A Modular Algorithm for Computing the Characteristic Polynomial of an Integer Matrix in Maple

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Abstract

Let $\mathbf{A}$ be an $n \times n$ matrix of integers. In this paper we present details of our Maple implementation of a modular method for computing the characteristic polynomial of $\mathbf{A}$. Our implementation considers several different representations for the computation modulo primes, including the use of double precision floats. The algorithm presently implemented in Maple releases 7–9 is the Berkowitz algorithm. We present some timings comparing the two methods on a large sparse matrix arising from an application in combinatorics, and also some randomly generated dense matrices.

1 Introduction

Let $\mathbf{A}$ be an $n \times n$ matrix of integers. One way to compute the characteristic polynomial $c(x) = \det(x\mathbf{I} - \mathbf{A}) \in \mathbb{Z}[x]$ is to evaluate the characteristic matrix at n points, compute n determinants of integer matrices, then interpolate to obtain the characteristic polynomial. The determinants of integer matrices can be computed using a fraction-free Gaussian elimination algorithm (see Chapter 9 of Geddes et. al [5]) in $O(n^3)$ integer multiplications and divisions. This approach will lead to an algorithm that requires $O(n^4)$ integer operations.

The algorithm presently implemented in Maple releases 7–9 is the Berkowitz algorithm [2]. It is a division free algorithm and thus can be used to compute the characteristic polynomial of a matrix over any commutative ring R. It does $O(n^4)$ multiplications in R. In [1], Abdeljaoued described a Maple implementation of a sequential version of the Berkowitz algorithm and compared it with the interpolation method and other methods. His implementation improves with sparsity to $O(n^3)$ multiplications when the matrix has $O(n)$ non-zero entries.

In section 2 we present details of our Maple implementation of a modular method for computing $c(x)$, the characteristic polynomial of $\mathbf{A}$. The algorithm computes the characteristic polynomial modulo a sequence of primes and applies the Chinese remainder theorem. Our implementation considers several different representations for the computation modulo primes, including the use of double precision floats. In section 3 we present some timings comparing our modular algorithm implementations and the Berkowitz algorithm on a 364×364 sparse matrix arising from an application in combinatorics from Quaintance [8], and also some timings comparing randomly generated large dense matrices. In section 4 we give a short asymptotic comparison of the algorithms.

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2 A Dense Deterministic Modular Algorithm

Let $\mathbf{A} \in \mathbb{Z}^{n\times n}$ be the input matrix, we want to compute the characteristic polynomial $c(x) = \det(x\mathbf{I} - \mathbf{A}) \in \mathbb{Z}[x]$. We will utilize a modular algorithm to compute $c(x)$ by computing the characteristic polynomial of $\mathbf{A}$ modulo a sequence of primes $p_1, p_2, p_3, ...$ using the Hessenberg matrix algorithm, then use the Chinese remaindering algorithm to reconstruct $c(x)$. The cost of the Hessenberg approach is $O(n^3)$ arithmetic operations in $\mathbb{Z}_p$ for each prime p. An alternative to the Hessenberg matrix approach would be a Krylov approach which has the same asymptotic complexity. In the Krylov approach one starts with a random vector $v \in \mathbb{Z}_p^n$ and computes the Krylov sequence of vectors

$$v, \mathbf{A}v, \mathbf{A}^2v, \mathbf{A}^3v, ..., \mathbf{A}^nv$$

stopping when a linear dependence between them is found. This linear dependence provides a factor of the minimal polynomial of $\mathbf{A}$. Here is our modular algorithm.

Input: Matrix $\mathbf{A} \in \mathbb{Z}^{n\times n}$
Output: Characteristic polynomial $c(x) = \det(x\mathbf{I} - \mathbf{A}) \in \mathbb{Z}[x]$

1. Compute a bound S (see below) larger than the largest coefficient of $c(x)$.
2. Choose t machine primes $p_1, p_2, \ldots, p_t$ such that $m = \prod_{i=1}^{t} p_i > 2S$.
3. **for** $i = 1$ **to** t **do**
   (a) $\mathbf{A}_i \leftarrow \mathbf{A} \bmod p_i$.
   (b) Compute $c_i(x)$ — the characteristic polynomial of $\mathbf{A}_i$ over $\mathbb{Z}_{p_i}$ via the Hessenberg algorithm.
4. Apply the Chinese remainder theorem:
   Solve $c(x) \equiv c_i(x) \pmod{p_i}$ for $c(x) \in \mathbb{Z}_m[x]$.
5. Output $c(x)$ in the symmetric range for $\mathbb{Z}_m$.

We can compute a bound S for the largest coefficient of $c(x)$ by modifying a bound for the determinant of $\mathbf{A}$. We have

$$\det(\mathbf{A}) \le n! \prod_{i=1}^{n} \max_{j=1}^{n} |a_{i,j}|$$

so a bound for S is

$$S \le \det(\mathbf{A}') \quad \text{where} \quad a'_{i,j} = \begin{cases} 1 + |a_{i,i}| & i = j \\ a_{i,j} & \text{otherwise.} \end{cases}$$

2.1 Hessenberg Algorithm

Recall that a square matrix $\mathbf{M} = (m_{i,j})$ is in upper Hessenberg form if $m_{i,j} = 0$ for all $i \ge j + 2$, in other words, the entries below the first subdiagonal are zero.

$$\begin{pmatrix} m_{1,1} & m_{1,2} & m_{1,3} & \cdots & m_{1,n-2} & m_{1,n-1} & m_{1,n} \\ m_{2,1} & m_{2,2} & m_{2,3} & \cdots & m_{2,n-2} & m_{2,n-1} & m_{2,n} \\ 0 & m_{3,2} & m_{3,3} & \cdots & m_{3,n-2} & m_{3,n-1} & m_{3,n} \\ 0 & 0 & m_{4,3} & \cdots & m_{4,n-2} & m_{4,n-1} & m_{4,n} \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & m_{n-1,n-2} & m_{n-1,n-1} & m_{n-1,n} \\ 0 & 0 & 0 & \cdots & 0 & m_{n,n-1} & m_{n,n} \end{pmatrix}$$

The Hessenberg algorithm (see [3]) consists of the following two main steps:

Step 1: Reduce the matrix $\mathbf{M} \in \mathbb{Z}_p^{n\times n}$ into the upper Hessenberg form using a series of row and column operations in $\mathbb{Z}_p$, while preserving the characteristic polynomial. This is a similarity transformation. $O(n^3)$ operations in $\mathbb{Z}_p$ are performed. To see that the upper Hessenberg form $\mathbf{H}$ has the same characteristic polynomial as $\mathbf{M}$, note that $\mathbf{M} = \mathbf{EHE}^{-1}$ where $\mathbf{E}^{-1} = \mathbf{E}^t$ and $\det(\mathbf{E}) = \pm 1$. Here $\mathbf{E}$ corresponds to the row operations, $\mathbf{E}^t$ corresponds to the column operations. We have

$$\begin{aligned}\det(x\mathbf{I} - \mathbf{M}) &= \det(x\mathbf{I} - \mathbf{EHE}^{-1}) \\ &= \det(\mathbf{E}(x\mathbf{I})\mathbf{E}^{-1} - \mathbf{EHE}^{-1}) \\ &= \det(\mathbf{E}(x\mathbf{I} - \mathbf{H})\mathbf{E}^{-1}) \\ &= \det(\mathbf{E})\det(x\mathbf{I} - \mathbf{H})\det(\mathbf{E}^{-1}) \\ &= \det(x\mathbf{I} - \mathbf{H}).\end{aligned}$$

The algorithm below reduces a matrix $\mathbf{M}$ into upper Hessenberg form. In the algorithm, $\mathbf{R}_i$ denotes the i'th row of $\mathbf{M}$ and $\mathbf{C}_j$ the j'th column of $\mathbf{M}$.

Input: Matrix $\mathbf{M} \in \mathbb{Z}_p^{n\times n}$
Output: Matrix $\mathbf{M}$ in upper Hessenberg form with the same eigenvalues

for $j = 1$ **to** $n - 2$ **do**
  search for a nonzero entry $m_{i,j}$ where $j + 2 \le i \le n$
  if found such entry **then**
    do $\mathbf{R}_i \leftrightarrow \mathbf{R}_{j+1}$ and $\mathbf{C}_i \leftrightarrow \mathbf{C}_{j+1}$ **if** $m_{j+1,j} = 0$
    for $k = j + 2$ **to** n **do**
      (reduce using $m_{j+1,j}$ as pivot)
      $u \leftarrow m_{k,j}\, {m_{j+1,j}}^{-1}$
      $\mathbf{R}_k \leftarrow \mathbf{R}_k - u\mathbf{R}_{j+1}$
      $\mathbf{C}_{j+1} \leftarrow \mathbf{C}_{j+1} + u\mathbf{C}_k$
    end for
  else
    first j columns of $\mathbf{M}$ is already in upper Hessenberg form
  end if
end for

Step 2: The characteristic polynomial $c(x) = p_{n+1}(x) \in \mathbb{Z}_p[x]$ of the upper Hessenberg form can be efficiently computed bottom up using $O(n^2)$ operations in $\mathbb{Z}_p[x]$ ($O(n^3)$ operations in $\mathbb{Z}_p$) from the following recurrence for $p_k(x)$.

$$p_{k+1}(x) = \begin{cases} 1 & k = 0 \\ (x - m_{k,k})\, p_k(x) - \sum_{i=1}^{k-1} (\prod_{j=i}^{k-1} m_{j+1,j})\, m_{i,k}\, p_i(x) & 1 \le k \le n+1 \end{cases}$$

The algorithm below computes the above recurrence bottom up, and clearly shows that $O(n^2)$ operations in $\mathbb{Z}_p[x]$ are required.

Input: Matrix $\mathbf{M} \in \mathbb{Z}_p^{n \times n}$ in upper Hessenberg form
Output: Characteristic polynomial $c(x) \in \mathbb{Z}_p[x]$ of $\mathbf{M}$

$p_1(x) \leftarrow 1$
for $k = 1$ **to** n **do**
  $p_{k+1}(x) \leftarrow (x - m_{k,k})\, p_k(x)$
  $t \leftarrow 1$
  for $i = 1$ **to** $k - 1$ **do**
    $t \leftarrow t\, m_{k-i+1,k-i}$
    $p_{k+1}(x) \leftarrow p_{k+1} - t\, m_{k-i,k}\, p_{k-i}(x)$
  end for
end for
output $p_{n+1}(x)$

3 Timings and Implementations

For a machine prime p, in order to improve the running time of our algorithm, we've implemented the Hessenberg algorithm over $\mathbb{Z}_p$ in the C programming language and the rest of the algorithm in Maple. We used the Maple external function interface to call the C code (see [7]). We've implemented both the 32-bit integer version and 64-bit integer versions, and also several versions using 64-bit double precision floating point values for comparison.

The following table consists of some timings (in seconds) of our modular Hessenberg algorithm for a sparse 364×364 input matrix arising from an application in combinatorics (see [8]). Rows 1-9 below are for the modular algorithm using different implementations of arithmetic for $\mathbb{Z}_p$. The accelerated floating point version **fprem** using 25-bit primes generally give the best times.

Versions	Xeon 2.8 GHz	Opteron 2.0 GHz	AXP2800 2.08 GHz	Pentium M 2.00 GHz	Pentium 4 2.80 GHz
64int	100.7	107.4			
32int	66.3	73.0	76.8	35.6	57.4
new 32int	49.7	54.7	56.3	25.5	39.6
fmod	29.5	32.1	33.0	35.8	81.1
trunc	67.8	73.7	69.6	88.5	110.6
modtr	56.3	62.5	59.5	81.0	82.6
new fmod	11.0	11.6	14.5	15.2	28.8
fprem	10.4	10.9	13.7	13.9	26.8
fLA	17.6	19.9	21.9	26.2	27.3
Berkowitz	2053.6	2262.6			

Implementations

64int The 64-bit integer version is implemented using the *long long int* datatype in C, or equivalently the *integer[8]* datatype in Maple. We can use 32-bit primes. All modular arithmetic first executes the corresponding 64-bit integer machine instruction, then reduces the result mod p because we work in $\mathbb{Z}_p$. We allow both positive and negative integers of magnitude less than p.

32int The 32-bit integer version is similar, but implemented using the *long int* datatype in C, or equivalently the *integer[4]* datatype in Maple. 16-bit primes are used here.

new 32int This is an improved **32int**, with various hand/compiler optimizations.

fmod This 64-bit float version is implemented using the *double* datatype in C, or equivalently the *float[8]* datatype in Maple. 64-bit float operations are used to simulate integer operations. Operations such as additions, subtractions, multiplications are followed by a call to the C library function *fmod()* to reduce the results mod p, since we are working in $\mathbb{Z}_p$. We allow both positive and negative floating point representations of integers with magnitude less than p.

trunc This 64-bit float version is similar to above, but uses the C library function *trunc()* instead of *fmod()*. To compute $b \leftarrow a \bmod p$, we first compute $c \leftarrow a - p \times \mathit{trunc}(a/p)$, then $b \leftarrow c$ if $c \neq \pm p$, $b \leftarrow 0$ otherwise. The *trunc()* function rounds towards zero to the nearest integer.

modtr A modified **trunc** version, where we do not do the extra check for equality to $\pm p$ at the end. So to compute $b \leftarrow a \bmod p$, we actually compute $b \leftarrow a - p \times \mathit{trunc}(a/p)$, which results in $-p \leq b \leq p$.

new fmod An improved **fmod** version, where we have reduced the number of times *fmod()* is called. In other words, we reduce the results mod p only when the number of accumulated arithmetic operations on an entry exceeds a certain threshold. In order to allow this, we are restricted to use 25-bit primes. We call this delayed mod acceleration. See the next subsection.

fprem Equivalent to **new fmod** version, but via direct assembly programming using *fprem* instruction, removing the function call overhead and making some efficiency improvements.

fLA An improved **trunc** version using delayed mod acceleration. It is the default used in Maple's `LA:-Modular` routines.

3.1 Efficiency Considerations

There are a few considerations for use of floating point for mod p computations. Keeping these in mind, one can implement faster external code for the algorithms than is possible with the integer codes, and still have the advantage of using larger primes on 32-bit machines.

1. Although floating point integer computations can represent 53-bit numbers accurately, we restrict the modulus to $p < 2^{25}$, which allows for more efficient mod operations, and multiple mod operations (up to 8) to occur before having to reduce modulo p. We call this the delayed mod acceleration.

2. Leveraging the smaller primes allows up to 8 computations (using a maximal size prime) to occur before we must perform a mod . This can be efficiently utilized in row-based algorithms, as a counter associated with each row can count the number of operations performed, and the algorithms can be made to only perform the mod once the maximal number of computations is reached.

3. Floating point computations have a number of ways in which a mod can be performed, including but not limited to subtracting the floor of the inverse of the modulus times the number from the number, the floating point mod operation *fmod* or *fprem*, using *trunc*, etc.

In our experiments we found the following: Use of the smaller primes, and delayed mod, mentioned in items 1 and 2 above increased performance by a factor of 2-3.

With these modifications, use of floating point modular arithmetic generally demonstrated better performance than integer modular arithmetic.

The use of the C-library *fmod* function or direct assembly programming using the *fprem* instruction (essentially equivalent modulo function call overhead and some efficiency improvements made available for our specific use of *fmod*) showed better performance than the other floating point schemes, except on the Pentium 4, on which it was approximately equal. Note also that on Pentium M the *fprem* performance was nearly a factor of 2 times better.

3.2 Timings for Dense Matrices

The following table consists of some timings (in seconds) of our modular Hessenberg algorithm using float (**fprem**) and integer (**new 32int**) implementations on dense $n \times n$ matrices, with uniformly random integer entries between -999 and 999. We also compare with Maple's Berkowitz algorithm. The timings were done on a dual Opteron 2.2Ghz processor running Unix.

n	float	integer	Berkowitz
50	<0.1	0.13	7.85
100	0.61	1.85	128.6
200	8.82	30.8	2248.1
300	45.4	153.2	
400	173.5	493.4	
600	1195.2	2973.1	
800	4968.8		

Note that the time for Berkowitz algorithm on a dense 200×200 integer matrix is even slower than a sparse 364×364 integer matrix, resulting from the cost of large integer arithmetic. Maple's Berkowitz algorithm is much much slower than the others, as the timings suggest.

From the above data, we can see that the float version is always faster than the integer version (about 3 times faster). A method to improve the running time still further would be to use the early termination technique (see [4]) to stop the Chinese remaindering. It would convert the deterministic algorithm into a Monte-Carlo type probabilistic algorithm, with a bounded probability of error. A good bound for the probability of error, such as 10^{-50} would be sufficient for all practical applications.

4 Asymptotic Comparison of the Methods

Let $\mathbf{A}$ be an $n \times n$ matrix of integers. To compare the running times of the Berkowitz algorithm and the modular algorithm, we suppose that the entries of $\mathbf{A}$ are bounded by B^m in magnitude, that is, they are m base B digits in length. For both algorithms, we need a bound S on the size of the coefficients of the characteristic polynomial $c(x)$. A generic bound on the size of the determinant of $\mathbf{A}$ is sufficient since this is the largest coefficient of $c(x)$. The magnitude of the determinant of $\mathbf{A}$ is bounded by $S = n!B^{mn}$ and its length is bounded by $n \log_B n + mn$ base B digits. If $B > 2^{15}$ then we may assume $\log_B n < 2$ in practice and hence the length of the determinant is $O(mn)$ base B digits.

In Berkowitz's algorithm, the $O(n^4)$ integer multiplications are on integers of average size $O(mn)$ digits in length, hence the complexity (assuming classical integer arithmetic is used) is $O(n^4(mn)^2)$.

Since Maple 9 uses the FFT for integer multiplication and division, the complexity is reduced to $\tilde{O}(n^5 m)$.

In the modular algorithm, we will need $O(mn)$ machine primes. The cost of reducing the n^2 integers in $\mathbf{A}$ modulo one prime is $O(mn^2)$. The cost of computing the characteristic polynomial modulo each prime p is $O(n^3)$. The cost of the Chinese remaindering assuming a classical method for the Chinese remainder algorithm (which is what Maple uses) is $O(n(mn)^2)$. Thus the total complexity is $O(mnmn^2 + mnn^3 + n(mn)^2) = O(m^2n^3 + mn^4)$.

If we assume $m = O(n)$, that is, the size of the integer grows proportionally with the size of the matrix, the complexity of the Berkowitz algorithm and the modular algorithm is $\tilde{O}(n^6)$ and $O(n^5)$ respectively.

If we have $|A_{i,j}| < B$ for all n (in the second set of timings $|A_{i,j}| < 10^3$), the complexity of the Berkowitz algorithm and the modular algorithm is $\tilde{O}(n^5)$ and $O(n^4)$ respectively. In concluding, we mention that algorithms which are asymptotically faster than $O(n^4)$ are known. Two recent reference are Kaltofen and Villard in [6] and Dumas, Pernet and Wan in [4]. We have not implemented any of these algorithms.

References

[1] J. Abdeljaoued. The Berkowitz Algorithm, Maple and Computing the Characteristic Polynomial in an Arbitrary Commutative Ring. *MapleTech* **5**(1), pp. 21–32, Birkhauser, 1997.

[2] S. J. Berkowitz, On computing the determinant in small parallel time using a small number of processors. *Inf. Porcessing Letters* **18**(3) pp. 147–150, 1984.

[3] H. Cohen. *A Course in Computational Algebraic Number Theory.* Graduate texts in mathematics, **138**, Springer-Verlag, 1995.

[4] J.-G. Dumas, C. Pernet, Z. Wan. Efficient Computation of the Characteristic Polynomial. To appear in *The proceedings of ISSAC 2005,* ACM Press, 2005

[5] K. O. Geddes, S. R. Czapor, and G. Labahn. *Algorithms for Computer Algebra.* Kluwer Academic Publ., Boston, Massachusetts, USA, 1992.

[6] E. Kaltofen, G. Villard. On the Complexity of Computing Determinants. *Journal of Computational Complexity* **13** pp. 91–130, 2004.

[7] M. Monagan, K. Geddes, K. Heal, G. Labahn, S. Vorkoetter, J. McCarron, P. deMarco. *Maple 9 Advanced Programming Guide*, Ch. 6, Maplesoft, 2003.

[8] J. Quaintance, $m \times n$ Proper Arrays: Geometric Construction and the Associated Linear Cellular Automata. *Proceedings of the 2004 Maple Summer Workshop*, 2004.