Fast reversion of formal power series

Fredrik Johansson
LFANT, INRIA Bordeaux

RAIM, 2016-06-29, Banyuls-sur-mer

Reversion of power series

$$F = \exp(x) - 1 = x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots$$

$$G = \log(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \ldots$$

$$F(G(x)) = G(F(x)) = x, \quad G = F^{-1} \text{ and } F = G^{-1}$$

Applications:

- Combinatorics, recurrences (example: counting binary trees)
- Numerical approximation of F^{-1}
- Asymptotic analysis

Operations in $R[[x]]/\langle x^n \rangle$

$$F = F(x) = \sum_{k=0}^{n-1} f_k x^k, \qquad [x^k]F(x) = f_k \in R$$

Addition	$F + G = \sum_{k=0}^{n-1} (f_k + g_k) x^k$
Multiplication	$FG = \sum_{k=0}^{n-1} \left(\sum_{i=0}^{k} f_i g_{k-i} \right) x^k$
Reciprocal	If f_0 is a unit, find G such that $FG = 1$
Composition	If $g_0 = 0$, $F(G) = \sum_{k=0}^{n-1} f_k G^k$
Reversion	If $f_0 = 0$ and f_1 is a unit, find G s.t. $F(G) = x$

Computational complexity

Counting operations in the base ring R.

$M(n)$: multiplying two length-n polynomials

Classical	$M(n) = O(n^2)$
Karatsuba	$M(n) = O(n^{\log_2(3)}) = O(n^{1.59})$
Fast Fourier Transform	$M(n) = O(n \log^{1+o(1)} n) = O(n^{1+o(1)})$

$MM(n) = O(n^\omega)$: multiplying two $n \times n$ matrices

Classical	$MM(n) = O(n^3)$
Strassen	$MM(n) = O(n^{\log_2(7)}) = O(n^{2.81})$
Coppersmith-Winograd-Le Gall	$MM(n) = O(n^{2.3728639})$

Newton iteration for power series

If $\varphi(G_k) = 0 \bmod x^n$, then (under natural assumptions)

$$\varphi(G_{k+1}) = 0 \bmod x^{2n}, \qquad G_{k+1} = G_k - \frac{\varphi(G_k)}{\varphi'(G_k)}$$

$O(M(n))$ computation of $1/F$: take $\varphi(G) = \dfrac{1}{G} - F$, giving:

$$G_{k+1} = 2G_k - FG_k^2.$$

Reversion using Newton iteration

Given $F = f_0 + f_1 x + \ldots$ with $f_0 = 0$ and f_1 invertible.

Take $\varphi(G) = F(G) - x$, giving:

$$G_{k+1} = G_k - \frac{F(G) - x}{F'(G)}.$$

Brent and Kung, 1978: up to constant factors:

composition $\Leftrightarrow$ reversion

Fast composition: elementary functions

Assume that $1, 2, \ldots, n-1$ are invertible in R.

$$F' = \sum_{k=0}^{n-2} (k+1) f_{k+1} x^k, \quad \int F = \sum_{k=1}^{n-1} \left(\frac{1}{k}\right) f_{k-1} x^k$$

$$\log(1+F) = \int \frac{F'}{1+F}, \quad \operatorname{atan}(F) = \int \frac{F}{1+F^2}$$

Newton iteration: log $\to$ exp, atan $\to$ tan.
sin, cos, sinh, cosh, asin ... using algebraic transformations.

Cost: $O(M(n)) = O(n^{1+o(1)})$.

Generalization: differential equations (hypergeometric, ...)

Composition of general power series

Horner's rule

$$F(G) = (\ldots(f_{n-1} \cdot G + f_{n-2}) \cdot G + \ldots + f_1) \cdot G + f_0$$

Complexity: $O(nM(n))$

Brent-Kung 2.1: baby-step, giant-step version of Horner's rule
Complexity: $O(n^{1/2}M(n) + n^{1/2}MM(n^{1/2}))$

Brent-Kung 2.2: divide-and-conquer Taylor expansion
Complexity: $O((n \log n)^{1/2}M(n))$

Brent-Kung algorithm 2.1

Example with $n = 9, \ m = \lceil \sqrt{n} \rceil = 3$
Computing $F(G)$ where $F = f_0 + f_1 x + \ldots + f_8 x^8$

$$(f_0 + f_1 G + f_2 G^2) + (f_3 + f_4 G + f_5 G^2) G^3 + (f_6 + f_7 G + f_8 G^2) G^6$$

$(m \times m) \times (m \times m^2)$ matrix multiplication:

$$\begin{pmatrix} f_0 & f_1 & f_2 \\ f_3 & f_4 & f_5 \\ f_6 & f_7 & f_8 \end{pmatrix} \times \begin{pmatrix} ----- & 1 & ----- \\ ----- & G & ----- \\ ----- & G^2 & ----- \end{pmatrix}$$

Final combination using Horner's rule.

Complexity of composition algorithms

Horner's rule: $O(nM(n))$

BK 2.1: $O(n^{1/2}M(n) + n^{1/2}MM(n^{1/2}))$

BK 2.2: $O((n \log n)^{1/2}M(n)) = O(n^{3/2+o(1)})$

$M(n)$	$MM(n)$	Horner	BK 2.1	BK 2.2
n^2	n^3	n^3	$n^{2.5}$	$n^{2.5} \log^{0.5} n$
$n^{1.59}$	n^3	$n^{2.59}$	$n^{2.09}$	$n^{2.09} \log^{0.5} n$
$n \log n$	n^3	$n^2 \log n$	n^2	$n^{1.5} \log^{1.5} n$
$n \log n$	$n^{2.3728639}$	$n^2 \log n$	$n^{1.687}$	$n^{1.5} \log^{1.5} n$
$(n \log n)$	(n^2)	$(n^2 \log n)$	$(n^{1.5} \log n)$	$(n^{1.5} \log^{1.5} n)$

BK 2.1 wins for small n, BK 2.2 wins for large n
BK 2.1 wins with hypothetical $O(n^2)$ matrix multiplication

The Lagrange inversion theorem

The coefficients of F^{-1} are given by

$$[x^k]F^{-1} = \frac{1}{k}[x^{k-1}]\left(\frac{x}{F}\right)^k.$$

$O(nM(n))$ algorithm: compute $H = x/F$ using Newton iteration for the reciprocal, then compute $H, H^2, H^3, \ldots, H^{n-1}$

Better than classical algorithms ($O(n^3)$)

Similar to Newton iteration + Horner's rule

Worse than Newton iteration + BK2.1 or BK2.2

Fast Lagrange inversion

We can extract a single coefficient in $H^{a+b} = H^a H^b$ using $O(n)$ operations:

$$[x^k]H^{a+b} = \sum_{i=0}^{k} \left([x^i]H^a\right) \cdot \left([x^{k-i}]H^b\right)$$

Compute $H, H^2, \ldots, H^{m-1}$, then $H^m, H^{2m}, H^{3m}, \ldots, H^{\lfloor n/m \rfloor m}$.

Choose $m \approx \sqrt{n} \Rightarrow$ need $O(\sqrt{n})$ polynomial multiplications, plus $O(n^2)$ coefficient operations.

Fast Lagrange inversion, first version

$m \leftarrow \lfloor \sqrt{n} \rfloor$
$H \leftarrow x/F$
for $1 \leq i < m$ **do**
  $H^{i+1} \leftarrow H^i \cdot H$
  $b_i \leftarrow \frac{1}{i}[x^{i-1}]H^i$
end for
$T \leftarrow H^m$
for $i = m, 2m, 3m, \ldots, \ell m < n$ **do**
  $b_i \leftarrow \frac{1}{i}[x^{i-1}]T$
  for $1 \leq j < m$ **while** $i + j < n$ **do**
    $b_{i+j} \leftarrow \frac{1}{i+j} \sum_{k=0}^{i+j-1} ([x^k]T) \cdot ([x^{i+j-k-1}]H^j)$
  end for
  $T \leftarrow T \cdot H^m$
end for
return $b_1 x + b_2 x^2 + \ldots + b_{n-1} x^{n-1}$

Using matrix multiplication

Example: $n = 8$, $m = \lceil \sqrt{8-1} \rceil = 3$. We want the coefficients $b_1, b_2, \ldots, b_7$ of $1, x, \ldots, x^6$ in the respective powers of H.

$$h_{k,i} = [x^i]H^k$$

$$A = \begin{pmatrix} h_{0,2} & h_{0,1} & h_{0,0} & 0 & 0 & 0 & 0 & 0 & 0 \\ h_{3,5} & h_{3,4} & h_{3,3} & h_{3,2} & h_{3,1} & h_{3,0} & 0 & 0 & 0 \\ - & - & h_{6,6} & h_{6,5} & h_{6,4} & h_{6,3} & h_{6,2} & h_{6,1} & h_{6,0} \end{pmatrix}$$

$$B = \begin{pmatrix} 0 & 0 & h_{1,0} & h_{1,1} & h_{1,2} & h_{1,3} & h_{1,4} & h_{1,5} & h_{1,6} \\ 0 & h_{2,0} & h_{2,1} & h_{2,2} & h_{2,3} & h_{2,4} & h_{2,5} & h_{2,6} & - \\ h_{3,0} & h_{3,1} & h_{3,2} & h_{3,3} & h_{3,4} & h_{3,5} & h_{3,6} & - & - \end{pmatrix}$$

$$AB^T = \begin{pmatrix} b_1 & b_2 & b_3 \\ b_4 & b_5 & b_6 \\ b_7 & - & - \end{pmatrix}$$

Fast Lagrange inversion, matrix version

$m \leftarrow \lceil \sqrt{n-1} \rceil$
$H \leftarrow x/F$
{Assemble $m \times m^2$ matrices B and A from $H, H^2, \ldots, H^m$ and $H^m, H^{2m}, H^{3m}, \ldots$}
for $1 \le i \le m,\ 1 \le j \le m^2$ **do**
    $B_{i,j} \leftarrow [x^{i+j-m-1}]\ H^i$
    $A_{i,j} \leftarrow [x^{im-j}]\ H^{(i-1)m}$
end for
$C \leftarrow AB^T$
for $1 \le i < n$ **do**
    $b_i \leftarrow C_i/i$ (C_i is the ith entry of C read rowwise)
end for
return $b_1 x + b_2 x^2 + \ldots + b_{n-1} x^{n-1}$

Comparison with BK 2.1

Let $m = \sqrt{n}$.

Fast Lagrange inversion for reversion:

1. $2m + O(1)$ polynomial multiplications
2. One $(m \times m^2)$ times $(m^2 \times m)$ matrix multiplication
3. $O(n)$ additional operations

"Fast Horner's rule" (BK 2.1) for composition:

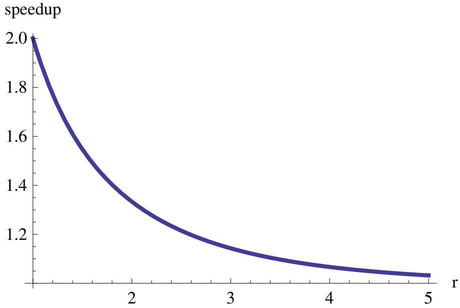
1. m polynomial multiplications, each with cost $M(n)$
2. One $(m \times m)$ times $(m \times m^2)$ matrix multiplication
3. m polynomial multiplications and additions

Both $O(n^{1/2}(M(n) + MM(n^{1/2})))$, same constant factor.

Speedup by avoiding Newton iteration

If composition costs $C(n) \sim cn^r$, reversion via Newton costs

$$C(n) + C(n/2) + C(n/4) + \ldots = cn^r \left(\frac{2^r}{2^r - 1} \right)$$

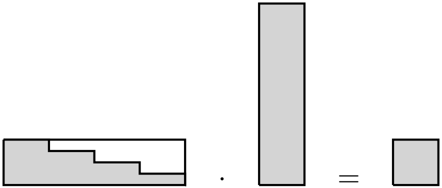


Classical polynomial multiplication: $\frac{4}{31}(8 + \sqrt{2}) \approx 1.214$
FFT polynomial multiplication, classical matrix multiplication: $4/3$

Faster matrix multiplication

Brent-Kung 2.1:

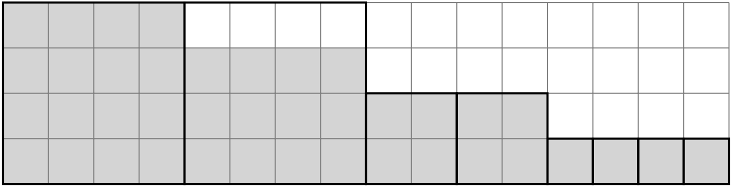
Fast Lagrange inversion:



Can we exploit the structure of A when $\omega < 3$?

Faster matrix multiplication, first algorithm

Decompose each $m \times m$ block of A into $(m/k) \times (m/k)$ blocks.

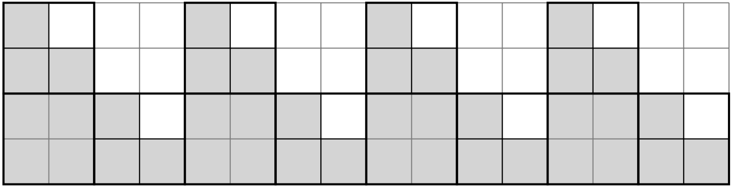


Asymptotic speedup s:

$$s = \frac{m^{\omega+1}}{\sum_{k=1}^{\infty} \left(\frac{m}{k} - \frac{m}{k+1}\right) k^2 \left(\frac{m}{k}\right)^{\omega}} > \frac{1}{\sum_{k=0}^{\infty} \frac{2^{k-1}}{2^{k\omega}}} = 2 - 2^{2-\omega} > 1$$

Faster matrix multiplication, second algorithm

Write $AB^T = (AP)(P^{-1}B^T)$ where P is a permutation matrix that makes each $m \times m$ block in A lower triangular.

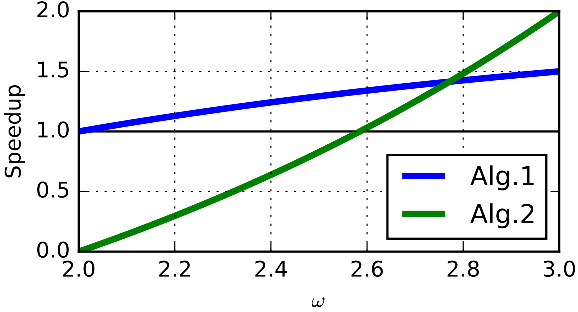


Recursive triangular multiplication:

$$R(k) = 4R(k/2) + 2(k/2)^\omega + O(k^2)$$

Speedup: $s = 2^{\omega-1} - 2$. Note: $s > 1$ when $\omega > \log_2 6 \approx 2.585$

Matrix multiplication speedup



Crossover at $\omega = 1 + \log_2(2 + \sqrt{2}) \approx 2.771$

$s = 2$ with classical matrix multiplication ($\omega = 3$)
$s = 1.5$ with Strassen multiplication
$s = 1.228$ with Coppersmith-Winograd-Le Gall

Using fast rectangular matrix multiplication

$MM(x, y, z)$: $(x \times y)$ by $(y \times z)$ matrix multiplication

Huang and Pan (1998):
$MM(m, m, m^2) = O(n^{1.667}) < mMM(m, m, m) = O(n^{1.687})$

By a transposition argument,
$MM(m, m^2, m) = (1 + o(1))MM(m, m, m^2)$

Open problem: can we get a speedup > 1?

Total speedup

Theoretical speedup of fast Lagrange inversion over BK 2.1 by both avoiding Newton iteration and speeding up matrix multiplication.

Dominant operation	Complexity	Newton	Matrix	Total
Polynomial, classical	$O(n^{5/2})$	1.214	1	1.214
Polynomial, Karatsuba	$O(n^{1/2+\log_2 3})$	1.308	1	1.308
Matrix, classical	$O(n^2)$	1.333	2.000	2.666
Matrix, Strassen	$O(n^{(1+\log_2 7)/2})$	1.364	1.500	2.047
Matrix, Cop.-Win.-LG	$O(n^{1.687})$	1.451	1.228	1.781
Matrix, Huang-Pan	$O(n^{1.667})$	1.458	1?	1.458?
(Polynomial, FFT)	$O(n^{3/2} \log^{1+o(1)} n)$	1.546	1	1.546

Implementation

Composition and reversion implemented in FLINT:

- $\mathbb{Z}/p\mathbb{Z}$, $p < 2^{64}$
- $\mathbb{Z}$
- $\mathbb{Q}$

In Arb (interval coefficients):

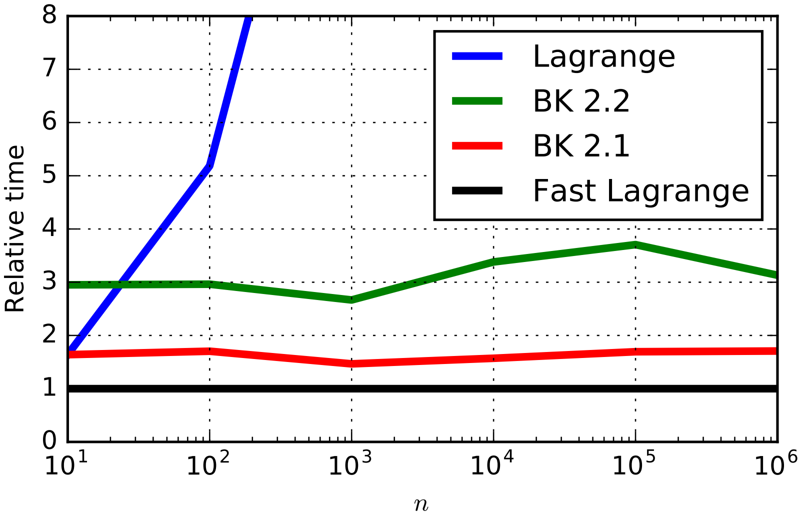
- $\mathbb{R}$
- $\mathbb{C}$

Reversion over $\mathbb{Z}/p\mathbb{Z}$ ($p = 2^{63} + 29$)

n	Lagrange	BK 2.1	BK 2.2	**Fast Lagrange**
10	$10 \cdot 10^{-6}$	$10 \cdot 10^{-6}$	$18 \cdot 10^{-6}$	$6.1 \cdot 10^{-6}$
10^2	0.0028	0.00092	0.0016	0.00054
10^3	0.690	0.066	0.120	0.045
10^4	110	3.3 (8%)	7.1	2.1
10^5	12100	144 (20%)	315	85
10^6	1900000	8251 (28%)	15131	4832

Time in seconds.
(Relative time spent on matrix multiplication.)

Reversion over $\mathbb{Z}/p\mathbb{Z}$ ($p = 2^{63} + 29$)



Reversion over $\mathbb{Z}$

$$F_1 = \sum_{k \geq 1} k! x^k, \quad F_2 = \frac{x}{\sqrt{1-4x}}, \quad F_3 = \frac{x+x^2}{1+x+x^2}$$

n	BK 2.1			**Fast Lagrange**		
	F_1	F_2	F_3	F_1	F_2	F_3
10	$10 \cdot 10^{-6}$	$10 \cdot 10^{-6}$	$10 \cdot 10^{-6}$	$4.9 \cdot 10^{-6}$	$4.3 \cdot 10^{-6}$	$4.1 \cdot 10^{-6}$
10^2	0.0078	0.0021	0.0021	0.0064	0.00096	0.00065
10^3	10	1.1	0.96	7.1	0.71	0.22
10^4	24356	1453	538	8903	426	152

Time in seconds.

Reversion over $\mathbb{Q}$

$$F_1 = \exp(x) - 1, \quad F_2 = x\exp(x), \quad F_3 = \frac{3x(1-x^2)}{2(1-x+x^2)^2}$$

n	BK 2.1			**Fast Lagrange**		
	F_1	F_2	F_3	F_1	F_2	F_3
10	$31 \cdot 10^{-6}$	$28 \cdot 10^{-6}$	$28 \cdot 10^{-6}$	$11 \cdot 10^{-6}$	$11 \cdot 10^{-6}$	$9.1 \cdot 10^{-6}$
10^2	0.012	0.021	0.0088	0.0089	0.0081	0.0019
10^3	8.8	17	3.1	14	13	0.65
10^4	13812	27057	1990	35633	27823	784

Time in seconds.

Reversion over $\mathbb{R}$

$$F_1 = \exp(x) - 1, \quad F_2 = \log(1+x), \quad F_3 = \Gamma(1+x) - 1$$

n	BK 2.1			**Fast Lagrange**		
	F_1	F_2	F_3	F_1	F_2	F_3
10	$26 \cdot 10^{-6}$	$24 \cdot 10^{-6}$	$52 \cdot 10^{-6}$	$17 \cdot 10^{-6}$	$17 \cdot 10^{-6}$	$39 \cdot 10^{-6}$
10^2	0.0042	0.059	0.0049	0.0031	0.044	0.0031
10^3	0.79	91	0.53	0.41	61	0.33
10^4	154		207	364		74

Precision doubled until the coefficient of x^{n-1} is a precise interval.
Time in seconds.

Conclusion and questions

Reversion algorithm analogous to BK 2.1, avoiding Newton iteration

Usually the fastest algorithm for reversion in practice.

Is there a Newton-free analog of BK 2.2 for reversion?
Can more be said about the structured matrix products?
Can denominators be handled better? Numerical stability?

Note: the algorithm has been published in FJ, *A fast algorithm for reversion of power series*, Math. Comp. 84, 475–484, 2015. Some more comments in my PhD thesis.