Sparse Polynomial Arithmetic with the BPAS Library

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The BPAS Library

Basic Polynomial Algebra Subprograms

The Basic Polynomial Algebra Subprograms (BPAS) is a free, open-source library providing support for polynomial arithmetic and system solving.

- ↳ Optimized fundamental operations support higher-level algorithms.
- ↳ Dense and **sparse** polynomial multiplication, division, pseudo-division.
- ↳ Normal forms, subresultants, regular chains.

`http://www.bpaslib.org`

Outline

Motivation

- To support the developement of our polynomial system solver we look to optimize some fundamental operations.
- Build from the ground up:
  - ↳ Polynomial multiplication, division, pseudo-division;
  - ↳ Normal forms, pseudo-division w.r.t a triangular set;
  - ↳ Subresultants (in progress);
  - ↳ Regular chains.
- For multivariate polynomials, sparsity must be exploited when possible.

Motivation

- Algorithm performance on modern computers is influenced by the *processor-memory gap* [2] and by the *memory wall* [8].
- Amount of memory used and how that memory is traversed is very important.
  ↳ Data locality, cache misses.
- Sparse algorithms, like that of Johnson [4], naturally make use of locality by producing the terms of the sum (difference, product, quotient, remainder) *in-order*.

Related and Previous Works

- Stephen C Johnson. "Sparse polynomial arithmetic". In: *ACM SIGSAM Bulletin* 8.3 (1974), pp. 63–71
- Michael Monagan and Roman Pearce. "Sparse polynomial division using a heap". In: *J. Symb. Comput.* 46.7 (2011), pp. 807–822
- Michael Monagan and Roman Pearce. "Polynomial division using dynamic arrays, heaps, and packed exponent vectors". In: *CASC 2007*. Springer. 2007, pp. 295–315
- Michael Monagan and Roman Pearce. "The design of Maple's sum-of-products and POLY data structures for representing mathematical objects". In: *ACM Communications in Computer Algebra* 48.3/4 (2015), pp. 166–186

From this work, MAPLE has become a leader in arithmetic performance and we use it as base of comparison.

Notations

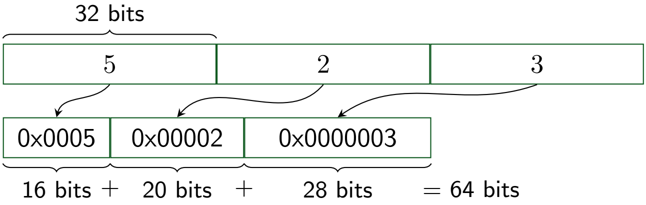
Throughout this presentation we use the following notation:

$$a = \sum_{i=1}^{n} a_i X^{\alpha_i} = \sum_{i=1}^{n} A_i$$

- The polynomial a has n terms.
- a_i are non-zero coefficients.
- α_i are **exponent vectors** for the variables $X = (x_1, x_2, \dots, x_m)$
- A_i are non-zero terms.
- $lm(a) = X^{\alpha_1}$ is the *leading monomial* of a.
- $lc(a) = a_1$ is the *leading coefficient* of a.
- $lt(a) = a_1 X^{\alpha_1} = A_1$ is the *leading term* of a.

Polynomial Data Structures: The Basics

- Polynomials are essentially collections of individual terms.
  - ↳ Must encode individual terms efficiently,
  - ↳ Must collect terms into a polynomial data structure effectively.
- An individual term is simply a coefficient and monomial.
  - ↳ Coefficients easily represented by GMP numbers.
  - ↳ With a consistent variable ordering, only exponent vectors need be encoded. This is done using exponent packing [1, 3] — bit-tricks.

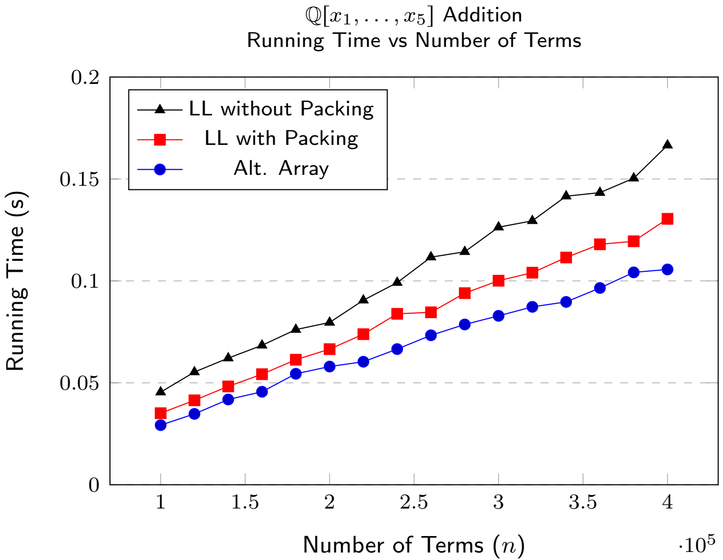


Polynomial Data Structures: The Collection

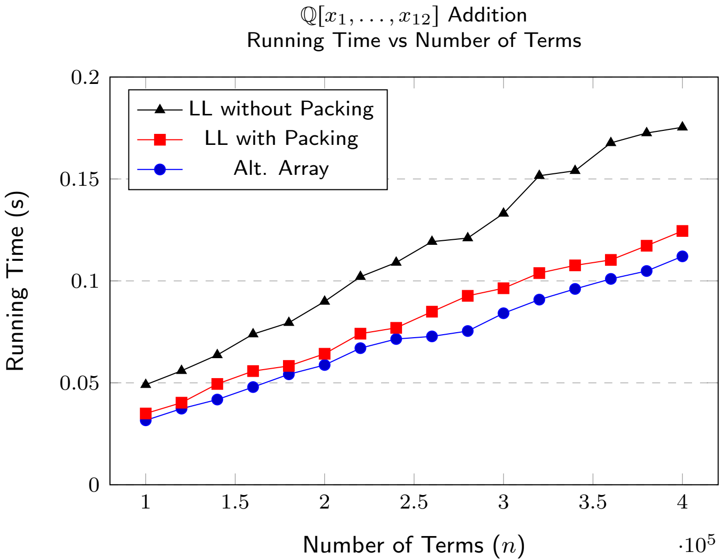
- A naïve approach would be to collect each term into a linked list.
  - ↳ Wasted memory storing a pointer for each node.
  - ↳ Indirection of pointers means adjacent terms not necessarily adjacet in memory.
- An *alternating array* is more succinct, removing pointers and alternating between coefficients and exponent vectors side-by-side in an array.
  - ↳ Adjacent terms are adjacent in memory, no overhead in encoding the structure (no pointers).
- In either case, maintain a canonical representation by keeping terms sorted using some term-order (lex).

$$\underbrace{\boxed{13}\boxed{x^2y^3}}_{\text{Term 1}}\underbrace{\boxed{5}\boxed{x^2y}}_{\text{Term 2}}\underbrace{\boxed{7}\boxed{y^3z}}_{\text{Term 3}}\boxed{\quad\cdots\quad}$$

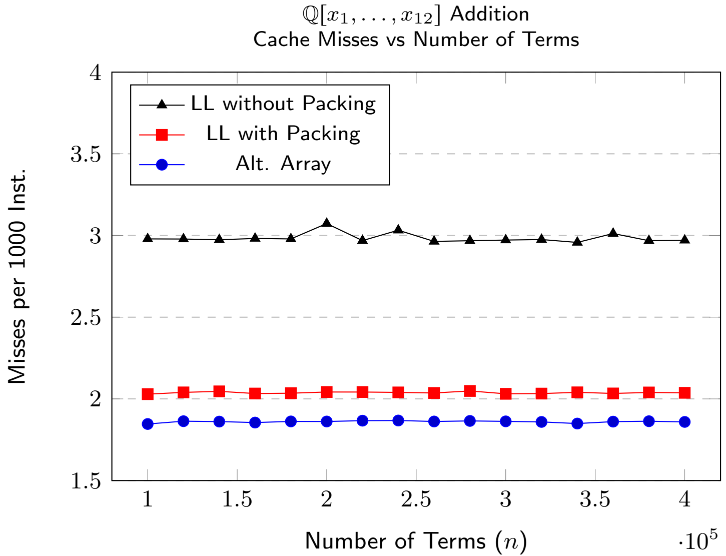
Polynomial Data Structures: Experimentation



Polynomial Data Structures: Experimentation



Polynomial Data Structures: Experimentation

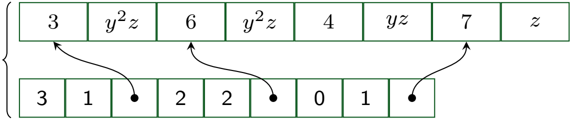


Polynomial Data Structures: Recursive Views

- Many polynomial operations are essentially univariate, viewing multivaraite polynomials recursively: pseudo-division, subresultants.

- It is useful to view a multivariate polynomial recursively, creating a univariate polynomial with polynomial coefficients.
  - ↳ Reuse the original polynomial array as coefficients → fast conversion
  - ↳ Create a small auxiliary alternating array for univariate exponents, coefficient size, and pointers to the original array.

Recursive View



$3x^3y^2z + 6x^2y^2z + 4x^2yz + 7z$ encoded recursively in x.

Sparse Polynomial Addition

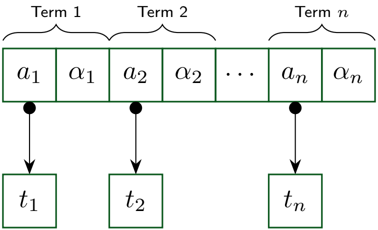
- Sparse polynomial addition highlights the general idea of our sparse arithmetic scheme: *generate terms in order* to exploit locality.

- Addition is essentially one step of merge-sort.
  - If terms are equal they are combined and appended to sum, otherwise simply append the maximum of the two.

$$\left.\begin{array}{l} a = 13x^2y^3 + 5x^2y \quad + \underset{\uparrow}{7}y^3z + \dots \\[2em] b = 6x^2y \quad\quad + \underset{\uparrow}{1}2xz^2 + \;\; 4y^2 \;\; + \dots \end{array}\right\} \; c = 13x^2y^3 + 11x^2y + \underset{\uparrow}{}$$

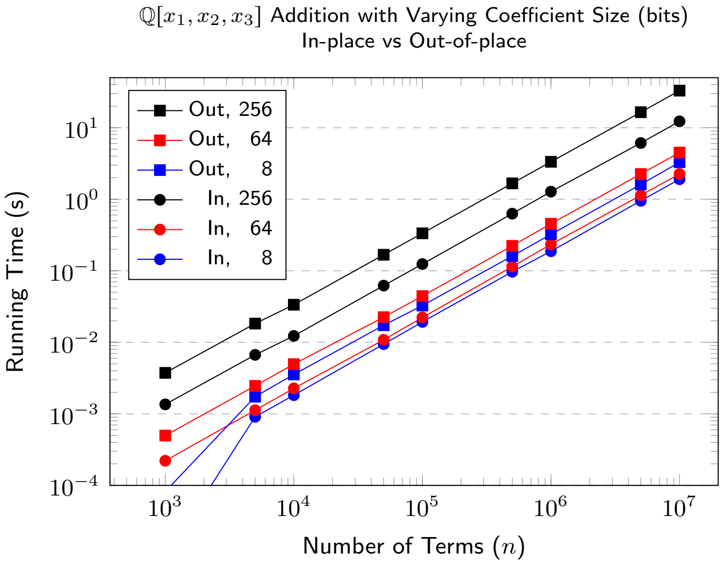
Polynomial Data Structures: "In-Place" Arithmetic

- In reality, GMP numbers are encoded as a *head* and a *tree*.
  - ↳ The head contains metadata: size, allocation, pointer to actual data.
  - ↳ The tree contains the actual encoding.



- For a lazy in-place implementation, simply copy all meta data *including pointers to trees*, do not copy the trees.

Sparse Addition: Experimentation



Sparse Polynomial Multiplication

- Multiplication performs an n-way merge of "streams", each stream being one term of a distributed over the entirety of b.
- Since b is sorted, multiplying by a single term of a keeps the sort order.
- Instead of choosing the maximum of 2 partitions as in addition, we choose the maximum among n.
  - ↳ This choice can be effectively implemented using a **heap**.
  - ↳ Optimize the heap $\implies$ Optimize arithmetic performance.

$$a \cdot b = \begin{cases} (a_1 \cdot b_1)\, X^{\alpha_1+\beta_1} + (a_1 \cdot b_2)\, X^{\alpha_1+\beta_2} + (a_1 \cdot b_3)\, X^{\alpha_1+\beta_3} + \dots \\ (a_2 \cdot b_1)\, X^{\alpha_2+\beta_1} + (a_2 \cdot b_2)\, X^{\alpha_2+\beta_2} + (a_2 \cdot b_3)\, X^{\alpha_2+\beta_3} + \dots \\ \quad \vdots \\ (a_n \cdot b_1)\, X^{\alpha_n+\beta_1} + (a_n \cdot b_2)\, X^{\alpha_n+\beta_2} + (a_n \cdot b_3)\, X^{\alpha_n+\beta_3} + \dots \end{cases}$$

Sparse Polynomial Arithmetic: Quantifying Sparsity

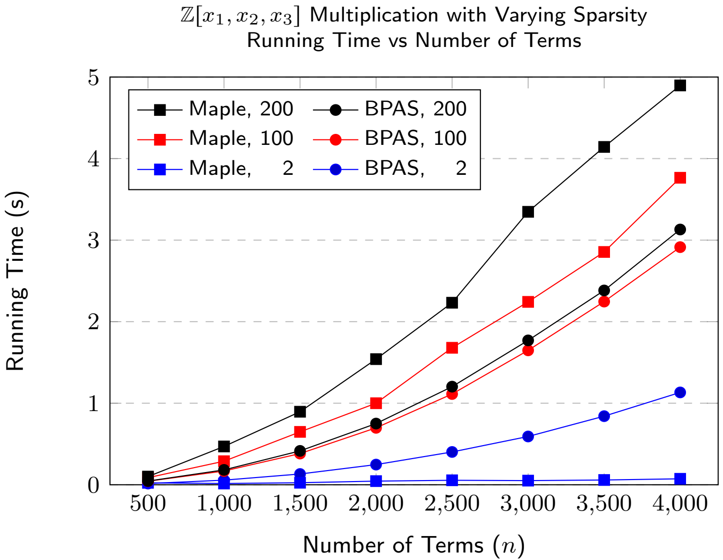
- For univariate polynomials, its sparsity can easily be described using the degree difference between any two adjacent terms. We quantify sparisty as the smallest integer larger than any such difference.

$$x^{12} + x^9 + x^2 + 1 \qquad \left.\begin{aligned} 12 - 9 &= 3 \\ \mathbf{9} - \mathbf{2} &= \mathbf{7} \\ 2 - 0 &= 3 \end{aligned}\right\} \implies \text{sparsity } = 8$$

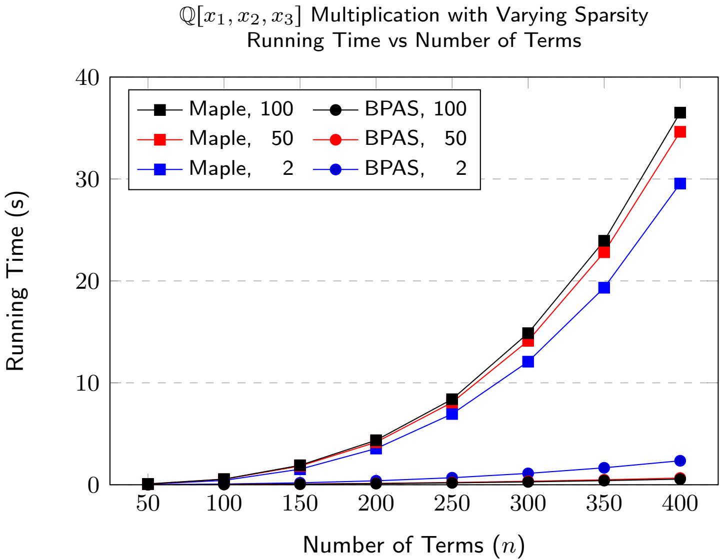
- *Kronecker Substituion* can map a multivariate polynomial to a univariate one in order to apply the same notion of sparsity. With d as an upper bound on partial degrees:

$$x_1^{e_1} x_2^{e_2} \ldots x_m^{e_m} \rightarrow y^{e_1 \cdot d \,+\, e_2 \cdot d^2 \,+\, \ldots \,+\, e_m \cdot d^m}$$

Sparse Polynomial Multiplication: Experimentation



Sparse Polynomial Multiplication: Experimentation



Sparse Polynomial Division

$$a = qb + r,\ deg(r) < deg(b)$$

Division is simply an application of multiplication.

- The quotient begins as $q^{(1)} = \mathrm{lt}(a)/\mathrm{lt}(b)$.
- Quotient and remainder terms are then produced from $q \cdot b$ with q updating throughout the computation.

The main idea is to repeatedly choose the leading term of $a - q^{(i)}b$

- Each new term of the quotient, q_{i+1}, is constructed to exactly cancel the leading term of $a - q^{(i)}b$

$$\begin{array}{r@{\,}l}
 & \underline{\ 3x^2 + 1\qquad\ } = q \\
2x & \big)\, 6x^3 + 2x + 1 \\
 & \underline{-3x^2(2x)\qquad\quad} \\
 & \qquad\qquad 2x + 1 \\
 & \underline{\qquad\quad -1(2x)\ \ } \\
 & \qquad\qquad\quad\ 1 = r
\end{array}$$

Sparse Polynomial Division

$$a = bq + r$$

Naïve Division

$q := 0$; $r := 0$
while $(\tilde{r} := \mathrm{lt}(a - qb - r)) \neq 0$ **do**
  if $\mathrm{lt}(b) \mid \tilde{r}$ **then**
    $q := q + \tilde{r}/\mathrm{lt}(b)$
  else
    $r := r + \tilde{r}$
end
return (q, r)

Heap Division

$(q, r, l) := 0$
$k := 1$
while $(\delta := \textbf{heapPeek}()) > -1$ **or** $k \leqslant n_a$ **do**
  if $\delta < \alpha_k$ **then**
    $\tilde{r} := A_k$
    $k := k + 1$
  else if $\delta = \alpha_k$ **then**
    $\tilde{r} := A_k - \textbf{heapExtract}()$
    $k := k + 1$
  else
    $\tilde{r} := -\textbf{heapExtract}()$
  if $B_1 \mid \tilde{r}$ **then**
    $\ell := \ell + 1$
    $Q_\ell := \tilde{r}/B_1$
    $q := q + Q_\ell$
    $\textbf{heapInsert}(Q_\ell, B_2)$
  else
    $r := r + \tilde{r}$
end
return (q, r)

Sparse Pseudo-Division

$$h^{deg(a)-deg(b)+1}a = qb + r,\ deg(r) < deg(b)$$

- The division algorithms can easily be adapted to pseudo-division. Repeatedly choose the leading term of $h^i a - q^{(i)}b,\ h = lc(b)$.
- However, performance is not as easily attained.
  - ↳ Delay multiplication by h as long as possible, performing only when strictly necessary.
  - ↳ Uses recursive data structure for efficient recursive, univariate view.
  - ↳ Careful implementation of *in-place* arithmetic to minimize memory movement when updating quotient and remainder.
- A *sparse* pseudo-division computes h^ℓ where $\ell \leqslant deg(a) - deg(b) + 1$ is the actual number of division steps performed.

Sparse Polynomial Arithmetic: Pseudo-Division

$$h^\ell a = qb + r$$

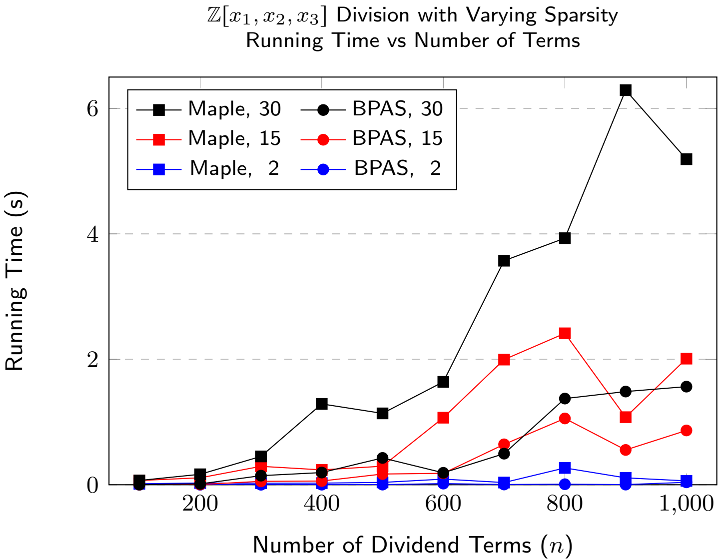
Naïve Pseudo-Division

$(q, r, \ell) := 0$
$h := \mathrm{lc}(b)$; $\gamma = \deg(b)$
while $(\tilde{r} := \mathrm{lt}(h^\ell a - qb - r)) \neq 0$ **do**
  if $x^\gamma \mid \tilde{r}$ **then**
    $q := hq + \tilde{r}/x^\gamma$
    $\ell := \ell + 1$
  else
    $r := r + \tilde{r}$
end
return (q, r, ℓ)

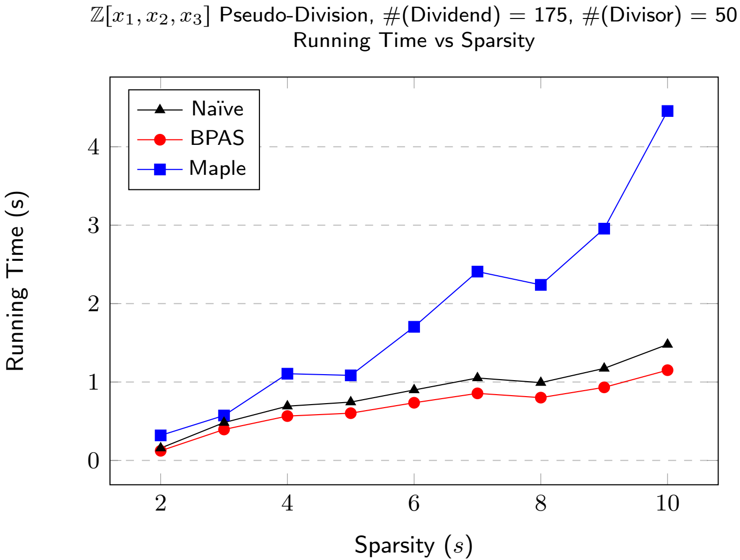
Heap Pseudo-Division

$(q, r, l) := 0$; $k := 1$
$h := \mathrm{lc}(b)$; $\gamma := \deg(b)$
while $(\delta := \mathbf{heapPeek}()) > -1$ **or** $k \leqslant n_a$ **do**
  if $\delta < \alpha_k$ **then**
    $\tilde{r} := h^\ell A_k$
    $k := k + 1$
  else if $\delta = \alpha_k$ **then**
    $\tilde{r} := h^\ell A_k - \mathbf{heapExtract}()$
    $k := k + 1$
  else
    $\tilde{r} := -\mathbf{heapExtract}()$
  if $x^\gamma \mid \tilde{r}$ **then**
    $q := hq$
    $\ell := \ell + 1$
    $Q_\ell := \tilde{r}/x^\gamma$
    $q := q + Q_\ell$
    $\mathbf{heapInsert}(Q_\ell, B_2)$
  else
    $r := r + \tilde{r}$
end
return (q, r, ℓ)

Sparse Polynomial Division: Experimentation



Sparse Pseudo-Division: Experimentation



Thank you!

Questions?

References

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[4] Stephen C Johnson. "Sparse polynomial arithmetic". In: *ACM SIGSAM Bulletin* 8.3 (1974), pp. 63–71.

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