Continued fractions and number systems: applications to correctly-rounded implementations of elementary functions and modular arithmetic.

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1. Continued fraction expansion reminders
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Notations

Let a real $0 < \alpha < 1$. There exists a unique integer sequence $(k_i)_{i\in\mathbb{N}}$ with $k_i \in \mathbb{N}^*$ such that

$$\alpha = \cfrac{1}{k_1 + \cfrac{1}{k_2 + \cfrac{1}{\ddots}}} := [0; k_1, k_2, \ldots].$$

This sequence is finite if α is rational, or infinite otherwise.

Notations

We denote by :

- $(r_i)_{i\in\mathbb{N}}$ the real sequence of the *tails* of α such that $\alpha = [0; k_1, k_2, \ldots, k_i + r_i]$;
- $(p_i/q_i)_{i\in\mathbb{N}}$ the rational sequence of the *convergents* such that $p_i/q_i = [0; k_1, k_2, \ldots, k_i]$;
- $(\theta_i)_{i\in\mathbb{N}}$ the real sequence of the such that $\theta_i = |q_i\alpha - p_i|$;

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- $(\theta_i)_{i\in\mathbb{N}}$ the real sequence of the such that $\theta_i = |q_i\alpha - p_i|$;

Leitmotif of the talk

Use the fact that $r_i = \theta_i/\theta_{i-1}$ to do modular arithmetic !

Recurrence relations

All sequences can be computed recursively :

$$\begin{array}{lll} p_{-1} = 1 & p_0 = 0 & p_i = p_{i-2} + k_i p_{i-1}, \\ q_{-1} = 0 & q_0 = 1 & q_i = q_{i-2} + k_i q_{i-1}, \\ \theta_{-1} = 1 & \theta_0 = \alpha & \theta_i = \theta_{i-2} - k_i \theta_{i-1}. \end{array}$$

with $k_i = \lfloor \theta_{i-2} / \theta_{i-1} \rfloor$.
k_i can be computed by subtraction (subtraction-based Euclidean algorithm) or by division (division-based Euclidean algorithm).

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The IEEE 754-2008 standard

Aim

Ensure predictable and portable numerical software.

Basic Formats

- single-precision (binary32)
- double-precision (binary64)
- quadruple-precision (binary128)

Rounding Modes

- Rounding to nearest
- Directed rounding (towards 0, $-\infty$ and $+\infty$)

Correctly rounded operations

$+, -, \times, /, \sqrt{\ }$

And for elementary mathematical functions ?

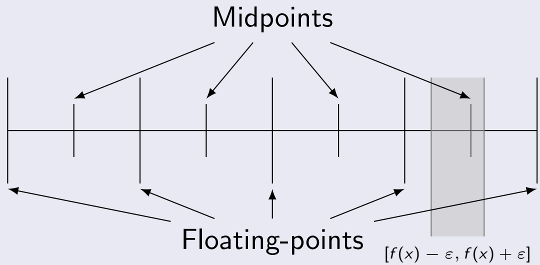
exp, log, sin, cos, tan, $\cdots$

$\Rightarrow$ IEEE-754-2008 only recommends correct rounding because of the Table Maker's Dilemma

Correct rounding

$$\circ_p(f(x) \pm \varepsilon) = \circ_p(f(x))$$

Hard-to-round case



Function Isolate(Exists ?, P, D, depth, k)

Input: `Exists?` (P, D) test the existence of (p, ϵ') HR-cases of P in D, P an approximation of f in D, depth and k two integers

if `Exists?` *(P, D)* **then**
  if *depth* $=$ *0* **then**
    retourner `ExhaustiveSearch` (P, D);
  else
    $(D_1, \ldots, D_k) :=$ `Subdivide` (D, k);
    $(P_1, \ldots, P_k) :=$ `Refine` (P, D, k);
    return $\bigcup_i$ `Isolate` (`Exists?`, P_i, D_i, depth - 1, k);
else
  return $\emptyset$;

Function Isolate(Exists?, P, D, depth, k)

Input: `Exists?` (P, D) test the existence of (p, ϵ') HR-cases of P in D, P an approximation of f in D, depth and k two integers

```
if Exists? (P, D) then
    if depth = 0 then
        retourner ExhaustiveSearch (P, D);
    else
        (D_1, ..., D_k) := Subdivide (D, k);
        (P_1, ..., P_k) := Refine (P, D, k);
        return ⋃_i Isolate (Exists?, P_i, D_i, depth - 1, k);
else
    return ∅;
```

HR-case existence test

Problem

Given $P \in \mathbb{R}[x]$, is there any $x \in [\![0, \#_p D]\!]$ such that

$$P(x) \mod 1 < \epsilon.$$

Solutions (with p the floating-point precision)

- Exhaustive search : $O(2^p)$;
- Lefèvre when $\deg P = 1$: $O(2^{2p/3})$ intervals in $O(p^2)$;
- SLZ when $\deg P > 1$: $O(2^{p/2})$ intervals in $O(\text{poly}(p, \deg P, \alpha))$.

Example of computation times

- e^x in full domain and $p = 53$ with Lefèvre : 5 years of CPU time ;
- 2^x in $[1/2, 1[$ and $p = 64$ with SLZ : 8 years of CPU time.

Challenges

- Binary128 is actually out of reach ;
- compute the hardest-to-round case for each of the 32 functions recommended by the IEEE std 754-2008 in binary64 ;
- tackle any function in reasonable time in binary64 ;
- and certify the results.

Lefèvre HR-case search

- Efficient for binary64 in practice : all known hardest-to-round in binary64 have been generated by Lefèvre ;

$$\left.\begin{array}{l}\bullet\ \text{Massively parallel ;}\\ \bullet\ \text{Fine-grain parallelism.}\end{array}\right\}\ \text{Perfect for GPU !}$$

Lefèvre HR-case existence test

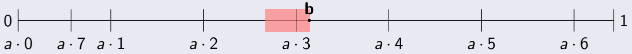
Problem

Given $b - ax \in \mathbb{R}[x]$, is there any $x \in [\![0, \#_p D]\!]$ such that

$$b - ax \mod 1 < \epsilon.$$

Geometrically

Is there any multiple of a in $\{ax \bmod 1 \mid x \leq \#_p D\}$ at a distance less than ϵ to the left of b?



The three distance theorem

Three distance theorem (Slater)

The points $\{a \cdot x \mod 1 \mid x < N\}$ split the segment $[0, 1[$ into N segments. Their lengths take at most three different values, one being the sum of the two others.

Link with continued fraction expansion

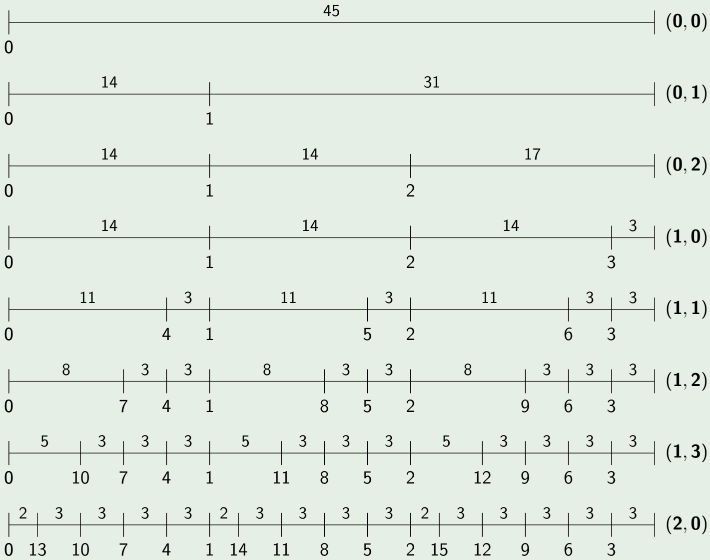
Given $a = [0; k_1, k_2, k_3, \dots]$ and $\frac{p_i}{q_i}$ the i^{th} convergent.

- The lengths are the $\theta_{i-1,t} = \theta_{i-1} - t \cdot \theta_i$, with $0 \leq t < k_{i+1}$.
  Their number are the $q_{i-1,t} = q_{i-1} + t \cdot q_i$, with $0 \leq t < k_{i+1}$.
- There are $O(\log N)$ two-length configurations and they verify

$$q_i \theta_{i-1,t} + q_{i-1,t} \theta_i = 1.$$

- Interpretation : if we place $N = q_i + q_{i-1,t}$ multiples of a,
  - there are q_i intervals of length $\theta_{i-1,t}$;
  - there are $q_{i-1,t}$ intervals of length θ_i.

Example : $a = 14/45$

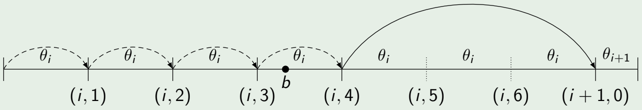


Lefèvre HR-case existence test

Idea

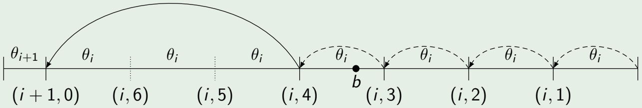
Write b in the basis $(\theta_{i,t})_{i\in\mathbb{N}}$ to get best approximations.

If i is even



$$(b-\tilde{b}_{i,t+1}) = (b-\tilde{b}_{i,t}) - \theta_i \quad \text{or} \quad (b-\tilde{b}_{i+1,0}) = (b-\tilde{b}_{i,t})$$

If i is odd



$$(b-\tilde{b}_{i+1,0}) = (b-\tilde{b}_{i,t}) - \theta_{i-1,t+1} \quad \text{or} \quad (b-\tilde{b}_{i,t+1}) = (b-\tilde{b}_{i,t})$$

An irregular control flow : bad for SIMD

Algorithm 1: Lefèvre HR-case existence test.

input : $b - a \cdot x$, ϵ'', N

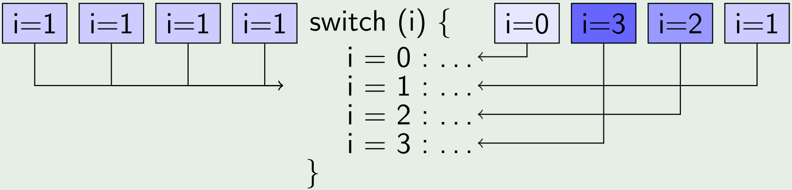
initialisation : $p \leftarrow \{a\}$; $q \leftarrow 1 - \{a\}$; $d \leftarrow \{b\}$;
$u \leftarrow 1$; $v \leftarrow 1$;

if $d < \epsilon''$ **then return** Failure;
while *True* **do**
    if $d < p$ **then**
        $k = \lfloor q/p \rfloor$;
        $q \leftarrow q - k * p$; $u \leftarrow u + k * v$;
        if $u + v \geq N$ **then return** Success;
        $p \leftarrow p - q$; $v \leftarrow v + u$;
    else
        $d \leftarrow d - p$;
        if $d < \epsilon''$ **then return** Failure;
        $k = \lfloor p/q \rfloor$;
        $p \leftarrow p - k * q$; $v \leftarrow v + k * u$;
        if $u + v \geq N$ **then return** Success;
        $q \leftarrow q - p$; $u \leftarrow u + v$;

SPMD on SIMD

- Develop a scalar program : a *kernel*
- Launch multiple threads running the same *kernel*
- Group their execution on SIMD units by *warps* of 32 threads

Control flow regularity

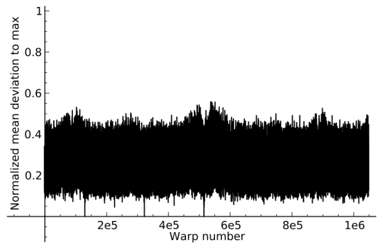


An irregular control flow : loop divergence

Normalized mean deviation to the maximum (NMDM)

$$1 - \frac{Mean(\{n_i, 0 \leq i < w\})}{Max(\{n_i, 0 \leq i < w\})}$$

Lefèvre existence test (e^x, $[1, 1+2^{-13}]$, $\epsilon = 2^{-32}$)



No implementation trick works !

- Re-organize data $\Rightarrow$ no *a priori* information
- Compute several sub-domains per thread without exiting the loop $\Rightarrow$ too few instructions to issue in the loop to offset the extra cost.

An irregular control flow

Why Lefèvre HR-case existence test is irregular ?

It goes from subtraction-based to division-based Euclidean algorithm depending on the position of b.
$\Rightarrow$ The number of loop iterations is hence conditioned by :

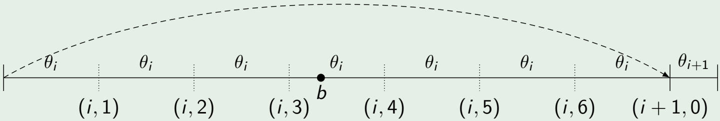
- the position of b on the unit segment,
- the number of quotient to compute and
- the value of the quotients.

Goal

Break this dependency by considering only $(i, 0)$ configurations.
$\Rightarrow$ Write b in the basis $(\theta_i)_{i\in\mathbb{N}}$ to obtain the same sequence of best approximations.

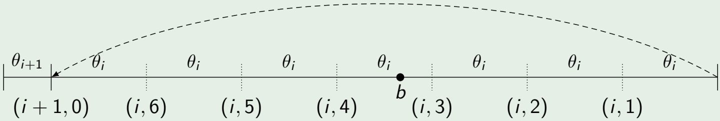
New reduction rules

If i is even



$$(b - \tilde{b}_{i+1}) = (b - \tilde{b}_i) \mod \theta_i$$

If i is odd



$$(b - \tilde{b}_{i+1}) = (b - \tilde{b}_i) - \theta_{i+1} \mod \theta_i$$

Divergence in the regular algorithm

Algorithm 2: Regular HR-case existence test.

input : $b - a \cdot x$, ϵ'', N

initialisation : $p \leftarrow \{a\}$; $q \leftarrow 1$; $d \leftarrow \{b\}$;
$u \leftarrow 1$; $v \leftarrow 0$;

if $d < \epsilon''$ **then return** Failure;

while *True* **do**

    if $p < q$ **then**

        $k = \lfloor q/p \rfloor$;

        $q = q - k * p$; $u = u + k * v$;

        $d = d \mod p$;

    else

        $k = \lfloor p/q \rfloor$;

        $p = p - k * q$; $v = v + k * u$;

        if $d \geq p$ **then**

            $d = (d - p) \mod q$;

    if $u + v \geq N$ **then return** $d > \epsilon''$;

Divergence on the main conditional branch

A deterministic test

i is alternatively odd and even.

$\Rightarrow$ We can avoid divergence by unrolling 2 loop iterations.

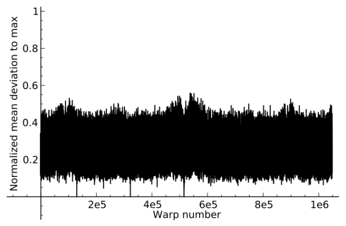
Algorithm 3: Regular HR-case existence test unrolled.

```
input : b − ax, ε'', N
initialisation :  p ← {a} ;   q ← 1 ;   d ← {b} ;
                  u ← 1 ;     v ← 0 ;
while True do
    k = ⌊q/p⌋;
    q = q − k ∗ p ; u = u + k ∗ v;
    d = d mod p;
    if u + v ≥ N then return d > ε'';
    k = ⌊p/q⌋;
    p = p − k ∗ q ; v = v + k ∗ u;
    if d ≥ p then
        d = d − p mod q;
    if u + v ≥ N then return d > ε'';
```

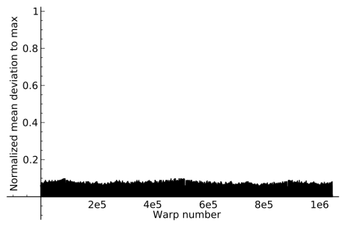
Normalized mean deviation to the maximum (NMDM)

$$1 - \frac{Mean(\{n_i, 0 \leq i < w\})}{Max(\{n_i, 0 \leq i < w\})}$$

Lefèvre Algorithm



New Algorithm



A regular control flow

Why the regular HR-case existence test is regular ?

It uses only division-based Euclidean algorithm.
$\Rightarrow$ The number of loop iterations only depend on the number of quotient to compute, which is very stable from one interval to the next.

	Seq.	MPI	CPU-GPU	$\frac{\text{Seq.}}{\text{MPI}}$	$\frac{\text{MPI}}{\text{CPU-GPU}}$
Pol. approx.	43300.81	5251.53	788.84	8.25	6.66
Lefèvre	36816.10	5292.67	2446.27	6.96	2.16
Regular	34039.94	4716.97	711.92	7.22	6.63
Lef. /Reg.	1.08	1.12	3.44	–	–

TABLE : Performance result on e^x in $[1, 2[$ for binary64 (Intel Xeon X5650 hexa-core , Nvidia C2070). Lefèvre MPI/New GPU : 7.4 .

Perspectives

Remaining development

- Argument reduction of periodic functions for large binades
- Implicit vectorization (OpenCL, ispc, . . .)

Lefèvre HR-case existence test

- Consider minimax approximations (libsollya) rather than Taylor to widen domains ?
- Generalize Lefèvre test to higher degree polynomial (change of variable + Hensel lifting) ?

SLZ

- Efficient parallel implementation of LLL
- Use structure of Coppersmith lattices
- Investigate structure in lattices involved in Coppersmith method over translated polynomials

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Modular arithmetic and CF

Notations

- $(\theta_i)_{i\in\mathbb{N}}$ sequence of the $|q_i\alpha - p_i|$ in CF,
- $(\theta'_i)_{i\in\mathbb{N}}$ sequence of the $|q_i a - p_i d|$ in extgcd(a, d).

Remark

- CF is arithmetic modulo 1,
- CF over a rational a/d and gcd(a, d) is identical, only difference is $\theta'_i = d \cdot \theta_i$.

Goal

Use $(\theta_i)_{i\in\mathbb{N}}$ number scale to perform modular operations.

Number systems based on CF

Ostrowski integer number system

Given $(q_i)_{i \in \mathbb{N}}$ the denominators of the convergents of any irrational $0 < \alpha < 1$, every positive integer b can be uniquely written as

$$b = 1 + \sum_{i=1}^{m} b_i q_{i-1}$$

where $\begin{cases} 0 \leq b_1 \leq k_1 - 1, 0 \leq b_i \leq k_i, \text{ for } i \geq 2, \\ b_i = 0 \text{ if } b_{i+1} = k_{i+1}. \end{cases}$

Associated number scale over real numbers : $((-1)^i \theta_i)_{i \in \mathbb{N}}$.
Decomposition algorithm : greedy algorithm by default.

Number systems based on CF

Signed Ostrowski integer number system

Given $(q_i)_{i\in\mathbb{N}}$ the denominators of the convergents of any irrational $0 < \alpha < 1$, every positive integer b can be uniquely written as

$$b = 1 + \sum_{i=1}^{m} (-1)^i b_i q_{i-1}$$

where $\begin{cases} 0 \leq b_1 \leq k_1 - 1, 0 \leq b_i \leq k_i, \text{ for } i \geq 2, \\ b_{i+1} = 0 \text{ if } b_i = k_i. \end{cases}$

Associated number scale over real numbers : $(\theta_i)_{i\in\mathbb{N}}$.
Decomposition algorithm : greedy algorithm by excess.

Modular multiplication

$$\text{Compute } c = a \cdot b \mod d.$$

Algorithm

1. Compute the sequences $(\theta'_i)_{i\in\mathbb{N}}$ and $(q_i)_{i\in\mathbb{N}}$ from extgcd(a, d)
2. Compute the sequence $(b_i)_{i\in\mathbb{N}}$ such that $b = 1 + \sum_{i=1}^{m} b_i q_{i-1}$
3. Return $a + \sum_{i=1}^{m} b_i (-1)^i \theta'_{i-1}$

Proof : Let $\alpha = a/d$ and $b = 1 + \sum_{i=1}^{m} b_i q_{i-1}$.

$$\alpha \cdot b = \alpha + \sum_{i=1}^{m} b_i q_{i-1} \alpha$$

As $(-1)^i \theta_i = q_i \alpha - p_i$,

$$\alpha \cdot b = \alpha + \sum_{i=1}^{m} b_i (-1)^i \theta_{i-1} + \sum_{i=1}^{m} b_i p_{i-1}$$

By the uniqueness of the decomposition,

$$0 \leq \alpha + \sum_{i=1}^{m} b_i (-1)^i \theta_{i-1} < 1.$$

And finally, by multiplying by d, we get

$$0 \leq a + \sum_{i=1}^{m} b_i (-1)^i \theta'_{i-1} < d$$

Modular division

Compute $c = a^{-1} \cdot b \mod d$.

Algorithm

1. Compute the sequences $(\theta'_i)_{i \in \mathbb{N}}$ and $(q_i)_{i \in \mathbb{N}}$ from $\mathrm{extgcd}(a, d)$
2. Compute the sequence $(b_i)_{i \in \mathbb{N}}$ such that
$$b = a + \sum_{i=1}^{m} b_i (-1)^{i-1} \theta'_{i-1}$$
3. Return $1 + \sum_{i=1}^{m} b_i q_{i-1}$

Proof : Similar to modular multiplication.

Complexity considerations

Compute the sequences $(\theta'_i)_{i\in\mathbb{N}}$ and $(q_i)_{i\in\mathbb{N}}$ from extgcd(a, d)

$$O(\log(d)^2)$$

Compute the sequence $(b_i)_{i\in\mathbb{N}}$ from $(q_i)_{i\in\mathbb{N}}$ (or $(\theta'_i)_{i\in\mathbb{N}}$)

$$O(\log(d)^2)$$

Evaluate the sequence $(b_i)_{i\in\mathbb{N}}$ in $(\theta'_i)_{i\in\mathbb{N}}$ (or $(q_i)_{i\in\mathbb{N}}$)

$$O(\log(d)^2)$$

Implementation considerations

Both algorithm

- Integrate multiplication and reduction
  $\Rightarrow$ we manipulate only words of size less than $\log d$;
- Quotients k_i and b_i can be computed only with subtractions as they are likely very small
  $\Rightarrow$ mean value is Khinchin constant ≈ 2.69.

Modular Multiplication

- $(q_i)_{i\in\mathbb{N}}$ is an increasing sequence
  $\Rightarrow$ every $q_i \leq b$ need to be stored to decompose b
  $\Rightarrow$ the needed part of the sequence is of size $O(\log(b)^2)$.

Modular Division

- $(\theta_i)_{i\in\mathbb{N}}$ is an decreasing sequence
  $\Rightarrow$ we can decompose b on-the-fly
  $\Rightarrow$ no extra storage is needed !

Perspectives

Algorithm enhancement

- Use other decompositions from Euclidean algorithm ?
  - compute remainders with centered division
  - use decomposition from three distance theorem (irregular control flow ? optimal ?)
- Find mean optimal decomposition (minimizing $\sum |b_i| + |k_i|$)
- Use binary GCD algorithm to build the sequences $(\theta_i)_{i\in\mathbb{N}}$ and $(q_i)_{i\in\mathbb{N}}$ and avoid divisions ?

Perspectives

Implementation

- We have a 64 bits proof of concept C implementation (speedup of $1.5 - 2.5$x over GMP). Now provide multiprecision.

Searching application...

- Compact hardware implementation of modular arithmetic ? (Jérémie ?)
- When multiple modular mult/div by the same value a are needed (e.g. Gauss elimination) ?

Thank you for your attention ! !

Any question, remark, recommendation ?

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