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Optimizing polynomials for floating-point implementation

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Abstract

The floating-point implementation of a function on an interval often reduces to polynomial approximation, the polynomial being typically provided by Remez algorithm. However, the floating-point evaluation of a Remez polynomial sometimes leads to catastrophic cancellations. This happens when some of the polynomial coefficients are very small in magnitude with respects to others. In this case, it is better to force these coefficients to zero, which also reduces the operation count. This technique, classically used for odd or even functions, may be generalized to a much larger class of functions. An algorithm is presented that forces to zero the smaller coefficients of the initial polynomial thanks to a modified Remez algorithm targeting an incomplete monomial basis. One advantage of this technique is that it is purely numerical, the function being used as a numerical black box. This algorithm is implemented within a larger polynomial implementation tool that is demonstrated on a range of examples, resulting in polynomials with less coefficients than those obtained the usual way.

Keywords: Polynomial evaluation, floating-point, elementary functions.

1 Introduction

Scientific and business applications need support for mathematical functions such as $e^x$, $\sin x$, $\log x$, $\text{erf} x$, and many others. Current processors offer little or no hardware for the evaluation of such functions. What they offer is high performance floating-point hardware for basic operations such as addition and multiplication, or their combination as a fused multiply-and-add. Other mathematical functions are usually approximated on a small domain by polynomials, which can then be evaluated using the high-performance operators of the processor [16, 14, 6]. This article addresses the design of such polynomial approximations. The difficulty is to obtain floating-point implementations of high quality with respect to both performance and precision.

1.1 Obtaining approximation polynomials

Several textbooks [13, 14, 16] discuss techniques to obtain good approximation polynomials. One may use Taylor polynomials, Chebychev approximations, or a minimax approximations given by Remez algorithm [17, 18]. The latter is preferred as it is theoretically the most accurate on a
domain: The minimax approximation of a function $f$ on a domain $I$ is defined as the polynomial $p$ that minimizes the infinite norm of the approximation error $\|p/f - 1\|_\infty$.

Throughout this article we focus on relative errors, which are more relevant to floating-point implementations. However, a good implementations of Remez algorithm can accommodate any kind of error through the use of an additional weight function $w$: Remez algorithm will actually minimize $\|p \cdot w - f\|_\infty$ for any $w$ provided by the user.

A few well-known tricks are used for certain classes of functions. For instance, for an odd/even function, a straightforward application of Remez algorithm will usually not provide an odd/even polynomial, although an odd/even approximation polynomial has several advantages. Firstly, it has twice as few coefficients as the minimax polynomial, and its evaluation will therefore be more economical. Secondly, the implementation will have the same symmetry properties as the function implemented. Thirdly, it is more stable numerically, as the sequel will show. The textbooks therefore advocate the use of an ad-hoc technique (which will be reviewed in Section 2.1) to compute, using standard Remez algorithm, a minimax approximation among the set of odd (resp. even) polynomials.

This article eventually offers a generalization of this ad-hoc technique to a much larger class of functions, but it didn’t start this way. The initial motivation of this work was to avoid a problem that makes the evaluation of some polynomials impractical using floating-point arithmetic. This problem is the occurrence of cancellations in the evaluation. It would in particular plague the evaluation of a straightforward minimax approximation to an odd/even function.

1.2 Floating-point evaluation of a polynomial

Let us consider the Horner evaluation of a polynomial of degree $d$:

$$p(x) = a_0 + x \cdot (a_1 + x \cdot (a_2 + ...) ...).$$

It can be described as a recurrence:

$$\begin{align*}
q_n &= a_n \\
q_i &= a_i + x \cdot q_{i+1} & \text{for } i = 0 \ldots n - 1 \\
p(x) &= q_0
\end{align*}$$

A cancellation happens when, for some values of $x$, the addition in $a_i + x \cdot q_{i+1}$ is effectively a subtraction and the two terms $a_i$ and $x \cdot q_{i+1}$ are very close to each other.

Cancellations in polynomial evaluation should be avoided for two reasons.

- Although a cancelling subtraction is an exact operation, in the sense that it never involves a rounding, some digits of the result are no longer significant. Consider for instance, in a decimal format with 4-digit significand, the subtraction 1.234 – 1.232. It is an exact subtraction that cancels three digits and returns $2.000 \cdot 10^{-3}$: the three zeroes do not correspond to significant information from the initial numbers. If this result is then multiplied by another value –which is precisely the case in Horner evaluation– this loss of information propagates to the result of the multiplication. As a side effect, error analysis becomes very difficult. This is the reason why useful theorems about the accuracy of Horner evaluation [1] have hypotheses that ensure that cancellation will not occur.

- Fast double-double [12] and triple-double [13] operations can only be used if the absence of cancellation can be proven beforehand. Otherwise, much slower versions have to be used [10].
The second reason leads us to avoid any cancellation. Usually this means that $x \cdot q_{i+1}$ should remain smaller than $a_i/2$ or that both always have the same sign – see Section 3 for the actual criterion used.

Other evaluation schemes exist and are better suited to current superscalar machines, from the family of Estrin schemes \cite{6,16,7} to Knuth/Eve transformations \cite{12,18}. The issue of cancellation is relatively independent of the choice of evaluation scheme, since it is mostly related to the orders of magnitude of the coefficients. More specifically, these other schemes can also be expressed as a tree of operations involving additions and partial polynomials, and the techniques developed for Horner should adapt to other schemes as well.

1.3 Contributions

It is quite simple to detect the possibility of cancellations in a polynomial evaluation scheme. We present an algorithm that starts with a standard minimax polynomial for a function, searches its Horner evaluation for cancellations, then tries to remove these cancellations by setting to zero the offending coefficients: if $a_i + x \cdot q_{i+1}$ may cancel, then set $a_i$ to zero. The algorithm then iterates using a modified Remez algorithm that forces some coefficients to zero.

It turns out that this algorithm numerically discovers the zero coefficients of odd/even functions, but also in many more cases when textbook recipes do not apply – examples will be given in Section 2.1. Even for odd/even functions, it widens the implementation space, as it explores implementations that are not strictly odd/even. It thus provides practical answers to questions such as: Is this odd polynomial really the optimal one with respect to my optimality criterion?

Moreover, this algorithm is purely numerical: all it requires is a black-box implementation of the function and its first two derivatives. This implementation has to return an enclosure of these functions in multiple precision, up to an accuracy sufficient with respect to the target precision. It may therefore be applied to arbitrary compound functions, but also to functions defined by integrals or iterative processes – in such cases the enclosures of the first two derivatives $f$ may have to be computed numerically out of those of $f$. We illustrate this in Section 2.1 on the example of \texttt{argerf = erf}^{-1}, which we compute by a Newton-Raphson-iteration out of on the function erf.

This algorithm may even be used for a class of applications studied by Remez \cite{17}, then Dunham \cite{8}, where a function is defined by a large set of points obtained from some physical experiment. A linear interpolation between these points allows one to recover the function, but one may want a more compact polynomial implementation. Provided the set of points is large enough and accurate enough, the technique presented here should apply to such problems, too.

Our algorithm has been implemented using the Sollya tool\footnote{http://sollya.gforge.inria.fr/}, in the Sollya scripting language. Sollya provides all the necessary building blocks. Internally, it uses multiple precision interval arithmetic based on the MPFR\footnote{http://www.mpfr.org/} library. Based on this, Sollya evaluates composite functions with faithful rounding to any precision. Functions written outside Sollya can also be linked dynamically. In addition, Sollya also provides a fast but nevertheless high-quality implementation of the infinite norm, and also a slower, certified one \footnote{http://sollya.gforge.inria.fr/}. Finally, Sollya integrates a Remez algorithm (presented in Section 2) which is more flexible than other implementations, for instance the minimax algorithm in the Maple \texttt{numapprox} package.
1.4 A complete implementation chain

The algorithm presented in this article provides a polynomial with real coefficients. What one eventually needs for a floating-point implementation is a polynomial with machine-representable coefficients: In the applications we target \([7]\), coefficients should be double-precision numbers, double-doubles, or triple-doubles \([11, 13]\). Techniques are known to obtain a minimax polynomial among the set of polynomial with such machine-representable coefficients \([2]\). These techniques have to be initialized with a good polynomial: the polynomial obtained by our algorithm fills this role. This final transformation of our polynomial is therefore out of the scope of the present article, although some of the examples provided in Section \([4]\) have gone through this final step, which is also automatic. The appropriate precision for each addition and multiplication step in the Horner scheme is chosen automatically. Let us just mention that one needs to ensure that this final step keeps our zero coefficient, which is easy within the framework of \([2]\). One also has to ensure that this final step does not introduce a possibility of cancellation. This can be checked a posteriori, and in practice the check always succeeds, because the algorithm of \([2]\) preserves the floating-point binade of the coefficients.

Finally one has to evaluate or certify a bound on the accumulated rounding error when this final polynomial is evaluated. This can be done using the Gappa tool \([8]\), and is also automated, but out of scope of this article.

To sum up, the algorithm presented in this article is integrated in a larger Sollya program that is capable of automatically generating certified C code for Horner’s scheme using expansion arithmetic from double to triple-double precision \([7]\). Let us now focus on this algorithm.

2 Minimax approximation on an incomplete monomial basis

This section first revisits the current textbook methodology for approximating a function with a polynomial, then introduces several useful generalizations and formalizations.

2.1 Introductory examples

Let us consider the example of an implementation of the sine function between \(-\pi/64\) and \(\pi/64\) (this interval is typical after a table-based argument reduction \([15, 16]\)). Let us assume that a target accuracy of \(2^{-60}\) is wanted, as would be the case for a quality double-precision implementation.

A first option is to use a Taylor approximation. As the sine function is odd, the corresponding series has only odd monomials. With degree 7, the relative approximation error is roughly \(2^{-53}\).

With degree 9, the error is smaller than \(2^{-68}\). This illustrates how discrete the quality of the approximation usually is with respect to the degree.

Another option is to use a minimax polynomial, provided by Remez algorithm. This will provide us with a polynomial that is not odd: its coefficients are

\[
\begin{align*}
a_1 &= 1.00000000000000000004553862129419953814366183346717373 \\
a_2 &= -0.874967378163014390017316615896238907007870683208826576 \cdot 10^{-16} \\
a_3 &= -0.166666666666639297309612035148824100626593835839529139 \\
a_4 &= -0.31797360730240662105040928632951877918380396824236704 \cdot 10^{-11} \\
a_5 &= 0.833333350548021113401528637698582467442968048220758103 \cdot 10^{-2} \\
a_6 &= -0.454284495616307678859183047154098436831822774513536551 \cdot 10^{-8} \\
a_7 &= -0.1983624855242322425486133528574705655050846399633158981546 \cdot 10^{-3}
\end{align*}
\]
The approximation error is now smaller than $2^{-64}$, and this polynomial fits our accuracy target. However, this full polynomial of degree 7 will require 7 multiplications and 6 additions when evaluated by Horner, whereas the Taylor of degree 9, considered as a degree-4 polynomial in $x^2$ multiplied by $x$, requires only 6 multiplications and 4 additions, and provides a much better approximation error ($2^{-68}$).

This is a good enough reason to prefer the degree-9 Taylor, but there is another critical problem with the minimax polynomial: when evaluated in finite precision, the alternation of comparatively very small and very large coefficients will lead to large cancellations.

Still, the approximation error of the Taylor polynomial is not balanced on the interval. One may think of zeroing out the smaller (even) coefficient of the minimax, but this provides a much worse approximation error ($2^{-49}$). Textbooks by Muller and Markstein therefore suggest the following better recipe for finding an odd polynomial with a better balanced error: perform the change of variable $X = x^2$, and compute a degree-4 minimax on the transformed function $\sin(\sqrt{X})/\sqrt{X}$, with a suitable weight function. This will provide a degree-4 polynomial in $X$. Multiplying the corresponding degree-8 polynomial in $x$ with $x$ yields an odd polynomial that approximates $\sin(x)$ well: the error is smaller than $2^{-60}$. This polynomial evaluates in only 6 multiplications, and without cancellation issues – this last point as a side effect, not mentioned in textbooks. Besides, a good choice of the weight function ensures that this polynomial is the minimax among the set of odd polynomials of degree 9.

This recipe is more or less the state of the art for finding an approximation polynomial, and the improvements over it have mostly consisted in obtaining minimax approximations over the set of polynomial with machine-representable coefficients [2]. Let us now try to apply it to more complex functions.

- $\cos(x^2)$ has a Taylor approximation of the form $1 - 1/2x^4 + 1/24x^8$ with only coefficients for powers of $x^4$. The recipe above can be accommodated to such cases.

- $\sin(x) + \cos(x^2)$ has the following Taylor approximation:
  
  $1 + x - 1/6x^3 - 1/2x^4 + 1/120x^5 - 1/5040x^7 + 1/24x^8 + 1/362880x^9$.... Here the zero coefficients – which will probably lead to cancelling coefficients in minimax approximation – are the coefficients of degree $2 + 4k$ for $k$ integer. This structure can be predicted fairly straightforwardly from the sums of the Taylor series of $\sin(x)$ and $\cos(x^2)$. However, the textbook recipe does not extend straightforwardly to this function: providing a minimax polynomial with this coefficient structure is not obvious. One may apply the recipe to $\sin(x)$, then to $\cos(x^2)$, then add the resulting polynomials coefficient-wise. This will provide a polynomial with the wanted coefficient structure, but there is no reason why it should be the one with minimal error.

- $e^{\sin(x) + \cos(x^2)}$ has a Taylor series with a single zero coefficient at degree 3. Again, this can be predicted analytically or using computer algebra, but it is getting less and less intuitive. And again, can the reader provide a change of variable allowing to compute a minimax polynomial for this function among the set of polynomial whose degree-3 coefficient is zero?

Looking back at the Taylor series for $\sin(x) + \cos(x^2)$, we also remark that even its non-zero coefficients will present risks of cancellation as the degree augments. Any methodology leading to an implementation has to study these cancellation issues at some point. Our approach is to attack the cancellation issues first by imposing the value 0 to some coefficients. It happens that such a
methodology will, as a side effect, zero out the coefficients which are zero in the Taylor series, and thus minimizes the number of operations required for the evaluation, just as the textbook recipe, but for more functions.

The core of this technique is a modified Remez algorithm that is able to compute a minimax polynomial on an incomplete monomial basis, which we present now.

### 2.2 Modifications to Remez algorithm

Refer to [16] for a good introduction to the Remez algorithm [17, 4]. Modifying this algorithm for an incomplete monomial basis \( \{x^{i_0}, x^{i_2}, \ldots, x^{i_n}\} \) is fairly straightforward. The core of Remez algorithm solves a linear interpolation problem on \( n + 2 \) points. In the general case, the matrix of this linear system is a Vandermonde matrix. For an incomplete basis, the matrix simply only contains columns corresponding to the given monomials. This possibility is already present in the initial formulation of the problem by Remez [17, 4].

### 2.3 Theoretical issues

Remez algorithm works iteratively. In order to ensure that the polynomial is really improved in each step, classical Remez algorithm requires the so-called Haar condition [17, 4]: the determinant of the formal matrix of the linear system does not vanish for any choice of approximation points in the interval \( I \). This Haar condition is always satisfied for Vandermonde matrices [17], hence for approximations on the complete monomial basis.

Unfortunately, the Haar condition is not fulfilled in general for incomplete bases, in particular if the interval comprises zero [17, 4]. Therefore the convergence of our modified Remez is not proven. Furthermore, when it converges, there is currently no proof that it converges to the expected minimax polynomial.

These issues are under investigation. To the best of our knowledge, there exists some literature addressing them, sometimes dating back to Remez himself [17, 19]. However there is no recent work on a multiple-precision implementation of a minimax without Haar condition.

### 2.4 The modified Remez algorithm in practice

In practice our modified Remez algorithm, implemented in the Sollya tool, satisfies our needs. The algorithm typically runs even without Haar condition until it converges to some polynomial [17], or until it can no longer exhibit \( n + 2 \) appropriate interpolation points. When it works, the returned polynomial might not be the actual best approximation polynomial. Nevertheless, it is possible to verify a posteriori whether or not this polynomial satisfies the target approximation error bound. This is enough to validate the implementation of a function. Experimentally, comparisons with minimax on the complete basis, as well as observed discrete jumps of errors with respect to the degree, suggest that the polynomial is not far from the optimal. Actually, the optimality can be proven a posteriori using a modification of the polytope exploration described in [3], but this is very costly and out of scope of this paper.

In addition, we use the modified Remez algorithm with care. For example, it is possible to ensure the Haar condition in cases when the incomplete monomial basis is even/odd: If the approximation interval \( I \) comprises zero, just take only the positive (or negative) half of the interval.
3 Computing cancellation-free approximation polynomials

The complete algorithm implementing our approach is sketched in the listing below. It first tests if the approximation polynomial in the complete basis is cancellation-free. If the test fails, all monomials on which cancellations occur are removed from the basis. An approximation polynomial is then computed in the resulting, incomplete basis. The algorithm iterates on increasing degrees
until the target error bound is fulfilled or an iteration limit is reached.

```
function multiplication of the (symbolic) polynomial $q$ until the target error bound is fulfilled or an iteration limit is reached.

Algorithm 1: The complete approximation algorithm

The $\text{guessdegree}$ Sollya function returns a guess of the degree needed for approximating a function $f$ in a domain $I$ with error less than $\varepsilon$. It is based on the first iteration of the Remez algorithm combined with a bisection search.

The assignment $q_i \leftarrow p_i^* + x \cdot q_{i+1}$ at line 19 of the algorithm must be understood as a symbolic multiplication of the (symbolic) polynomial $q_{i+1}$ by a free variable $x$ and a symbolic addition of $p_i^*$.
As mentioned in section 2.4, care is needed in the calls to the Remez algorithm. Lines 24 and 28 of the algorithm above refer to sub-routines that represent a few hundreds of lines of code in the Sollya scripting language.

All computations of infinite norms, infima and suprema occurring in the algorithm can be performed by uncertified, quick-and-dirty numerical algorithms. This permits to use a black-box implementation for the function \( f \). Certification of the infinite norm of the final polynomial can be performed a posteriori [5].

An iteration limit \( l \) is taken in input of the algorithm. We introduce it for ensuring the termination of the algorithm on degenerated problems that we believe to exist. Currently we can neither prove the convergence of the algorithm nor exhibit an example on which it would not terminate. In mathematical terms, we are currently unable to analyze whether the set of cancellation-free polynomials (as defined above) of arbitrary degree is dense for any function and approximation interval. In practice, the iteration limit is not reached.

4 Examples

4.1 From a function to a C implementation

Let us first reconsider the function \( f \) defined by \( f(x) = e^{\sin x - \cos x^2} \) in the domain \( I = [-2^{-8}; 2^{-8}] \). The function is to be approximated by a polynomial with a relative error less than \( 2^{-90} \). Our algorithm chooses the monomial basis \( \{ x^0, x^1, x^3, x^4, x^5, x^6, x^7, x^8, x^9 \} \), leaving out the monomial \( x^3 \). The implemented polynomial \( p(x) = \sum_{i=0}^{9} p_i x^i \) is given by

\[
\begin{align*}
p_0 &= 11938370416962674428469396878343 \cdot 2^{-108} \\
p_1 &= 2984592604206685857117349204375 \cdot 2^{-106} \\
p_2 &= 11938370416962674428436621385363 \cdot 2^{-109} \\
p_4 &= 4970345142530923 \cdot 2^{-55} \\
p_5 &= 358969371405011 \cdot 2^{-51} \\
p_6 &= 6516674741954513 \cdot 2^{-56} \\
p_7 &= 589077943038783 \cdot 2^{-57} \\
p_8 &= 5559725200690211 \cdot 2^{-59} \\
p_9 &= 5320394595779079 \cdot 2^{-58}
\end{align*}
\]

As can be easily verified by computing \( \|p/f-1\|_\infty \), its error is bounded by \( 2^{-90.4} \). It can be evaluated using Horner’s scheme with IEEE 754 double and double-double arithmetic with an round-off error of less than \( 2^{-93.6} \). This bound has been shown with the Gappa tool [6], and in the process Gappa formally shows a posteriori that no cancellation may occur.

4.2 Adaptation of the monomial basis to the target accuracy

Let us consider now the function \( f \) defined by \( f(x) = e^{\cos x^2 + 1} \) in the domain \( I = [-2^{-8}; 2^{-5}] \). The table below shows the monomial basis chosen by our algorithm, as a function of the relative approximation accuracy target.
### 4.3 An example of black-box function

The following example illustrates that the algorithm works well on black-box functions. The function $\operatorname{argerf} = \operatorname{erf}^{-1}$ is not currently available in the MPFR library, and the Sollya tool is based on MPFR. It is nevertheless relatively easy – although probably very inefficient – to implement using a Newton-Raphson-iteration on the function $\operatorname{erf}$. Its first two derivatives can be computed based on the code for $\operatorname{argerf}$ itself. We have implemented such a black-box function $\operatorname{argerf}$ and have dynamically bound it to Sollya.

For an approximation polynomial in the domain $I = [-1/4; 1/4]$ and a relative error bound of $2^{-60}$, our algorithm finds the monomial basis $\{x^1, x^3, x^5, x^7, x^9, x^{11}, x^{13}, x^{15}, x^{17}, x^{19}\}$. As $\operatorname{argerf}$ is given as a binary executable, there is no formal knowledge that it is an odd function. Nevertheless, the algorithm chooses an odd monomial basis for this odd function. The polynomial $p(x) = \sum_{i=0}^{19} p_i x^i$ implemented using IEEE 754 doubles and double-doubles is given by

<table>
<thead>
<tr>
<th>accuracy target</th>
<th>monomial basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-40}$</td>
<td>${x^0, x^4}$</td>
</tr>
<tr>
<td>$2^{-50}$</td>
<td>${x^0, x^4, x^8}$</td>
</tr>
<tr>
<td>$2^{-60}$</td>
<td>${x^0, x^4, x^8}$</td>
</tr>
<tr>
<td>$2^{-70}$</td>
<td>${x^0, x^4, x^8, x^{12}}$</td>
</tr>
<tr>
<td>$2^{-80}$</td>
<td>${x^0, x^4, x^8, x^{12}}$</td>
</tr>
<tr>
<td>$2^{-90}$</td>
<td>${x^0, x^4, x^8, x^{12}}$</td>
</tr>
<tr>
<td>$2^{-100}$</td>
<td>${x^0, x^4, x^8, x^{12}, x^{13}, x^{14}, x^{15}}$</td>
</tr>
<tr>
<td>$2^{-110}$</td>
<td>${x^0, x^4, x^8, x^{12}, x^{13}}$</td>
</tr>
<tr>
<td>$2^{-120}$</td>
<td>${x^0, x^4, x^8, x^{12}, x^{16}, x^{17}, x^{18}}$</td>
</tr>
</tbody>
</table>

Its approximation error is bounded by $2^{-62.9}$. The polynomial can be evaluated using Horner’s scheme and double and double-double arithmetic. The corresponding evaluation error is bounded by $2^{-62.4}$.
5 Conclusion and future works

Obtaining a floating-point C implementation of an arbitrary function has never been so automatic. The tools presented in this article are able to provide a high quality implementation of reasonably complex functions functions in a few seconds. Some of the a-posteriori validation steps may require many hours, though.

In the process of developing these tools, much insight has been gained in the issue of cancellation in polynomial evaluation, and its relationship to the monomial basis in which polynomials should be searched. The proposed modifications to Remez algorithm are simple in principle but complex in the details, and in the supporting theory. More solid mathematical foundations remain to be built, or rediscovered from ancient literature – the reference books on the subject date back to the ’60s. Meanwhile, we have demonstrated an implementation that works in practice.

Of course, expertise remains necessary in the implementation of an elementary function. A clever argument reduction can bring in accuracy and performance improvements by orders of magnitude above polynomial approximation alone, and this is totally function-dependent. Even in this case, the presented tool will be very helpful in the hands of the expert. Modern table-based argument reduction techniques are often parameterized, and lead to wide trade-offs. Choosing the best set of parameters may be very tedious, and performance-wise, it will be very dependent on the target machine. The tools presented here will help the designer navigate these trade-offs quickly. They have been used (at various stages of maturity) to build some of the functions in the CRLibm library.

Another, longer-term application of this kind of tool is the construction at compile-time of ad-hoc polynomial evaluators for composite functions appearing in application code. Many problems remain to be solved in this context, in particular the determination of a pertinent input interval – this is a difficult problem of static analysis in compilation. This approach could lead to higher performance, but also better accuracy than the composition of elementary functions currently used.

References


http://lipforge.ens-lyon.fr/www/crlibm/


