said interval, the range of acceptable function values. The heuristic either fails or produces as output a fully-specified straight-line program of fused multiply-adds that produces an acceptable function value for every machine-representable number in the specified interval.

The heuristic presented in this paper can be understood as a refinement of Brisebarre, Muller, and Tisserand’s polyhedral approach. Importantly, this heuristic accounts for round-off error that occurs while evaluating the function. Further, this heuristic can take explicit account of any argument-reduction and reconstruction steps necessary in the mathematical function implementation. The key recent advance in optimisation technology that makes this heuristic practical is the exact linear optimisation package \texttt{QSopt\_ex} of Applegate, Cook, Dash, and Espinoza [1].

An implementation of the heuristic in this paper, together with a distribution of \texttt{QSopt\_ex}, is available at [http://github.com/tmyklebu/funapprox](http://github.com/tmyklebu/funapprox).

3. Notation

C99’s hexfloat notation is used extensively in this paper. In this notation, a finite, normal \texttt{binary32} floating-point constant is written unambiguously in the form \texttt{0x1.mmmmp+ef}, where \texttt{0x} is literal, each \texttt{m} is a hexadecimal digit in the significand, \texttt{p} is literal, \texttt{+ee} is the exponent, and \texttt{f} is a literal suffix indicating that the number is \texttt{binary32}. See the recent C11
standard’s description of “hexadecimal floating-point constants” for a formal definition. As an example, \(0x1.1f2p+1f\) is the constant \(1 \cdot 2^1 + 1 \cdot 2^{-3} + 15 \cdot 2^{-7} + 2 \cdot 2^{-11}\).

“Ulp” is a shorthand for “unit in the last place.” Ignoring special cases, this is the difference between one floating-point number and the smallest floating-point number larger than it in magnitude. If \(x\) is a real number, then an “ulp of \(x\),” written ulp\(x\), is the difference between the largest floating-point number less-than-or-equal-to \(x\) and the smallest floating-point number larger than \(x\). \(^{1}\)

4. A RUNNING EXAMPLE

The following partially-specified C program will be used as a running example:

```c
float sin_poly(float a) {
    float s = a * a;
    float r5 = fmaf(s, c9, c7);
    float r4 = fmaf(s, r5, c5);
    float r3 = fmaf(s, r4, c3);
    float r2 = s * r3;
    float r1 = fmaf(a, r2, a);
    return r1;
}
```

Here, \(\text{fmaf}\) is the “fused multiply-add” for \texttt{binary32} numbers; \(\text{fmaf}(a, b, c)\) is the closest machine-representable number to \(ab + c\).

The program \texttt{sin\_poly} above attempts to compute the Horner form

\[
a + a \cdot a^2(c_3 + a^2(c_5 + a^2(c_7 + a^2c_9)))
\]

in \texttt{binary32} arithmetic. (Note that simple multiplications such as \(s = a \ast a\); may be computed as \(s = \text{fmaf}(a, a, 0.0f)\); if only for the sake of uniformity.)

It is desired that coefficients \(c_3, c_5, c_7,\) and \(c_9,\) each in \([-1, 1]\), are computed such that, for every \texttt{binary32} number \(a\) between \(-\pi/4\) and \(\pi/4\), the value returned from the call \texttt{sin\_poly}(\(a\)) is within 0.65 ulp of \(\sin\ a\). The choice of \([-1, 1]\) for every coefficient is arbitrary, but finite and reasonably small bounds on every coefficient are necessary so that the error bounds in the next section can give useful results.

Two obstacles present themselves. First, each coefficient \((c_3, c_5, c_7,\) and \(c_9)\) must be a \texttt{binary32} number. Second, \(s, r_5, r_4, r_3, r_2,\) and \(r_1\) are evaluated in \texttt{binary32} arithmetic—it is not enough that \((\text{1})\) is within 0.65 ulp of \(\sin\ a\) for every \(a \in [-\pi/4, \pi/4]\).

5. ERROR BOUNDS

The fused multiply-add (FMA) is available on many modern processors. The fused multiply-add computes \(ab + c\), for machine numbers \(a, b,\) and \(c,\) with only a single rounding at the end. This calculation is written as \(\text{fma}(a, b, c)\). The lack of rounding of the intermediate product \(ab\) often results in greater accuracy in a larger computation that makes use

\(^{1}\)There are several other definitions of ulp \(x\) that differ when \(x\) is equal to or near a signed power of two. See [15] for an extended discussion of various definitions of “ulp.” Any reasonable definition will do for the purpose of understanding this paper.
of the FMA. The IEEE standard for floating-point arithmetic \cite{12}, as of 2008, requires that \( \text{fma}(a, b, c) \) delivers the closest machine-representable number to \( ab + c \).

A very useful property of the FMA is that, as a univariate function of \( a \), \( \text{fma}(a, b, c) \) is a monotone (increasing or decreasing) function. Thus, given lower and upper bounds, say \( f \) and \( \overline{f} \), on \( \text{fma}(a, b, c) \), and values of \( b \) and \( c \), one can use binary search to find, quickly and exactly, the interval of representable numbers \( a \) such that \( f \leq \text{fma}(a, b, c) \leq \overline{f} \).

As mentioned, if \( a \), \( b \), and \( c \) are machine-representable numbers, the fused multiply-add \( \text{fma}(a, b, c) \) is the closest machine-representable number to \( ab + c \). Thus, absent exponent overflow or underflow, one can bound

\[
|\text{fma}(a, b, c) - (ab + c)| \leq \frac{1}{2} \text{ulp}(ab + c).
\]

If \( a \) and \( c \) are machine approximations to real numbers \( a + \delta a \) and \( c + \delta c \) but \( b \) is a machine-representable number known exactly, one can use the triangle inequality to bound

\[
|\text{fma}(a, b, c) - ((a + \delta a)b + (c + \delta c))| 
\leq \frac{1}{2} \text{ulp}(ab + c) + |\delta c + b\delta a| 
\leq \frac{1}{2} \text{ulp}(ab + c) + |\delta c| + |b\delta a|.
\]

Thus, if one has bounds on \( ab + c \), \( |\delta a| \), and \( |\delta c| \), one can compute an explicit bound on the difference between \( \text{fma}(a, b, c) \) and the exact-arithmetic result \( (a + \delta a)b + (c + \delta c) \).

Applying this bound naively (i.e. taking no account of possible cancellation) to the example of \( \sin_{\text{poly}}(0.5f) \), one can compute \( s = 0.25 \) and then find

\[ r_5 + \delta r_5 = 0.25c_9 + c_7 \]

with \( |\delta r_5| \leq \frac{1}{2} \text{ulp} 1.25 = 2^{-25} \) and \( |r_5| \leq 1.25 + 2^{-25} \).

Then

\[ r_4 + \delta r_4 = c_5 + 0.25c_7 + 0.25^2c_9 \]

with

\[ |\delta r_4| \leq \frac{1}{2} \text{ulp}(1.3125 + 2^{-25}) - 0.25\delta r_5 \leq 2^{-25} + 2^{-27} \]

and \( |r_4| \leq 1.3125 + 2^{-25} + 2^{-27} \).

Bounds on \( |\delta r_3|, |r_3|, |\delta r_2|, |r_2|, |\delta r_1|, \) and \( |r_1| \) can be computed analogously.

Note also that, given \( a \), bounds that must be satisfied by \( r_1 \) can be computed. For \( a = 0.5f \), we desire that \( r_1 \) is within 0.65 \text{ulp} of \( \sin \frac{1}{2} \). Since \( \sin \frac{1}{2} \) is roughly \( 0x1.eaee8744b0p-2f \), this means that we desire

\[ 0x1.eaee86p-2f \leq r_1 \leq 0x1.eaee88p-2f. \]

Note that these lower and upper bounds are adjacent binary32 numbers. In some other cases, such as \( a = 0.625f \), these lower and upper bounds are equal.

Since \( r_1 \) is computed using only \( r_2 \) and \( a \), this implies bounds on \( r_2 \). One can use binary search to find the smallest and largest binary32 numbers such that

\[ 0x1.eaee86p-2f \leq \text{fma}(a, r_2, a) \leq 0x1.eaee88p-2f. \]

This yields the bounds

\[ -0x1.5117aep-5f \leq r_2 \leq -0x1.511790p-5f. \]
These bounds are nonadjacent binary32 numbers. Since \( r_2 \) is computed using only \( r_3 \) and \( s \), this implies bounds on \( r_3 \):

\[
-0x1.5117aep-3f \leq r_3 \leq -0x1.511790p-3f.
\]

Unfortunately, \( r_3 \) is computed using the coefficient \( c_3 \), so similar bounds on \( r_4 \) cannot be obtained. However, if \( c_3 \) is fixed, this can be done.

6. Formulating linear constraints

Given a value of the abscissa \( a \), the value of \( s \) can be computed directly and acceptable bounds on \( r_1 \) can be derived from the value of \( \sin a \). As in the previous section, upper and lower bounds on the difference between the computed value \( \sin_{\text{poly}}(a) \) and the exact-arithmetic value of the Horner form (1) can be found.

Suppose this difference is at least \( \delta \) and at most \( \delta \). Then the coefficients \( c_3, \ldots, c_9 \) must satisfy the linear inequalities

\[
\begin{align*}
\sin(a) - 0.65 \text{ulp}(\sin(a)) + \delta 
\leq a + a \cdot s(c_3 + s(c_5 + s(c_7 + sc_9)))) \\
\leq \sin(a) + 0.65 \text{ulp}(\sin(a)) + \delta.
\end{align*}
\]

An acceptable list of coefficients \( c_3, \ldots, c_9 \) must satisfy (4) for every \( a \) of interest. However, one need not formulate all such constraints in the beginning. One can generate the inequalities (4) for some small subset of the points of interest, find a solution, and then look for points \( a \) not yet considered for which (4) is violated. This is often called a cutting-plane method.

Indeed, a classical theorem of Helly [9] (see also [17]) implies that a (possibly very large) system of linear inequalities in \( n \) variables is either satisfiable or there exists an unsatisfiable subsystem of at most \( n + 1 \) inequalities.

Given a list of linear inequalities that must be satisfied by some variables that take on real values, one can compute lower and upper bounds on the variables using linear optimisation. The linear optimisation problems that arise from (4) are very ill-conditioned. The left-hand side is a Vandermonde matrix and the bounds on each row of this Vandermonde, called \( \delta \) and \( \delta \) in (4), are often very close together. Conventional inexact linear optimisation, as implemented in systems such as Gurobi [8] and IBM’s CPLEX [11], can give meaningfully incorrect bounds and even confuse feasible systems of linear inequalities with infeasible systems. Therefore, fast, exact linear optimisation is necessary.

Note also that, if \( c_3 \) is fixed to some value, different (likely tighter) linear inequalities on \( c_5, c_7, \) and \( c_9 \) may be formulated since, for each abscissa \( a \), the interval of acceptable values of \( r_4 \) can now be derived.

7. The heuristic

The state of the heuristic has several components:

- A nonempty list of test points.
- Finite lower and upper bounds on each variable.

The heuristic runs the following loop until something fails:

1. Find a solution \( c \) such that \( p_c(x) \) is an acceptable rounding of \( f(x) \) for every test point \( x \).
Fix an ordering of the coefficients \([c_1, \ldots, c_k]\). 

\textbf{loop} some number of times 

\begin{algorithmic}
  \FOR {\(i = 1\) to \(k\)}
    \IF {\(i = k\)}
      report success.
    \ENDIF
    Compute lower and upper bounds on \(c_i\) by exact linear optimisation—say \(c_\underline{i} \leq c_i \leq c_\overline{i}\).
    \IF {infeasible, break.}
      Fix \(c_i\) to a randomly-chosen representable number between \(c_\underline{i}\) and \(c_\overline{i}\).
    \ENDIF
  \ENDFOR
\end{algorithmic}

\textbf{end loop}

Fail.

\begin{figure}
\caption{Pseudocode for Step 1.}
\end{figure}

(2) Find a point \(x\) such that \(p_c(x)\) is not an acceptable rounding of \(f(x)\) and add \(x\) to the list of test points.

(3) Go to 1.

Step 1 is done roughly as in Figure 1 but with some refinements described later. If step 1 fails, the heuristic reports failure. This does not necessarily imply that the problem is infeasible.

Step 2 is done by trying every abscissa of interest until at least one results in an unacceptable function value. This is only practical for smaller domains, such as those arising from IEEE binary32 functions.

Choosing a distribution other than the uniform distribution on \([c_\underline{i}, c_\overline{i}]\) may result in better performance. I use the average of two uniform samples on \([c_\underline{i}, c_\overline{i}]\); better choices may exist.

It is also wasteful to take only a single sample of \(c_{i+1}, \ldots, c_k\) after fixing \(c_i\). The linear optimisation problems later in the for loop tend to solve faster than those earlier in the loop. Further, a single bad coefficient choice later in the variable fixing process can scuttle a good choice of an earlier coefficient. Instead, I recursively try a constant number (four) of choices of \(c_{i+1}\) after fixing \(c_i\). The first choice of \(c_i\) made is always the value of \(c_i\) that most recently yielded an acceptable list of coefficients.

8. Examples

This section gives examples of C functions that compute arctan on \([-1, 1]\) and on \((-\infty, \infty)\) using fused multiply-add. The arctan function was chosen because it admits an especially simple argument reduction to \([-1, 1]\), yet some care must be taken to get a faithfully-rounded result on that interval.

8.1. Arctangent on \([-1, 1]\). The C function in Figure 2 is a faithfully-rounded approximation to \(\arctan x\) for \(x\) a binary32 number in \([-1, 1]\). On every binary32 number \(a\) in \([-1, 1]\), \texttt{atan}_poly(a) produces a result that differs from \(\arctan a\) by less than 0.95 ulp. This was computed in about five minutes from the partial straight-line program in Figure 3 fixing variables in the order \(c_3, c_5, c_7, c_9, c_{11}, c_{13}, c_{15}, c_{17}\).

By way of comparison, SLEEF’s implementation \texttt{xatanf} has a maximum error of roughly 1.773 ulp on \([-1, 1]\), which drops to roughly 1.707 ulp if \texttt{mlaf} is replaced by \texttt{fmaf}.
float atan_poly(float a) {
    float s = a * a;
    float r = 0x1.6d2026p-9f;
    r = fmaf(r, s, -0x1.03f2d4p-6f);
    r = fmaf(r, s, 0x1.5beeb4p-5f);
    r = fmaf(r, s, -0x1.33194ep-4f);
    r = fmaf(r, s, 0x1.b403a8p-4f);
    r = fmaf(r, s, -0x1.22f5c2p-3f);
    r = fmaf(r, s, 0x1.997748p-3f);
    r = fmaf(r, s, -0x1.5554d8p-2f);
    r = r * s;
    return fmaf(r, a, a);
}

Figure 2. A faithful approximation to arctan on $[-1, 1]$.

float atan_poly(float a) {
    float s = a * a;
    float r = c17;
    r = fmaf(r, s, c15);
    r = fmaf(r, s, c13);
    r = fmaf(r, s, c11);
    r = fmaf(r, s, c9);
    r = fmaf(r, s, c7);
    r = fmaf(r, s, c5);
    r = fmaf(r, s, c3);
    r = r * s;
    return fmaf(r, a, a);
}

Figure 3. A partially-specified approximation to arctan.

The Sollya tool [5], when given input

```
fpminimax(atan(x), [1,3,5,7,9,11,13,15,17],
[24,24,24,24,24,24,24,24,24], [1e-6, 1]);
```

produces the coefficients given in Figure 4. Sollya’s \texttt{fpminimax} uses an implementation of the method of Brisebarre and Chevillard. When the coefficients of this polynomial are substituted into Figure 3, the resulting function has a maximum error of roughly 1.067 ulp. The proposed heuristic therefore gives an improvement in the maximum error of about 0.117 ulp over Sollya.

8.2. \textbf{Arctangent everywhere.} The proposed approach allows one to specify the function to be approximated by means of a function taking an argument $x$ and returning the range
float c17 = 2.90188402868807315826416015625e-3f;
float c15 = -1.6290735453367232763671875e-2f;
float c13 = 4.30826172232627865234375e-2f;
float c11 = -7.5408883392810821533203125e-2f;
float c9 = 0.1066047251224517822265625f;
float c7 = -0.14209578931331634521484375f;
float c5 = 0.19993579387664794921875f;
float c3 = -0.333314359188079833984375f;

Figure 4. Sollya’s coefficients for approximating arctan on $[-1, 1]$.

float juffa_atanf(float a) {
    float r, t;
    t = fabsf(a);
    r = t;
    if (t > 1.0f) r = 1.0f / r;
    r = atan_poly(r);
    if (t > 1.0f) r = fmaf(0x1.ddcb02p-1f, 0x1.aee9d6p+0f, -r);
    r = copySignf(r, a);
    return r;
}

Figure 5. N. Juffa’s arctan skeleton. This calls $\text{atan\_poly}$ from Figure 3.

of acceptable values of $f(x)$. This can be used to find approximations that make a given mathematical function implementation (including, say, an argument reduction step) more accurate. Consider the partially-specified implementation of arctan (due to N. Juffa [14]) in Figure 5.

Suppose one desires a binary32 approximation of arctan that is within 1.2 ulp of arctan everywhere. This can be cast as an approximation problem on $[0, 1]$. For every binary32 number $x$ in $[0, 1]$, one wants

- the straight-line program given by $\text{atan\_poly}$ in 5 to yield a result within 1.2 ulp of arctan($x$), and
- for every $y \in (1, \infty)$ such that $1/y$ rounds to $x$, for the straight-line program given by $\text{atan\_poly}$ in 5 to yield a result such that, after line 18 is run, $r$ is within 1.2 ulp of arctan($y$).

One can find the interval of machine-representable $y \in (1, \infty)$ such that $1/y$ rounds to $x$ by binary search. It is straightforward to write a function that computes, given $x$, the range of acceptable values of $\text{atan\_poly}(x)$ under the above two conditions.

The proposed heuristic finds the coefficients in Figure 6 in about ten minutes. These coefficients yield an error less than 1.1978 ulp everywhere. By way of comparison, Sollya’s polynomial yields a maximum error of more than 1.535 ulp. I also tried asking for a maximum error of 1.1 ulp, but the heuristic failed to find a solution.
float c17 = 0x1.686c56p-9;
float c15 = -0x1.01dec8p-6;
float c13 = 0x1.5a901p-5;
float c11 = -0x1.32b648p-4;
float c9 = 0x1.b3f558p-4;
float c7 = -0x1.22f90cp-3;
float c5 = 0x1.99782cp-3;
float c3 = -0x1.5554d8p-2;

Figure 6. Coefficients for Figure 5.

9. Concluding remarks

This paper presented a heuristic for designing floating-point approximations to univariate elementary functions. It takes as input a straight-line program structure, an interval, and a function giving the range of acceptable values for each input in the interval. If the heuristic succeeds, it outputs a straight-line program implementing the function on the desired interval that satisfies the desired error bound.

This paper also presented two nontrivial examples of approximations to arctan. These produced binary32 numbers approximating the arctangent of binary32 numbers using binary32 arithmetic.

For larger floating-point types such as IEEE binary64, it is not clear to me how to prove in a reasonable amount of time that a given straight-line program either satisfies the desired error bound on an interval or to find an abscissa where it fails. Moreover, this approach might not scale to the higher-degree polynomials necessary for such approximations. I leave these considerations to future work.

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