Overview

This is the final report for my Google Summer of Code 2020 project with Boost.Multiprecision. The aim of the project was to ensure that core arithmetic functions are efficient for numbers of up to 10K digits. This encompassed:

- implementation, testing and benchmarking of the:
  - square root function,
  - k-th root function (where k is an integer),
  - logarithm function,
  - several algorithms for computing digits of π.
- testing the implementation of existing basic arithmetic operations

I implemented the following algorithms (more specific links to my implementations are also given at the subtitle of each section):

- For the square root function, I implemented Newton-Raphson iteration and Karatsuba square root. The performance (and correctness) tests indicated that Karatsuba square root implementation is >20x faster than the existing implementation at 10K digits.
- For the k-th root function, I implemented the Newton-Raphson iteration, where performance (and correctness) tests showed that it is >300x faster than the power-based implementation for small (<1K) integer values at 10K digits.
- For the log function, I implemented the log AGM method, where performance tests (and correctness tests) showed that it is >30x faster than the existing implementation at 10K digits.
- For pi computation, I implemented several algorithms (GL Un, Cub Un, GL, Qd, Cub, Qr, Qn, Non) with the trivial tests.

The above implementations turned out to be quite efficient for up to tens of thousands (and even more) of digits.

In case the math does not display well, you can download this report here.

SQRT implementation

code: Newton-Raphson iteration, Karatsuba square root, tests

The square root function is one of the most commonly used mathematical functions either as a standalone function or as a component of more complicated ones (see $\log$ and π computations, below).

Implementations

The existing implementation for floating point numbers converts the number to an integer and then performs the square root operation in the integer space. To recover the square root of the floating point number, only the exponent needs to be adjusted. This is why the descriptions of the algorithms below focus on computing the square root of an integer.

Existing implementation: The current implementation of the sqrt function uses the binary method which operates in two phases:

1. Using binary search find the largest power of two 2^i whose square is smaller than the given number.

2. Go through the bits $i-1$ to 0 and decide whether it should be a 1 or a 0, by checking if $(p+2^i)^2 \leq a$, where p is the suffix of the square calculated up to i.

The second check can be performed using just additions, so each iteration requires just additions. So, the computation requires additions linear to the number of precision bits.

Newton-Raphson's method: Newton's method is an iterative method which can be used to find a root of a (sufficiently smooth, see below) function f:

1. Choose an initial point x_0.
2. Set $x_{t+1} := x_t - \frac{f(x_t)}{f'(x_t)}$.
3. Repeat step (2) until two iterates x_t and x_{t+1} are sufficiently close (smaller than epsilon, the precision of the representation).

By choosing $f(x) = x^2 - a$, $f(x)$ has its only positive root at $x = \sqrt{a}$. The Newton-Raphson iteration becomes:

$$x_{t+1} := \frac{1}{2}\left(x_t + \frac{a}{x_t}\right)$$

For quadratic convergence, the initial value has to be within twice of the square root. For a value $a = y2^e$, a good initial value is $x_0 = y2^{e/2}$, which can be calculated efficiently by right shifting the number.

The implementation for Newton Raphson's method can be found [here](#).

In theory, for a good initial value, the convergence rate is quadratic. However, in practice, the algorithm has several calls to the division subroutine, making the execution slower.

Karatsuba square root:

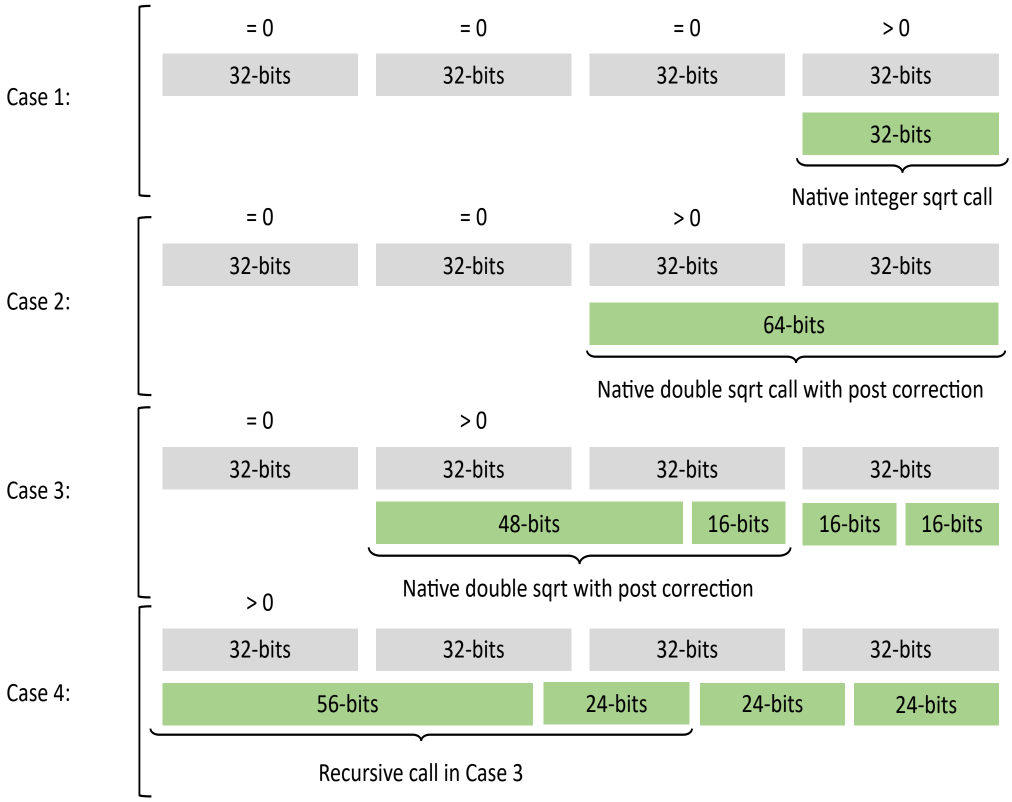
The Karatsuba square root method is a method that recursively computes the square root for the upper half of the digits and uses the division algorithm (and the lower half of the digits) to compute the square root of the entire number (see Algorithm 1). It is named like this due to its similarity with Karatsuba's multiplication algorithm that also splits the digits into four parts. The pseudocode for the algorithm (based on (Zimmerman 1998) and (Brent and Zimmerman 2010)) is given below:

Algorithm 1 SqrtKaratsuba

1: **procedure** $\textsc{SqrtKaratsuba}(x)$
2: $\qquad\triangleright$ Returns: s, r s.t. $s^2 \leq x = s^2 + r < (s+1)^2$
3: $\quad x = c_{n-1}\beta^{n-1} + \ldots + c_1\beta + a_0$ with $c_{n-1} \neq 0$
4: $\quad \ell \leftarrow \lfloor (n-1)/4 \rfloor$
5: $\quad$ **if** $\ell = 0$ **then**
6: $\qquad$ **return** $\textsc{SqrtKaratsubaBaseCase}(x)$
7: $\quad$ **end if**
8: $\quad$ Decompose $x = a_3\beta^{3\ell} + a_2\beta^{2\ell} + a_1\beta^{\ell} + a_0$ with $0 \leq a_0, a_1, a_2 < \beta^{\ell}$
9: $\quad (s', r') \leftarrow \textsc{SqrtKaratsuba}(a_3 b^{\ell} + a_2)$
10: $\quad t \leftarrow r'\beta^{\ell} + a_1$
11: $\quad q \leftarrow \lfloor t/(2s') \rfloor$
12: $\quad u \leftarrow \mathrm{rem}(t, 2s')$
13: $\quad s \leftarrow s'\beta^{\ell} + q$
14: $\quad r \leftarrow u\beta^{\ell} + a_0 - q^2$
15: $\quad$ **if** $r < 0$ **then**
16: $\qquad r \leftarrow r + 2s - 1$
17: $\qquad s \leftarrow s - 1$
18: $\quad$ **end if**
19: $\quad$ **return** (s, r)
20: **end procedure**

The implementation of the core part can be found here.

The other part which is not covered in the algorithm descriptions is how to solve the base case. The problem here is that we will be left with four (because of line 5) 32-bit limbs and there is no built-in method to compute the square root of 128-bit integers. Continuing the splitting at the bit level at non-fixed positions will be tedious and not very efficient. However, I noticed that it is possible instead to handle all cases as one of the following four:



The second case relies on the fact that we can fix the rounding problems in double sqrt for 64-bit integers (see code). The third case splits into 32-bit integers which means that the recursive call can be handled by Case 2 (see code). The fourth case splits into 64-bit integers which means that the recursive call can be handled by Case 3 (see code).

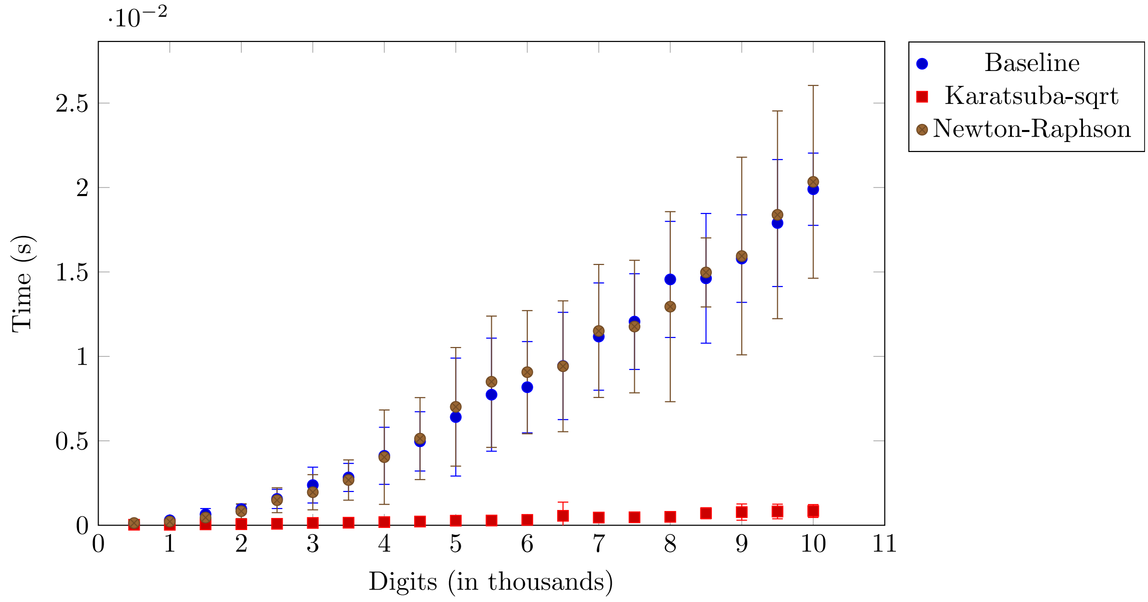
Correctness tests

The following correctness tests (see here) were run for each of the implementations:

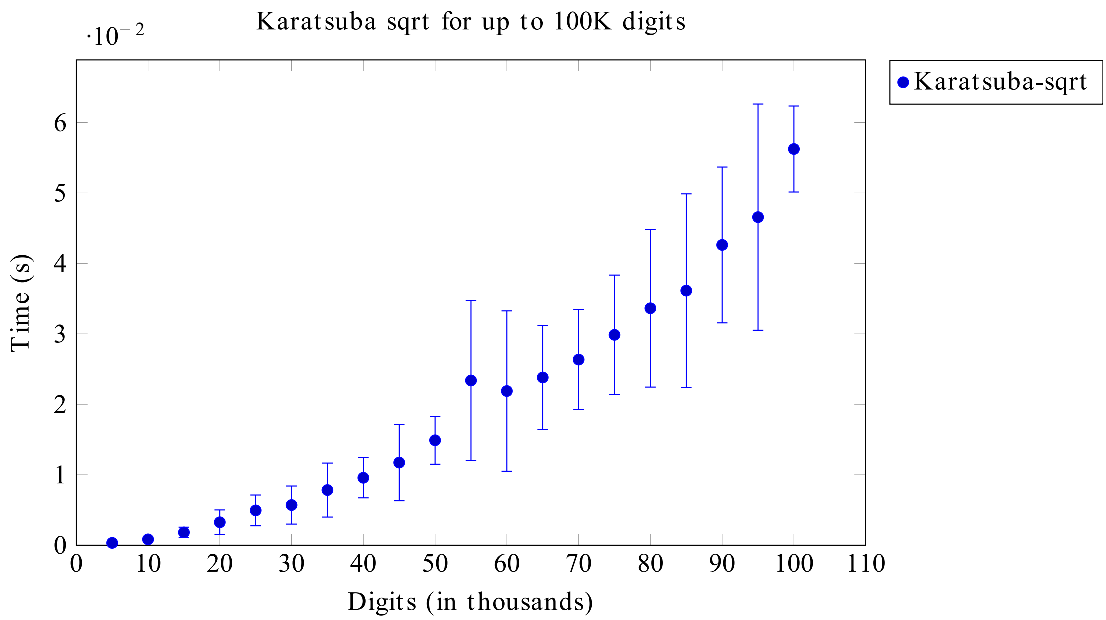
- A number of randomly chosen values in $[1,\ 10^{10000}]$:
  - with some of which the response was compared to hardcoded values from Wolfram Alpha.
  - with some of which the response was verified using the following integer square root check (requiring only multiplications): x is the square of a iff $(x+1)^2 > a$ and $x^2 \leq a$.
- A number of edge cases (containing 0, 1, powers of two)
- A number of cases that are difficult for specific algorithms:
  - powers of two,
  - powers of two minus one,
  - numbers with different 1, 2, 3 or 4 limbs.
  - all possible squares of numbers in $[1,\ 2^{32}]$ (must enable `EXHAUSTIVE_TESTS`),
  - $x^2 + 2x$ for all numbers in $[1,\ 2^{32}]$ (these trigger the greatest possible remainder).

Performance tests

The tests where performed on the same 20 randomly sampled numbers. The error bars represent confidence intervals at 95% assuming each trial is i.i.d.



As an extension we show that Karatsuba square root is efficient for up to 100K (and even more).



k-th root implementation

code: Newton-Raphson and tests

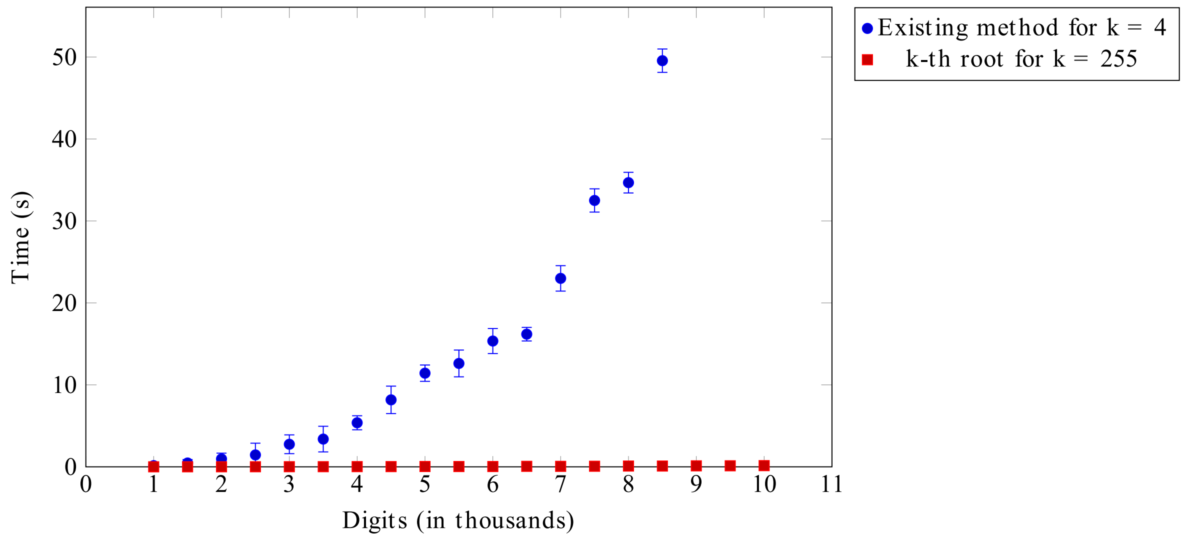
Some of the π algorithms require taking the fourth or fifth root of a number. The general case for this is taking the k-th integer root of a number x. The current way of doing this in Boost.Multiprecision is through $\mathrm{pow}(x, 1/k)$ which is not very efficient for small integer k.

Newton-Raphson method: Similarly to the Newton-Raphson implementation of the square root, we define $f(x) = x^k - a$, whose derivative is $f'(x) = (k-1)x$and which gives the iteration method,

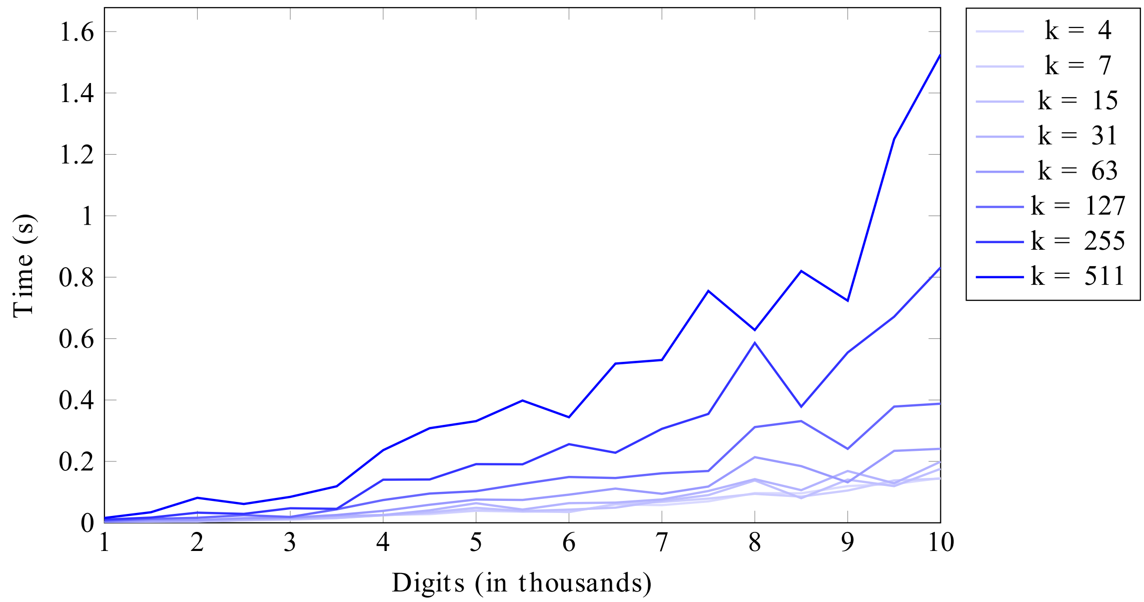
$$x_{t+1} := \frac{1}{k}((k-1)x_t - a)$$

Performance tests

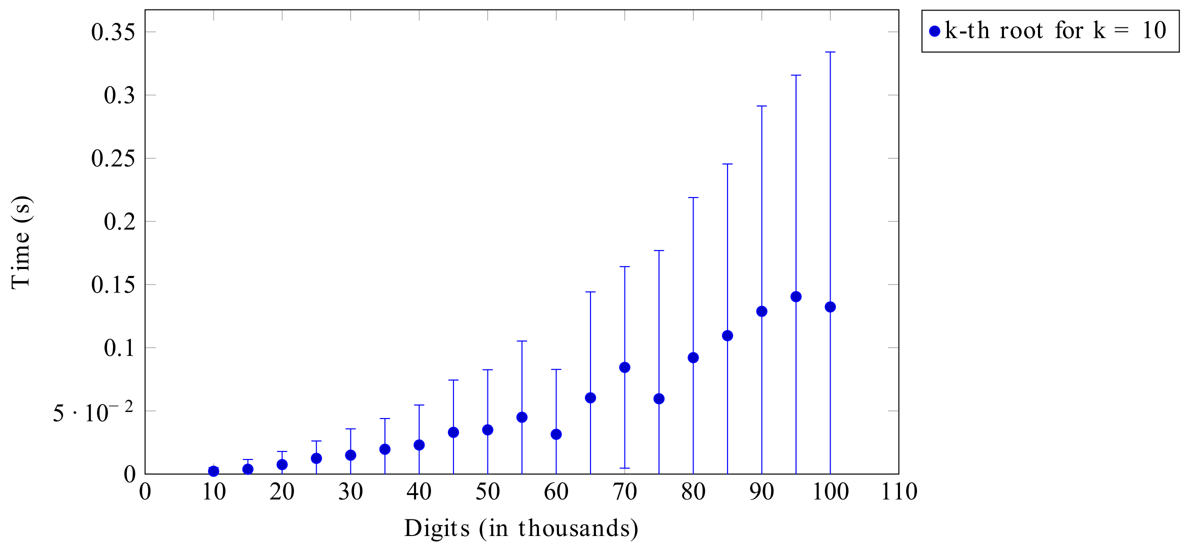
Comparing with the existing implementation, the new implementation is 300x faster for 10K digits,



See below the performance for various values of k,



As an extension, the performance tests for up to 100K digits, show that the implementation is efficient for an even wider range of values.



Log implementation

code: log AGM, correctness tests and performance tests

Implementations

Existing implementation: The existing implementation computes $\log(x)$, by writing x as $a \cdot 2^n$ and setting $y = a - 1$. Then $\log(x) = n\log(2) + \log(a) = n\log(2) + \log(1 + y)$. The constant $\log(2)$ is hardcoded and $\log(1 + y)$ is computed using Maclaurin series:

$$\log(1 + y) = \sum_{i=1}^{\infty}(-1)^{i+1}\frac{y^i}{i}$$

AGM-based: Gauss introduced the arithmetic-geometric method (AGM), where two initial values a_0 and b_0 are chosen and

$$a_n := \frac{a_{n-1} + b_{n-1}}{2} \quad \text{and} \quad b_n := \sqrt{a_{n-1}b_{n-1}}.$$

For any initial values with $a_0 \geq b_0$, the sequence converges to a finite value $M(a_0, b_0)$by Bolzanno-Weirstrass as $a_0 \leq a_1 \leq \ldots \leq b_1 \leq b_0$.

Gauss proved that a sequence with $a_0 = 1$ and $b_0 = x$ converges to $\frac{\pi}{2E(x)}$, where

$$E(x) = \int_0^{\pi/2}\frac{d\theta}{\sqrt{1-(1-x^2)\sin^2\theta}}dx$$

The elliptic function $E(x)$ satisfies $E(4/x) = \ln(x) + \frac{4\ln(x) - 4}{x^2} + o(x^{-2})$. Hence, one can evaluate x to p digits of precision using

$$\ln(x) \approx \frac{\pi}{2M(1,\ 4/s)} - m\ln(2)$$

where $s = x2^m > 2^{p/2}$. This algorithm has $\mathcal{O}(\log p)$ operational complexity and $\mathcal{O}(M(p)\log p)$, where $M(p)$ is the time complexity of multiplication. The implementation is based on the description in (Borwein and Borwein, 1987) and Section 7.5.2 in (Muller 2006)

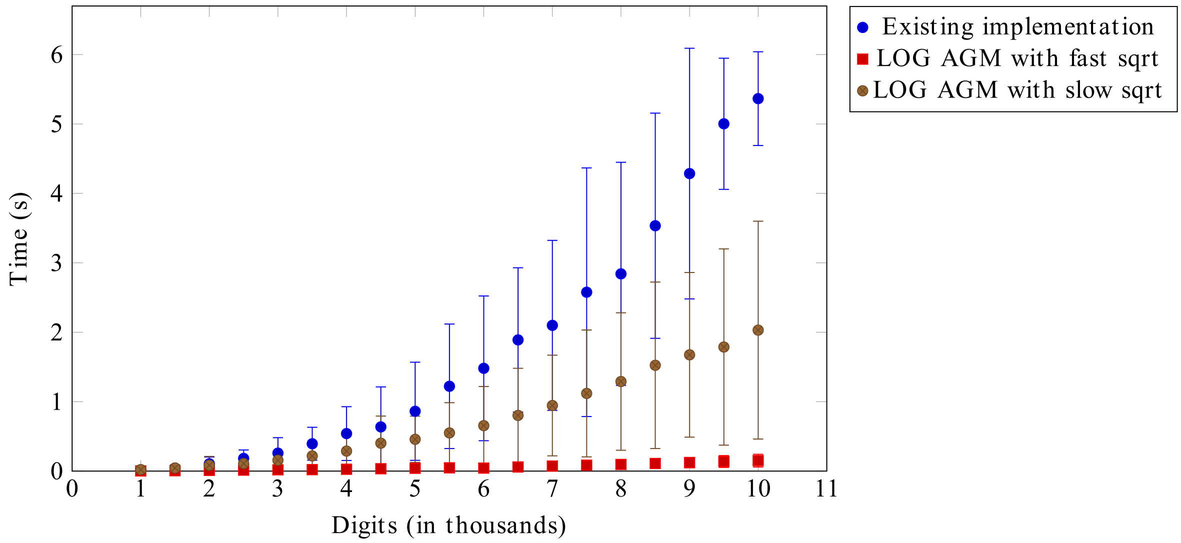
Correctness tests

The following correctness tests were run (see here):

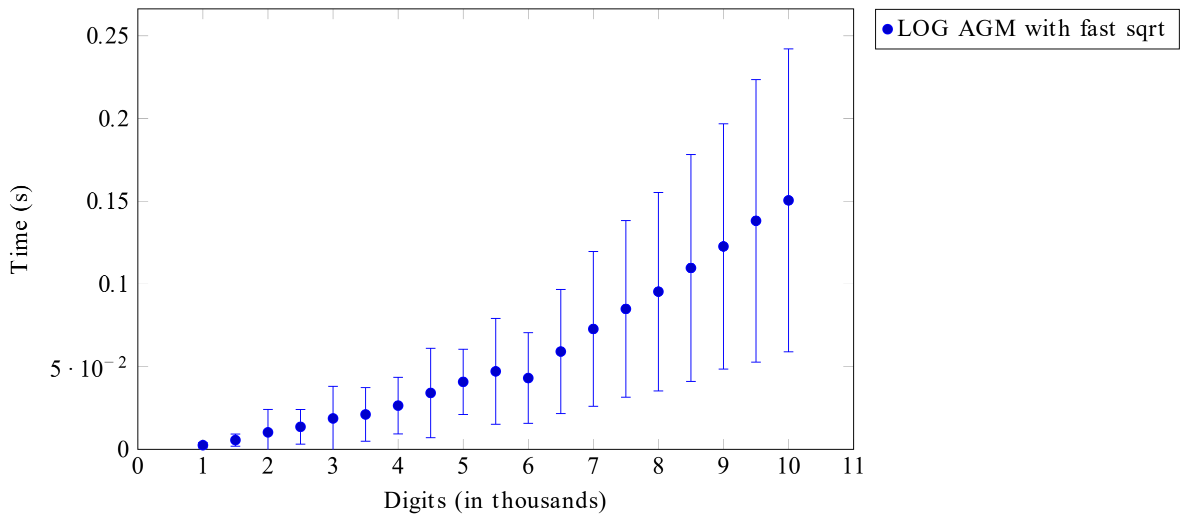
- Tests of extreme values (infinity, zero)
- Tests of edge cases (1, e)
- Tests for various pseudo-random values.
- Stress tests by comparing the log() of 50 random values with the output of MPFR.
- Tests for different ranges: close to zero, just below 1/2, just above 1/2, just below 1, just above 1

Performance tests

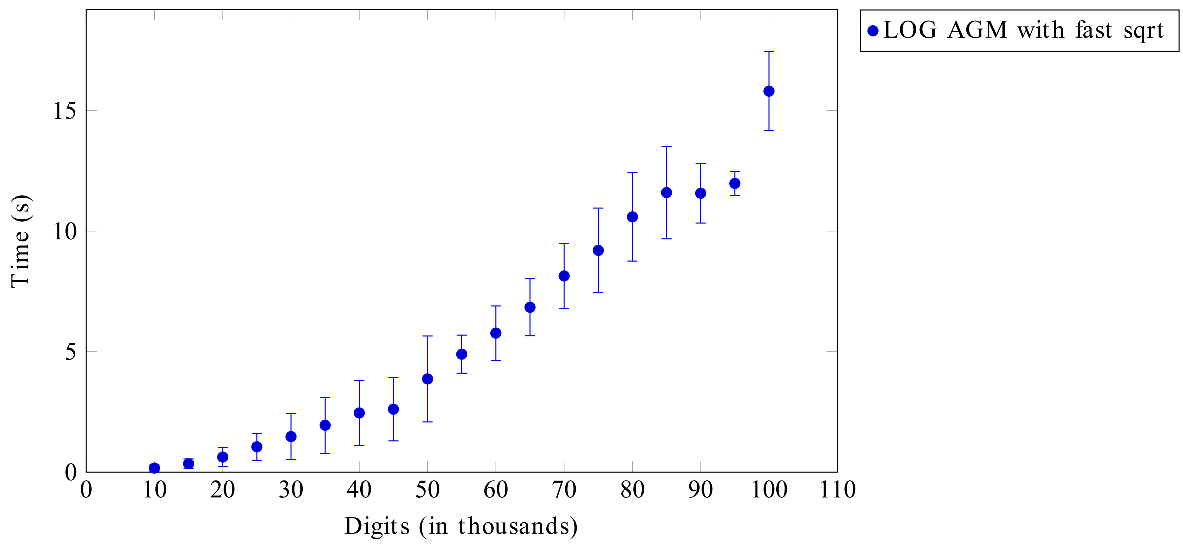
The tests where performed on the same 20 randomly sampled numbers. The error bars represent confidence intervals at 95% assuming each trial is i.i.d.



For more emphasis on the newly implemented method using the log AGM function:



As an extension we show that the log AGM implementation performance for up to 100K.



PI algorithms

code: pi algorithms (GL Un, Cub Un, GL, Qd, Cub, Qr, Qn, Non) and tests

Implementations

Existing implementation: The existing implementation simply has a hardcoded value for pi.

New implementations: We added the Gauss-Legendre algorithm and some of the variants introduced by the Borwein brothers:

- Gauss-Legendre (GL Un), with implementation based on Algorithm 16.148 of (Arndt and Haenel, 2001) (mentor's implementation).
- Cubic Borwein (Cub Un) with implementation based on Algorithm 16.151 of (Arndt and Haenel, 2001) (mentor's implementation).

- Gauss-Legendre (GL) (the non-Schoenhage variant).
- Quadratic Borwein (Qd) (uses sqrt) based on Algorithm 2.1 on p.46 of (Borwein and Borwein, 1987).
- Cubic Borwein (Cub) basic implementation (uses cbrt method, so it is not expected to benefit from any of the improvements) based on p.47 of (Borwein et al. 1994).
- Quartic Borwein (Qr) (uses sqrt twice) based on Algorithm 5.3 on p.170 of (Borwein and Borwein 1987).
- Quintic Borwein (Qn) (uses 5-th root) based on (Borwein and Borwein, 1989).
- Nonic Borwein (Non) (uses cbrt) based on (Bailey et al. 1997).

Correctness tests

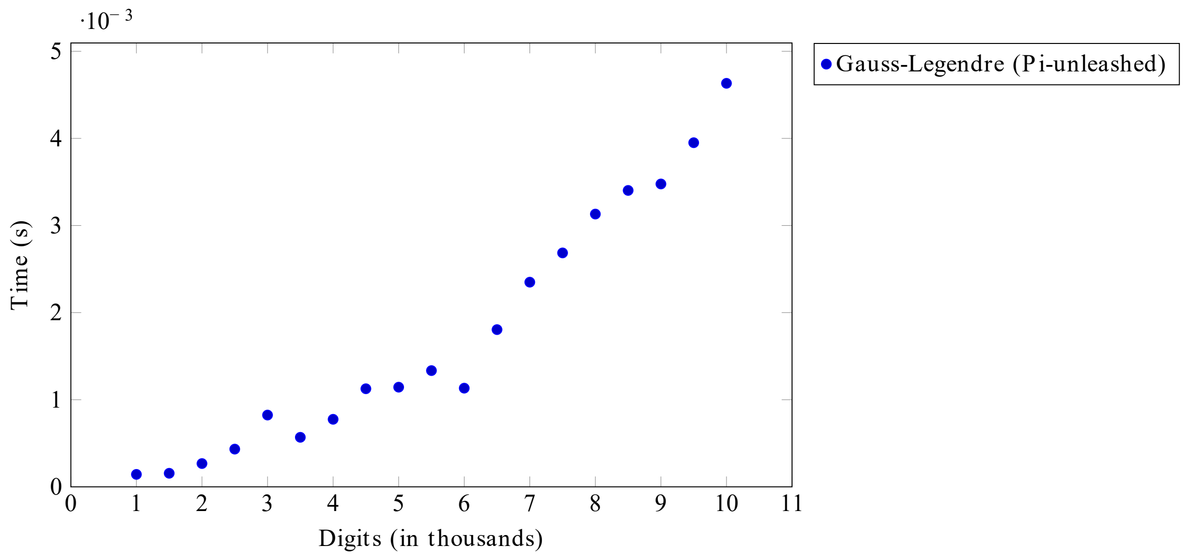
The tests simply compared the digits with various publicly available collections of pi digits.

Performance tests

Below is a table with the performance of each implementation on a set of digits. The shaded rows show the performance of the algorithms without the newest changes (efficient sqrt and kth-root). With the exception of cubic Borwein (which uses cbrt), all others show a significant improvement. The fastest method was Gauss-Legendre (with the Unleash Pi implementation).

Method/N	GL Un	Cub Un	GL	Qd	Cub	Qr	Qn	Non
1K	0.003268s	0.003646s	0.000948s	0.002509s	0.003997s	0.001952s	0.012384s	0.006122s
	0.017836s	0.004957s	0.009617s	0.008635s	0.004179s	0.013524s	0.208164s	0.005892s
5K	0.012640s	0.113406s	0.020494s	0.063762s	0.116883s	0.029694s	0.313708s	0.149207s
	0.255039s	0.130431s	0.268763s	0.263724s	0.126375s	0.284409s	18.019207s	0.163338s
10K	0.047336s	0.473562s	0.064468s	0.298860s	0.433946s	0.096938s	1.32719s	0.548498s
	1.094545s	0.517367s	1.091298s	0.969387s	0.485853s	1.050066s	155.949646s	0.686482s
50K	1.075196s	10.947395s	1.115937s	5.745923s	11.148762s	2.091759s	41.4093s	15.325591s
	27.866652s	13.622281s	28.721098s	26.763367s	12.883669s	35.426968s		17.174911s
100K	3.919699s		4.652693s	26.834837s		9.370837s		
500K	97.616852s		121.964401s					

Below, we show a more detailed plot of the performance of GS Un, against various digits up to 10K.



VC builds for MPFR and MPIR

This GSoC work also created basic support for VC builds of MPIR and MPFR. The MPIR build is based on the original work of https://github.com/wbhart/mpir (GMP_VERSION version 6.0.0 and MSC_MPIR_VERSION 3.0.0). Instructions for building and running MPIR and MPFR with Boost are the following:

1. Obtain a copy of vsyasm.
2. Copy the file `yasm` to `C:\Program Files\yasm\`.
3. Set a user variable `YASMPATH=<path to YASM assembler>` (e.g. `C:\Program Files\yasm\`).
4. Ensure that path you have selected matches that in `example\mpfr_vc_and_mpir_vc\mpir_vc\yasm\vsyasm.props`.
5. Supply a custom build rule to Visual Studio 2019:
    1. Identify a directory such as: `C:\Program Files (x86)\Microsoft Visual Studio\2019\Community\MSBuild\Microsoft\VC\v160\BuildCustomizations`
    2. Here, custom build rules reside in files with extensions ".props" and ".targets"
    3. Copy `vsyasm.props`, `vsyasm.targets` and `vsyasm.xml` to this directory, so that VS can find the custom rules for yasm.
6. (Make sure that you have set `BOOST_ROOT` to the root directory of the Boost version you want to run).
7. Open `example\mpfr_vc_and_mpir_vc\test_with_boost\test_with_boost.sln` (here) and run.

Future work:

- Using Newton-Raphson method, we can compute the complex exponential function (see preliminary work: code and tests). In turn, this will give efficient implementations for sine and cosine.
- The following functions could be optimised further: eval_msb, create a function that computes and returns both the remainder and the quotient.

References

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