

Real root isolation for univariate polynomials on GPUs and multicores

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Direction of the research activities of Marc Moreno Maza's team :

- Study theoretical aspects of systems of polynomial equations and try to answer the question “what is the best form for the set of solutions ?”
- Study algorithmic answers to the question “how can we compute this form of the set of solutions at the lowest cost ?”
- Study implementation techniques for algorithms to make the best use of today's computers.
- Apply it to unsolved problems when the prototype solver is ready.

Main purpose of the Lab

The laboratory works in close cooperation with *Maplesoft*.



Maple 16

Current main purpose of the laboratory :

- Provide Maple's end-users with symbolic computation tools.
- Take advantage of hardware acceleration technologies, using GPUs and multicores, using the best computer ressources.
- Develop the library *cumodp* which will be integrated into Maple so as to provide fast arithmetic operations over prime fields.

Purpose of my internship

- contribute to the library *cumodp*
- develop code for exact calculation of the real roots of univariate polynomials
- use mathematical tools : *Descartes' rule of signs*, *Fast Fourier transform*, computing by *homomorphic images*...
- realize algorithms using GPUs

Descartes' rule of sign

Descartes' rule of signs (DRS)

Consider a univariate polynomial $P \in \mathbb{R}[X]$ and the sequence (a_n) of its non-zero coefficients. Let c be the number of sign changes of the sequence (a_n) . Then the number of positive roots of P is at most c .

Gauss' property

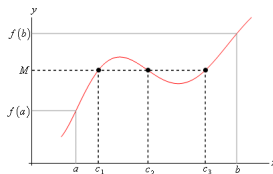
If we consider the previous rule of signs and count the roots with their multiplicities, then the number of positive real roots of P has the same parity as c .

This rule can also be used to determine the number of negative real roots of polynomials.

Intermediate values theorem

Intermediate values theorem (IVT)

If f is a real-valued continuous function on the interval $[a, b]$ and M is a number between $f(a)$ and $f(b)$, then there exists $c \in [a, b]$ such that we have $f(c) = M$.



In particular if $M = 0$, then there exists $c \in [a, b]$ such that $f(c) = 0$ holds.

Horner's method

- We want to evaluate the following polynomial :

$$P(X) = \sum_{i=0}^n a_i X^i = a_0 + a_1 X + a_2 X^2 + \cdots + a_n X^n$$

A better way to evaluate it is to use **Horner's method**, that is, represents P in the following form :

$$P(X) = a_0 + X (a_1 + X (a_2 + X (\cdots (a_{n-1} + (a_n X) \cdots))))$$

- costs of operations : $\Theta(n)$ for *Horner's method*, $\Theta(n^2)$ for naive method.

Example of real root search

Let's consider $P(X) = X^3 + 3X^2 - X - 2$: $c = 1$ so P has 1 positive root.
 $P(-X) = -X^3 + 3X^2 + X - 2$: $c = 2$ so P has 2 or 0 negative roots.

$P(-1) = 1$, $\lim_{X \rightarrow -\infty} P(X) = -\infty \Rightarrow \exists r_1 \in]-\infty; -1[\mid P(r_1) = 0$
 $\Rightarrow P$ has 2 negative roots.

Let's use the IVT for $M = 0$:

The following evaluations of P can be done using the *Horner's method*.

As $P(-1) = 1$ and $P(-2) = -2$, then $r_1 \in]-2, -1[$.

As $P(0) = -2$ and $P(-1) = 1$, then $r_2 \in]-1, 0[$.

As $P(0) = -2$ and $P(1) = 1$, then $r_3 \in]0, 1[$.

Vincent-Collins-Akritas' algorithm

The **Vincent-Collins-Akritas' algorithm** (VCA) computes a list of disjoint intervals with rational endpoints for a polynomial P such that :

- each real root of P belongs to a single interval, and
- each interval contains only one real root of P .

Algorithm 1: RealRoots(p)

Input: a univariate squarefree polynomial p of degree d
Output: the number of real roots of p

```

1 begin
2   Let  $k \geq 0$  be an integer such that
   the absolute value of all the real
   roots of  $p$  is less than or equal to
    $2^k$ ;
3   if  $x \mid p$  then  $m := 1$  else  $m := 0$ ;
4    $p_1 := p(2^k x)$ ;
5    $p_2 := p_1(-x)$ ;
6    $m' := \text{RootsInZeroOne}(p_1)$ ;
7    $m := m + \text{RootsInZeroOne}(p_2)$ ;
8   return  $m + m'$ ;
9 end
```

Algorithm 2: RootsInZeroOne(p)

Input: a univariate squarefree polynomial p of degree d
Output: the number of real roots of p in $(0, 1)$

```

1 begin
2    $p_1 := x^d p(1/x)$ ;
3    $p_2 := p_1(x+1)$ ; // Taylor shift
4   Let  $v$  be the number of sign
   variations of the coefficients of  $p_2$ ;
5   if  $v \leq 1$  then return  $v$ ;
6    $p_1 := 2^d p(x/2)$ ;
7    $p_2 := p_1(x+1)$ ; // Taylor shift
8   if  $x \mid p_2$  then  $m := 1$  else  $m := 0$ ;
9    $m' := \text{RootsInZeroOne}(p_1)$ ;
10   $m := m + \text{RootsInZeroOne}(p_2)$ ;
11  return  $m + m'$ ;
12 end
```

The algorithm 2 is called several times and inside it, *Taylor shift by 1* also \implies : *Taylor shift by 1* needs to be optimized at the lowest cost possible.

Modular arithmetic

A current problem : expressions in the coefficients swell when computing with polynomial or matrices over a field (\mathbb{Z} e.g.) \Rightarrow performance bottleneck for computer algebra.

Two solutions :

- use highly optimized multiprecision libraries (e.g. Gmp), and
- compute by **homomorphic images**.

Ways to compute by homomorphic images :

- use the *Chinese Remainder Theorem*, or
- use the *Hensel's Lemma*.

Chinese Remainder Theorem (1)

Chinese Remainder Theorem 1st version (CRT1)

Consider m_1, m_2, \dots, m_r a sequence of r positive integers which are pairwise coprime. Consider also a sequence (a_i) of integers and the following system (S) of congruence equations :

$$(S) : \begin{cases} x \equiv a_1 \pmod{m_1} \\ x \equiv a_2 \pmod{m_2} \\ \vdots \\ x \equiv a_r \pmod{m_r} \end{cases}$$

Then (S) has a unique solution modulo $M = m_1 \times m_2 \times \dots \times m_r$:

$$x = a_1 \times M_1 \times y_1 + a_2 \times M_2 \times y_2 + \dots + a_r \times M_r \times y_r$$

with $\forall i \in \llbracket 1, r \rrbracket$, $M_i = \frac{M}{m_i}$ and $y_i \times M_i \equiv 1 \pmod{m_i}$.

Chinese Remainder Theorem (2)

Lemma

Let $f \in \mathbb{Z}[x]$ be nonzero of degree $n \in \mathbb{N}$ and $a \in \mathbb{Z}$. If the coefficients of f are absolutely bounded by $B \in \mathbb{N}$, then the coefficients of $g = f(x + a) \in \mathbb{Z}[x]$ are absolutely bounded by $B(|a| + 1)^n$.

Our future results will be given in $\mathbb{Z}[x]/M\mathbb{Z}$. Thanks to lemma, if M is sufficiently big, we could consider our results in $\mathbb{Z}[x]$. The algebraic form of the *Chinese Remainder Theorem* will be also used for *homomorphic images* :

Chinese Remainder Theorem 2nd version (CRT2)

Let us consider m_1, m_2, \dots, m_r a sequence of r positive integers which are pairwise coprimes and $M = m_1 \times m_2 \times \dots \times m_r$. Then :

$$\mathbb{Z}/M\mathbb{Z} \cong \mathbb{Z}/m_1\mathbb{Z} \times \mathbb{Z}/m_2\mathbb{Z} \times \dots \times \mathbb{Z}/m_r\mathbb{Z}$$

Taylor shift by a

Definition

The **Taylor shift by a** of a polynomial $P \in R[x]$, with R a field (e.g., \mathbb{Z}) consists of evaluating the coefficients of $P(x + a)$.

So, for a polynomial $P = \sum_{0 \leq i \leq n} f_i x^i \in \mathbb{Z}[x]$ and $a \in \mathbb{Z}$, we want to compute the coefficients $g_0, \dots, g_n \in \mathbb{Z}$ of the Taylor expansion :

$$Q(x) = \sum_{0 \leq k \leq n} g_k x^k = P(x + a) = \sum_{0 \leq i \leq n} f_i (x + a)^i$$

There are several methods to compute this, the classical ones deal with the *Horner's method*. There are also asymptotically fast methods, and in particular **Divide & Conquer method (D&C)** which we will use.

Divide & Conquer method (D&C)

Definition

The **size of a polynomial** of degree d is $d + 1$.

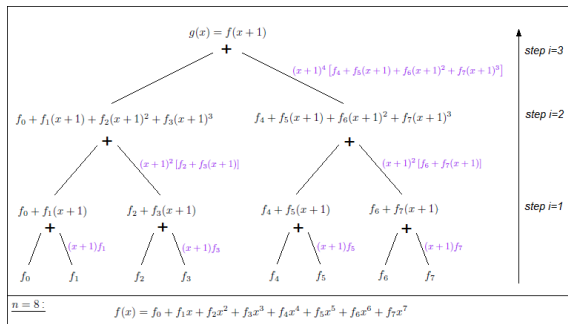
size of the polynomials considered : $n = 2^e$ (so degree : $d = 2^e - 1$)

The Divide & Conquer method consists of :

- ① **split** the polynomial as : $P(x) = P^{(0)}(x + 1) + (x + 1)^{n/2} \times P^{(1)}(x + 1)$
- ② **evaluate** $P^{(0)}(x + 1)$ and $P^{(1)}(x + 1)$ **recursively**
- ③ **compute a product** when $P^{(1)}(x + 1)$ is evaluated
- ④ **compute a sum** when $P^{(0)}(x + 1)$ and the product are evaluated

These are the four main things to implement to realize the *Taylor shift* by 1.

D&C tree for $n = 8 = 2^3$



D&C computing tree

In parallel, we consider the tree by levels (from its base) and not recursively.

Compute the $(x + 1)^{2^i}$ s

For multiplication, we need to compute the polynomials $(x + 1)^{2^i}$ for $i \in \llbracket 0, e - 1 \rrbracket$.

Consequence of the binomial theorem

According to the binomial theorem, we have in general :

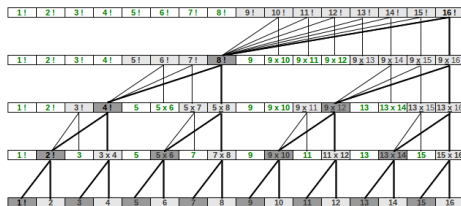
$$\forall n \in \mathbb{N}, (x + 1)^n = \sum_{k=0}^n \binom{n}{k} x^k \text{ with } \binom{n}{k} = \frac{n!}{k! (n - k)!}$$

Consequence : we need to compute the sequence $(i!)_{0 \leq i \leq n}$.

Factorial sequence

We compute only the sequence $(i!)_{1 \leq i \leq n}$ (power of 2).

Notation : $a \times b = \prod_{k=a}^b k$ (e.g. $9 \times 13 = 9 \times 10 \times 11 \times 12 \times 13$).

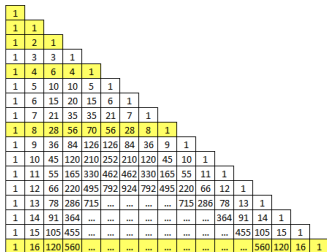


Mapping of the computation of the sequence $(i!)_{1 \leq i \leq 16}$

$n/2$ threads do products using a “pillar” factor (in the darkest boxes).

Work : $\Theta(n \log(n))$

Store the $(x+1)^{2^i}$ s



Pascal triangle

Array Monomial shift device for $n = 16 = 2^4$:

1	1	2	1	4	6	4	1	8	28	56	70	56	28	8	1
---	---	---	---	---	---	---	---	---	----	----	----	----	----	---	---

At step i , *local* $n = 2^i$:

$$\forall j \in \llbracket 0, local_n - 1 \rrbracket, Monomial_shift[local_n + j] = \binom{local_n}{j+1}$$

Divide & Conquer method

Recall how we can realize the *D&C method*.

The Divide & Conquer method consists of :

- 1 **split** the polynomial as : $P(x) = P^{(0)}(x+1) + (x+1)^{n/2} \times P^{(1)}(x+1)$
- 2 **evaluate** $P^{(0)}(x+1)$ and $P^{(1)}(x+1)$ **recursively**
- 3 **compute a product** when $P^{(1)}(x+1)$ is evaluated
- 4 **compute a sum** when $P^{(0)}(x+1)$ and the product are evaluated

These are the four main things to implement to realize the *Taylor shift by 1*. We will only focus on the multiplication, which is the most hard and tricky operation to realize our code.

Multiplication : concept

- **Small sizes ($n \leq 512$) :**

We can use a procedure called *list_Plain_Mul* which computes a list of pairwise products of polynomials of same size.

- **Big sizes ($n > 512$) :**

We can use *FFT* whic several procedures which compute a list pairwise products of polynomials of same size.

Polynomials considered at step i :

Polynomials $P^{(1)}$ (of size 2^i) and $(x + 1)^{2^i}$ (of size $2^i + 1$).

Multiplication : a challenge

Problems :

- Polynomials considered must be of the same size (rather 2^i) so as to use the procedures of the lab.
- Size of the product of two such polynomials is not a power of 2 (but $2^{i+1} - 1$).

Solutions :

- Modify procedure *list_Plain_Mul* and adapt it for my case.
- Consider another product with polynomials of same sizes.

Multiplication : decomposition

We can decompose the product desired as follows :

$$\begin{aligned}P^{(1)}(X) \times (X+1)^{2^i} &= \left(\sum_{i=0}^{2^i-1} a_i X^i \right) \times (X+1)^{2^i} \\&= P^{(1)}(X) \times \left[(X+1)^{2^i} - 1 + 1 \right] \\&= P^{(1)}(X) \times \left[(X+1)^{2^i} - 1 \right] + P^{(1)}(X) \\&= P^{(1)}(X) \times X \times \frac{(X+1)^{2^i} - 1}{X} + P^{(1)}(X) \\&= X \cdot \left(P^{(1)}(X) \times \frac{(X+1)^{2^i} - 1}{X} \right) + P^{(1)}(X)\end{aligned}$$

Multiplication : technic

Taylor shift multiplication concept

Using the following formula :

$$P^{(1)}(X) \times (X + 1)^{2^i} = X \cdot \left(P^{(1)}(X) \times \frac{(X + 1)^{2^i} - 1}{X} \right) + P^{(1)}(X)$$

The multiplication desired amounts to :

- ① *multiplying* $P^{(1)}(X)$ by $[(X + 1)^{2^i} - 1]/X$ of sizes 2^i ,
- ② *doing a right shift* (multiplication by X), and
- ③ *semi-adding* the result of the two first steps with $P^{(1)}(X)$.

We will just detail how to do the multiplication for the two cases of polynomial sizes.

Multiplication : arrays considered (artificial ex.)

If we consider polynomials at step 1 :

$$\text{Polynomial_shift_device}[0] = \begin{array}{|c|c||c|c||c|c||c|c|} \hline 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline \end{array}$$

Then for the two multiplication techniques used, we consider :

- "Small sizes" ($n \leq 512$) :

$$M_{gpu} = \begin{array}{|c|c||c|c||c|c||c|c|} \hline 3 & 4 & 2 & 1 & 5 & 6 & 2 & 1 \\ \hline \end{array}$$

- "Big sizes" ($n > 512$) :

$$\text{fft_device} = \begin{array}{|c|c|c|c||c|c|c|c||c|c|c|c||c|c|c|c|} \hline 3 & 4 & 0 & 0 & 2 & 1 & 0 & 0 & 5 & 6 & 0 & 0 & 2 & 1 & 0 & 0 \\ \hline \end{array}$$

Multiplication according to the size of the polynomials

- "Small sizes" ($n \leq 512$) :

We use *Mgpu* and multiply directly pairwise polynomials inside, then do a right shift. Product size is still a power of 2. So

list_Plain_Mul_and_right_shift is used to do :

$$X \cdot \left(P^{(1)}(X) \times [(X + 1)^{2^i} - 1]/X \right).$$

- "Big sizes" ($n > 512$) :

We transform *Mgpu* in *fft_device* and then use *FFT* for the multiplication $P^{(1)}(X) \times [(X + 1)^{2^i} - 1]/X$.

The *FFT* will be explained in the following section.

First definition

Definition

Let n be a positive integer and $\omega \in R$.

- ω is a n -th root of unity if $\omega^n = 1$.
- ω is a primitive n -th root of unity if :
 - (1) $\omega^n = 1$.
 - (2) ω is a unit in R .
 - (3) $\forall t$ prime s.t. $t|n$, $\omega^{n/t} - 1$ is neither 0 nor a 0 divisor.

We now take $\omega \in R$ to be a primitive n -th root of unity.

Discrete Fourier transform (DFT)

Definition

The R -linear map

$$DFT_{\omega} : \begin{cases} R^n & \rightarrow R^n \\ f & \mapsto (f(1), f(\omega), f(\omega^2), \dots, f(\omega^{n-1})) \end{cases}$$

which evaluates a polynomial at the powers of ω is called the **Discrete Fourier Transform (DFT)**.

Proposition (consequence of the Lagrange's theorem)

The R -linear map DFT_{ω} is an isomorphism.

Then we can represent a polynomial f by the DFT representation with ω determined in our code.

Convolution

Definition

The **convolution** w.r.t. n of $f = \sum_{0 \leq i < n} f_i x^i$ and $g = \sum_{0 \leq i < n} g_i x^i$ in $R[x]$ is $h = f * g = \sum_{0 \leq k < n} h_k x^k$ s.t.

$$\forall k \in \llbracket 0, n-1 \rrbracket, h_k = \sum_{i+j \equiv k \pmod n} f_i g_j.$$

One can prove that $fg = f * g \pmod{x^n - 1}$.

Lemma (DFT product amounts to a scalar product)

For $f, g \in R[x]$ univariate polynomials of degree less than n we have

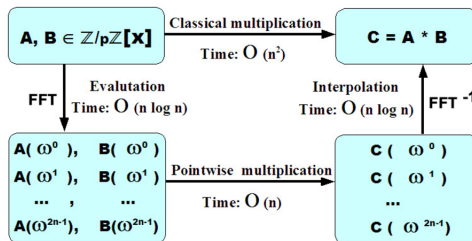
$$DFT_\omega(f * g) = DFT_\omega(f) DFT_\omega(g).$$

FFT Mapping

Definition

The **Fast Fourier Transform (FFT)** is an efficient algorithm to compute *DFT* and its inverse.

We use the **Cooley-Tukey** algorithm following a *D&C* strategy.



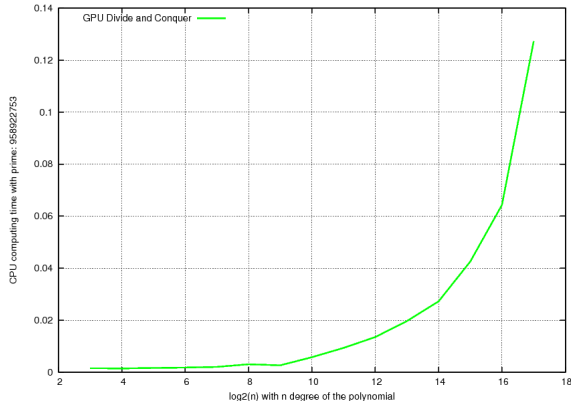
FFT-based univariate polynomial multiplication over $\mathbb{Z}/p\mathbb{Z}$

Taylor shift by 1 execution times

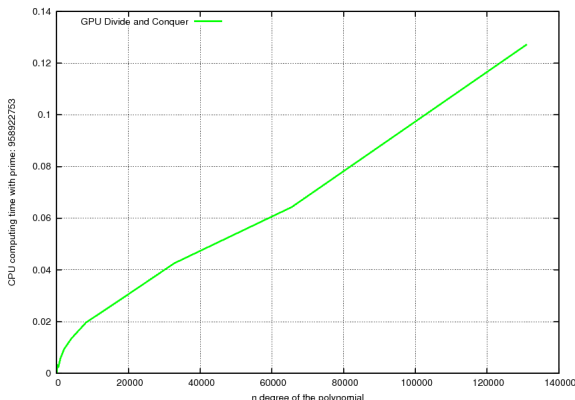
Results are for polynomials of sizes $n = 2^e$:

Execution time in seconds					
e	n	GPU	CPU : HOR	CPU : DNC	Maple 16
3	8	0.001518	0.000128	0.000141	<0.001
4	16	0.001432	0.000186	0.000172	<0.001
5	32	0.001590	0.000167	0.000191	<0.001
6	64	0.001773	0.000192	0.000294	0.008
7	128	0.002016	0.000261	0.000628	0.024
8	256	0.003036	0.000593	0.002331	0.084
9	512	0.002624	0.001278	0.006304	0.320
10	1024	0.005756	0.005940	0.032073	1.400
11	2048	0.009317	0.015312	0.095027	5.640
12	4096	0.013475	0.076866	0.376543	24.478
13	8192	0.019674	0.324029	1.498890	104.438
14	16384	0.027229	1.282708	6.861433	437.848
15	32768	0.042561	5.110919	23.907799	1781.427
16	65536	0.064306	15.184347	114.988129	7407.063
17	131072	0.127214	80.625801	477.934692	>10000

Execution time of the GPU in function of e

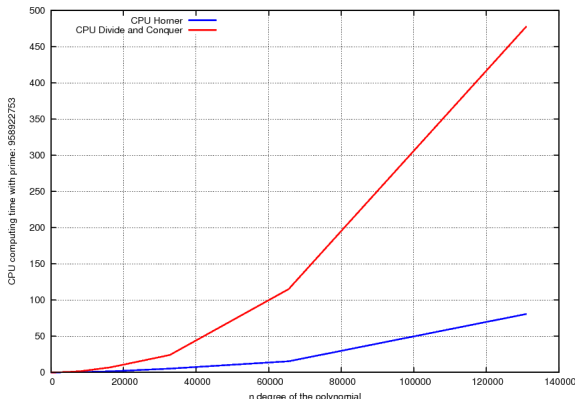


Execution time of the GPU in function of n

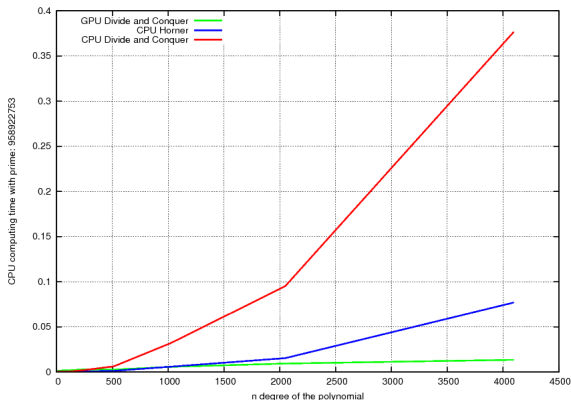


This execution time is approximatively linear.

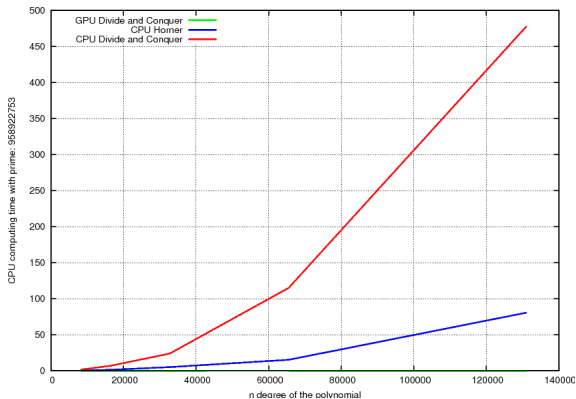
Execution times of the CPU in function of n



Execution times in function of n for small degrees



Execution times in function of n for big degrees



We clearly improve performances using GPUs.

Remark : the behaviour of the CPU times is the same for the different sizes.

Possible improvements & FFT primes

- We need to improve the parallel computation of the sequence $(i!)_{1 \leq i \leq n}$, and
- We can reduce the size of the array storing the elements of $(x + 1)^{2^i}$ as these polynomials are symmetric.

The *Taylor shift* modulo p is needed several times to get the *Taylor shift* in \mathbb{Z} . Two questions arises :

- 1 What prime numbers must we use ?
- 2 How many such primes numbers must we use ?

Primes numbers of the form $p = M \times 2^j + 1$ yield the best performance for *FFT*, with $p > n$ and $M < 2^j$ odd integer.

Combination with the Chinese Remainder thm.

We need to Taylor shift by a prime number $(m_i)_{1 \leq i \leq s}$ s times.
For each coefficient in \mathbb{Z} , we obtain a vector $\mathbf{x} = (x_1, \dots, x_s)$.

Objective : using the CRT2, compute the image a of \mathbf{x} by

$$\mathbb{Z}/m_1\mathbb{Z} \times \dots \times \mathbb{Z}/m_s\mathbb{Z} \cong \mathbb{Z}/m_1 \dots m_s\mathbb{Z}.$$

Representation : we can represent a by $\mathbf{b} = (b_1, \dots, b_s)$ s.t.

$$a = b_1 + b_2 m_2 + b_3 m_1 m_2 + \dots + b_s m_1 \dots m_{s-1}.$$

Then we will use the conversion of modular numbers to their **mixed radix representation by a matrix formula** to compute \mathbf{b} .

Definition (1)

Let us consider m_1, m_2, \dots, m_s distinct prime numbers.

Definition $((m_{i,j})$ and $(n_{i,j}))$

We define the sequences $(m_{i,j})_{1 \leq i < j \leq s}$ and $(n_{i,j})_{1 \leq i < j \leq s}$ such that :

$$\begin{cases} m_{i,j} \times m_i \equiv 1 \pmod{m_j} & | \quad 0 \leq m_{i,j} < m_j \\ n_{i,j} = m_j - m_{i,j} \end{cases}$$

Definition (2)

Definition (matrix A)

We define the matrix $(A_k)_{1 \leq k \leq s-1}$ as the following :

$$A_k = \left(\begin{array}{c|c} I_{k-1} & 0 \\ \hline 0 & B_k \end{array} \right) \text{ with}$$

$$B_k = \begin{pmatrix} 1 & n_{k,k+1} & n_{k,k+2} & \dots & n_{k,s} \\ 0 & m_{k,k+1} & 0 & \dots & 0 \\ \vdots & \ddots & m_{k,k+2} & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \dots & \dots & 0 & m_{k,s} \end{pmatrix}$$

Mixed radix representation by a matrix formula

Theorem

$$\mathbf{b} = (\dots (((\mathbf{x}A_1) A_2) A_3) \dots) A_{s-1}$$

Definition

As A_k is sparse, we don't really need to multiply our results by a matrix. Thus, we will consider sequences $(L_k)_{1 \leq k \leq s-1}$ and $(D_k)_{1 \leq k \leq s-1}$ respectively the first row of A_k and the diagonal of A_k such that :

$$(L_k) = (n_{k,j} \mid k+1 \leq j \leq s),$$

$$(D_k) = (m_{k,j} \mid k+1 \leq j \leq s).$$

This gives the following algorithm (with $d = n - 1 = 2^e - 1$) :

Algorithm for the mixed radix representation

Input : $X[0..d][1..s]$, s , $(m_i)_{1 \leq i \leq s}$, $(L_k)_{1 \leq k \leq s-1}$, $(D_k)_{1 \leq k \leq s-1}$

Y := X

for $k = 1..s - 1$ do

 for $i = 0..d$ do

 for $j = k + 1..s$ do

$Y_{i,j} := [(Y_{i,j}L_{k,j} \bmod m_j) + (Y_{i,j}D_{k,j} \bmod m_j)] \bmod m_j$

 end do

 end do

end do

Output : $Y[0..d][1..s]$

This algorithm can be parallelized but the different loops in k need less and less computations, parallelization must be done with reflection.