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Computing Krylov iterates in the time of matrix multiplication

Vincent Neiger

Sorbonne Université, CNRS, LIP6
F-75005 Paris, France

Clément Pernet

Univ. Grenoble Alpes, Grenoble INP
CNRS, LJK UMR 5224
Grenoble, France

Gilles Villard

CNRS, Univ. Lyon, ENS de Lyon, Inria,
UCBL, LIP UMR 5668
Lyon, France

ABSTRACT

Krylov methods rely on iterated matrix-vector products $A^k u_j$ for an $n \times n$ matrix A and vectors u_1, \dots, u_m . The space spanned by all iterates $A^k u_j$ admits a particular basis — the *maximal Krylov basis* — which consists of iterates of the first vector $u_1, Au_1, A^2 u_1, \dots$, until reaching linear dependency, then iterating similarly the subsequent vectors until a basis is obtained. Finding minimal polynomials and Frobenius normal forms is closely related to computing maximal Krylov bases. The fastest way to produce these bases was, until this paper, Keller-Gehrig’s 1985 algorithm whose complexity bound $O(n^\omega \log(n))$ comes from repeated squarings of A and logarithmically many Gaussian eliminations. Here $\omega > 2$ is a feasible exponent for matrix multiplication over \mathbb{F} . We present an algorithm computing the maximal Krylov basis in $O(n^\omega \log \log(n))$ field operations when $m \in O(n)$, and even $O(n^\omega)$ as soon as $m \in O(n/\log(n)^c)$ for some fixed real $c > 0$. As a consequence, we show that the Frobenius normal form together with a transformation matrix can be computed deterministically in $O(n^\omega \log \log(n)^2)$, and therefore matrix exponentiation A^k can be performed in the latter complexity if $\log(k) \in O(n^{\omega-1-\epsilon})$, for $\epsilon > 0$. A key idea for these improvements is to rely on fast algorithms for $m \times m$ polynomial matrices of average degree n/m , involving high-order lifting and minimal kernel bases.

1 INTRODUCTION

We present a new deterministic algorithm for the computation of some specific Krylov matrices, which play a central role in determining the structure of linear operators. To a matrix $A \in \mathbb{F}^{n \times n}$ over an arbitrary commutative field \mathbb{F} , a (column) vector $u \in \mathbb{F}^n$ and a nonnegative integer $d \in \mathbb{N}$, we associate the *Krylov matrix* $K_d(A, u)$ formed by the first d iterates of u through A :

$$K_d(A, u) = \begin{bmatrix} u & Au & \dots & A^{d-1}u \end{bmatrix} \in \mathbb{F}^{n \times d}. \quad (1)$$

More generally, to m vectors $U = [u_1 \ \dots \ u_m] \in \mathbb{F}^{n \times m}$ and a tuple $d = (d_1, \dots, d_m) \in \mathbb{N}^m$, we associate the Krylov matrix

$$K_d(A, U) = \begin{bmatrix} K_{d_1}(A, u_1) & \dots & K_{d_m}(A, u_m) \end{bmatrix} \in \mathbb{F}^{n \times |d|}, \quad (2)$$

where $|d|$ is the sum $d_1 + \dots + d_m$. (Note that it will prove convenient to allow $m = 0$ and $d_i = 0$.) Such matrices are used to construct special bases of the A -invariant subspace

$$\text{Orb}(A, U) = \text{Span}_{\mathbb{F}}(\{A^i u_j, i \in \mathbb{N}, j \in \{1, \dots, m\}\}).$$

Indeed, for a given A and U there always exists a tuple d such that the columns of $K_d(A, U)$ form a basis of $\text{Orb}(A, U)$ (Section 3.1.1). In this paper, we focus on the computation of the unique such basis of $\text{Orb}(A, U)$ whose tuple d is the lexicographically largest one [11, Sec. 5]. We call this d the *maximal (Krylov) indices* of $\text{Orb}(A, U)$, and the corresponding basis the *maximal Krylov basis*.

Our main result is a deterministic algorithm that computes the maximal Krylov basis in $O(n^\omega \log \log(n))$ field operations when $m \in O(n)$, where $\omega > 2$ is a feasible exponent for the cost of square matrix multiplication over \mathbb{F} [2, 23]. As soon as the number m of initial vectors in U is in $O(n/\log(n)^c)$ for some fixed $c > 0$, the bound becomes simply $O(n^\omega)$ (Theorem 4.1). This is an improvement over the best previously known complexity bound $O(n^\omega \log(n))$, for an algorithm due to Keller-Gehrig [11]. In particular, to get down to $O(n^\omega)$, we avoid an ingredient that is central in the latter algorithm and related ones, which is to compute logarithmically many powers of A by repeated squaring (see Section 3.1.1).

Overview of the approach. The main idea is to use operations on polynomial matrices rather than linear transformations. In this direction, we are following in the footsteps of e.g. [26], where polynomial matrix inversion is exploited to compute sequences of matrix powers, and [15], where polynomial matrix normal forms and block-triangular decompositions allow the efficient computation of the characteristic polynomial. A key stage we introduce consists in transforming between left and right matrix fraction descriptions:

$$S(x)T(x)^{-1} = (I - xA)^{-1}U = \sum_{k \geq 0} x^k A^k U, \quad (3)$$

with $S \in \mathbb{F}[x]^{n \times m}$ and $T \in \mathbb{F}[x]^{m \times m}$. For $m \leq n$, one may see Eq. (3) as considering a compressed fraction description ST^{-1} of $(I - xA)^{-1}U$, with larger polynomial degrees and smaller matrix dimensions. The power series expansion of ST^{-1} , when suitably truncated, produces a Krylov basis.

After some preliminary reminders on polynomial matrices in Section 2, the first algorithms are given in Section 3. There, our contribution is specifically adapted to the case where the compression is fully effective, that is, when m is away from n (at least slightly, see below). In this case, thanks to the kernel basis algorithm of [25] and its analysis in [8, 15], appropriate S and T are computed using $O(n^\omega)$ arithmetic operations (Section 2.1).

The next steps are to determine the maximal indices and to compute a truncated series expansion of ST^{-1} . First we explain in Section 3.1 that the maximal indices of $\text{Orb}(A, U)$ are obtained by working, equivalently to Eq. (3), from certain denominator matrices of $(xI - A)^{-1}U$ (see Eq. (4)). The indices are computed as diagonal degrees if the denominator is triangular (Lemma 3.1). It follows that a Hermite form computation allows us to obtain them efficiently [12]. We then give in Section 3.2 an algorithm for computing a Krylov matrix $K_d(A, U)$ for an arbitrary given d , which we will apply afterwards with the maximal indices for d . According to Eq. (3) and given a tuple $d = (d_1, \dots, d_m) \in \mathbb{N}^m$, this Krylov matrix can be obtained from the expansion of ST^{-1} with column j truncated modulo x^{d_j} for $1 \leq j \leq m$. To deal with the unbalancedness of degrees and truncation order, this expansion is essentially computed using high-order lifting [21], combined with the partial linearization

technique of [6]. (To keep things concise in Section 3, details about this are deferred until Section 6.) If $m \in O(n/\log(n)^c)$, then the maximal indices and $K_d(A, U)$ for any d such that $|d| = O(n)$ can be computed using $O(n^\omega)$ arithmetic operations.

Our general algorithm computing maximal Krylov bases is given in Section 4. The ability to reduce the cost for certain m , as seen above, allows to improve the general case $m = O(n)$ and obtain the complexity bound $O(n^\omega \log \log(n))$. Algorithm `MaxKrylovBasis` is a hybrid one, using the Keller-Gehrig strategy as well as polynomial matrices. In the same spirit as the approach in [11, Sec. 5], we start with the computation of a partial Krylov basis $\tilde{K}(A, U)$ from the whole U , but for only a few iterations, i.e. up to degree $\tilde{d} \sim \log(n)^c$. This allows us to isolate $O(n/\log(n)^c)$ vectors for which iterations should be continued. A maximal basis is then computed only from these vectors, based on polynomial matrix operations. The final maximal basis is obtained by appropriately merging the short and long sequences of Krylov iterates henceforth available, via fast Gaussian elimination [11, Sec. 4].

Frobenius normal form and extensions. Krylov matrices are a fundamental tool for decomposing the space \mathbb{F}^n with respect to a linear operator (see e.g. [5, 19] for detailed algorithmic treatments), or linear dynamical systems [9, 10]. The Frobenius normal form and the Kalman decomposition are briefly discussed in Section 5. The best known deterministic algorithm for the Frobenius form can be found in [19, Prop. 9.27]; the employed approach reveals in particular that the problem can essentially be reduced to computing $O(\log \log(n))$ maximal Krylov bases. The cost for the Kalman decomposition is bounded by that of the computation of a constant number of Krylov bases. Thus our results reduce the complexity bounds for these two problems. Matrix exponentiation is also accelerated, as a direct consequence of the cost improvement for the Frobenius normal form [5, Thm. 7.3].

Computational model. Throughout this paper, \mathbb{F} is an effective field. The cost analyses consist in giving an asymptotic bound on the number of arithmetic operations in \mathbb{F} used by the algorithm. The operations are addition, subtraction, multiplication, and inversion in the field, as well as testing whether a given field element is zero. We use that two polynomials in $\mathbb{F}[x]$ of degree bounded by d can be multiplied using $O(d \log(d) \log \log(d))$ field operations [4, Chap. 8]. On rare occasions, mostly in Section 6, we use a multiplication time function $d \mapsto M(d)$ for $\mathbb{F}[x]$ to develop somewhat more general results [4, Chap. 8]. This multiplication time function is subject to some convenient assumptions (see Section 6.1), which are satisfied in particular for an $O(d \log(d) \log \log(d))$ algorithm.

Notation. For an $m \times n$ matrix A , we write a_{ij} for its entry (i, j) . Given sets I and J of row and column indices, $A_{I,J}$ stands for the corresponding submatrix of A ; we use $*$ to denote all indices, such as in $A_{I,*}$ or $A_{*,J}$. We manipulate tuples $d \in (\mathbb{N} \cup \{-\infty\})^m$ of indices or polynomial degrees, and write $|d|$ for the sum of the entries of the tuple. For a polynomial matrix $A \in \mathbb{F}[x]^{m \times n}$, the column degree $\text{cdeg}(A)$ is the tuple of its column degrees $\max_{1 \leq i \leq m} (\deg a_{i,j})$, for $1 \leq j \leq n$.

2 KERNEL BASIS, HERMITE NORMAL FORM

We recall the complexity bounds for two fundamental problems which we rely on: kernel basis and Hermite normal form. The more

technical presentation of some of the other ingredients needed to manipulate polynomial matrices, such as truncated inversion, is deferred to Section 6.

2.1 Minimal kernel basis

A core tool in Algorithms 1 and 2 is the computation of minimal kernel bases of polynomial matrices [9, Sec. 6.5.4, p. 455]. The matrix fraction description in Eq. (3) can indeed be rewritten as

$$\begin{bmatrix} I - xA & -U \end{bmatrix} \begin{bmatrix} S \\ T \end{bmatrix} = 0.$$

For a matrix $F \in \mathbb{F}[x]^{n \times m}$, its (right) kernel is the $\mathbb{F}[x]$ -module formed by the vectors $p \in \mathbb{F}[x]^m$ such that $Fp = 0$; it has rank $m - \text{rank}(F)$. A kernel basis is said to be minimal if it is column reduced, that is, its leading matrix has full column rank [9, Sec. 6.3, p. 384]. An efficient algorithm for minimal kernel bases was described in [25], and its complexity was further analyzed in the case of a full rank input F in [8, App. B] and [15, Lem. 2.10]. We will use the following particular case of the latter result:

LEMMA 2.1. ([25, Algo. 1], and analyses in [8, 15].) *Let $F \in \mathbb{F}[x]^{n \times (m+n)}$ have rank n and degree ≤ 1 , with $m \in O(n)$. There is an algorithm `MinimalKernelBasis` which, on input F , returns a minimal kernel basis $B \in \mathbb{F}[x]^{(m+n) \times m}$ for F using $O(n^\omega)$ operations in \mathbb{F} . Furthermore, $|\text{cdeg}(B)| \leq n$.*

The complexity bound in [15] uses a multiplication time function with assumptions that are satisfied in our case (see [15, Sec. 1.1]). Apart from supporting degree > 1 , the three listed references above also consider the more general *shifted* reduced bases [1]. The non-shifted case is obtained by using the uniform shift $s = (1, \dots, 1) \in \mathbb{N}^{m+n}$, for which s -reduced bases are also (non-shifted) reduced bases. This shift does satisfy the input requirement $s \geq \text{cdeg}(F)$ and it has sum $|s| = m + n$; [25, Thm. 3.4] then guarantees that B has sum of s -column degrees at most $m + n$, which translates as $|\text{cdeg}(B)| \leq n$.

2.2 Hermite normal form

A nonsingular polynomial matrix $H \in \mathbb{F}[x]^{m \times m}$ is in Hermite normal form if it is upper triangular, with monic diagonal entries, and all entries above the diagonal have degree less than that of the corresponding diagonal entry: $\deg(h_{ij}) < \deg(h_{ii})$ for $1 \leq i < j \leq m$. Given a nonsingular matrix $T \in \mathbb{F}[x]^{m \times m}$, there is a unique matrix $H \in \mathbb{F}[x]^{m \times m}$ in Hermite normal form which can be obtained from T via unimodular column operations, meaning $TV = H$ for some $V \in \mathbb{F}[x]^{m \times m}$ with $\det(V) \in \mathbb{F} \setminus \{0\}$. It is called the Hermite normal form of T .

In fact, in this paper we are only interested in the diagonal degrees of the Hermite form (see Section 3.1.2). By the uniqueness of the form (off-diagonal degrees can always be reduced relative to the diagonal ones), these degrees are the same for all triangular forms unimodularly right equivalent to T .

LEMMA 2.2. ([12, Prop. 3.3].) *Let T be nonsingular in $\mathbb{F}[x]^{m \times m}$. There is an algorithm `HermiteDiagonal` which takes T as input and returns the diagonal entries $(h_{11}, \dots, h_{mm}) \in \mathbb{F}[x]^m$ of the Hermite normal form of T using $O(m^{\omega-1} n \log(n)^{c_1})$ operations in \mathbb{F} , where $n = \max(m, |\text{cdeg}(T)|)$ and c_1 is a positive real constant.*

The algorithm as described in [12, Algo. 1] works with an equivalent lower triangular variation of the form. It involves two main tools: kernel bases, whose cost does not have dominant logarithmic factors (Lemma 2.1), and column bases [24], for which there is no analysis of the number of logarithmic factors in the literature, to the best of our knowledge. In Lemma 2.2 we introduce the latter as a constant $c_1 > 0$, and this remains to be thoroughly analyzed.

3 KRYLOV BASIS VIA POLYNOMIAL KERNEL

The key ingredients in our approach for computing Krylov bases transform the problem into polynomial matrix operations. In this section, we present two algorithms which involve matrix fraction descriptions as in Eq. (3), or equivalent formulations (see also Appendix B). In Section 3.1, given $A \in \mathbb{F}^{n \times n}$ and $U = [u_1 \cdots u_m]$ formed from m vectors in \mathbb{F}^n , Algorithm `MaxIndices` computes the maximal Krylov indices of $\text{Orb}(A, U)$. It exploits the fact that these indices coincide with the degrees of certain minimal polynomial relations between the columns of $[xI - A \quad -U]$, allowing the use of polynomial matrix manipulation tools. In Section 3.2, we consider the problem of computing the Krylov matrix $K_d(A, U)$ for a given tuple $d \in \mathbb{N}^m$. Based on Eq. (3), after computing a kernel basis to obtain S and T , Algorithm `KrylovMatrix` proceeds with a matrix series expansion, using the truncation orders given by d .

Joining both algorithms, from A and U one obtains the maximal Krylov basis of $\text{Orb}(A, U)$, at a cost of $O(n^\omega)$ field operations as soon as the number m of vectors forming U is in $O(n/\log(n)^c)$. This will be done explicitly in Lines 1 to 5 of Algorithm `MaxKrylovBasis` in Section 4.

3.1 Computing the maximal indices

We begin in Section 3.1.1 with a brief reminder of a useful characterization of the maximal Krylov indices in terms of linear algebra over \mathbb{F} . We then show how to reduce their computation to operations on polynomial matrices, by explaining that they coincide with the degrees of certain polynomials in a kernel basis (Lemma 3.1).

Linear dependencies between vectors in Krylov subspaces are translated into polynomial relations using the $\mathbb{F}[x]$ -module structure of \mathbb{F}^m based on $xu = Au$ for $u \in \mathbb{F}^n$ [7, Sec.3.10]. Some of these dependencies in $\text{Orb}(A, U)$ are given by the coefficients of the entries of the triangular matrices $H \in \mathbb{F}[x]^{m \times m}$ such that

$$(xI - A)^{-1}U = LH^{-1} \quad (4)$$

with $L \in \mathbb{F}[x]^{n \times m}$ [9, Sec. 6.7.1, p. 476]. In particular, if L and H are (right) coprime then the maximal indices of $\text{Orb}(A, U)$ are given by the diagonal degrees of H . We explain this in Section 3.1.2, considering equivalently that $[L^\top \quad H^\top]^\top$ is a kernel basis of $[xI - A \quad -U]$. The computation of the indices follows in Section 3.1.3, it is a combination of the kernel algorithm of [25] with the Hermite form algorithm of [12].

3.1.1 Keller-Gehrig's branching algorithm. The most efficient algorithm so far for computing the lexicographically largest tuple d such that $K_d(A, U)$ is a Krylov basis is given in [11, Sec. 5]. For a general U ($m \in O(n)$), the associated cost bound $O(n^\omega \log(n))$ is mainly due to raising A to powers in order to generate Krylov vector sequences. A characterization of the maximal indices d which we will need (a proof can be found in Appendix A), is used in particular

by Keller-Gehrig: for $1 \leq j \leq m$, d_j is the first integer such that

$$A^{d_j}u_j \in \text{Span}(u_j, Au_j, \dots, A^{d_j-1}u_j) + \text{Orb}(A, U_{*,1..j-1}). \quad (5)$$

A recursive construction allows independent and increasingly long Krylov chains $u_j, Au_j, \dots, A^l u_j, l \geq 0$, to be joined together in order to reach the maximal basis of $\text{Orb}(A, U)$; with independence guaranteed by Gaussian elimination [11, Sec. 4]. We will return to this in our general Krylov basis method in Section 4.

3.1.2 Links with Hermite normal form. The following is to be compared with known techniques for matrix fraction descriptions [9, Sec. 6.4.6, p. 424], or to a formalism occasionally used to efficiently compute matrix normal forms [22; 19, Chap. 9].

LEMMA 3.1. *Given $A \in \mathbb{F}^{n \times n}$ and $U \in \mathbb{F}^{n \times m}$, let $[L^\top \quad H^\top]^\top$ be a kernel basis of $[xI - A \quad -U]$ such that $H \in \mathbb{F}[x]^{m \times m}$ is upper triangular. The matrix H is nonsingular and its diagonal degrees are the maximal Krylov indices of $\text{Orb}(A, U)$.*

PROOF. We first note that $(xI - A)^{-1}UP$ is a polynomial matrix with P upper triangular in $\mathbb{F}[x]^{m \times m}$ if and only if we have

$$p_{jj}(A)u_j + \sum_{i=1}^{j-1} p_{ij}(A)u_i = 0, \quad 1 \leq j \leq m. \quad (6)$$

In fact, using the expansion $(xI - A)^{-1} = \sum_{k \geq 0} \frac{A^k}{x^{k+1}}$ at $x = \infty$, we see that the coefficient of $1/x^{k+1}$ in the j th column of the expansion of $(xI - A)^{-1}UP$ is

$$\sum_{l=0}^{\deg p_{jj}} p_{jj}^{(l)} A^{l+k} u_j + \sum_{i=1}^{j-1} \sum_{l=0}^{\deg p_{ij}} p_{ij}^{(l)} A^{l+k} u_i = 0, \quad k \geq 0.$$

Here we have denoted the coefficient of degree l of $p_{i,j}$ by $p_{ij}^{(l)}$, for $1 \leq i \leq j \leq m$. Then the ‘‘if’’ direction is obtained with $k = 0$ since the coefficient of $1/x$ in the expansion of the polynomial matrix $(xI - A)^{-1}UP$ is zero. Conversely, if Eq. (6) holds then it can be multiplied by any power A^k with $k \geq 0$. Thus the corresponding coefficients of $1/x^{k+1}$ are zero in the expansion of $(xI - A)^{-1}UP$, which is thus a polynomial matrix.

Now let d be the maximal indices tuple, and let d' be the tuple of the diagonal degrees of H . We have that H is nonsingular hence $d' \in \mathbb{N}^m$. Indeed, since $L = (xI - A)^{-1}UH$, $Hu = 0$ for $u \neq 0$ would lead to $[L^\top \quad H^\top]^\top u = 0$, which is impossible by definition of bases.

To conclude the proof, we first show that d is lexicographically greater than d' , and then the converse. The characterization of d given by Eq. (5) leads to linear dependencies as in Eq. (6), hence to P with diagonal degrees given by d . Since $(xI - A)^{-1}UP$ is a polynomial matrix, say R , the columns of $[R^\top \quad P^\top]^\top$ are in the kernel of $[xI - A \quad -U]$ and we must have $P = HQ$ for some polynomial matrix Q . Here we have used that $[L^\top \quad H^\top]^\top$ is a basis of the kernel. Since both P and H are triangular we conclude that d is greater than d' . On the other hand, considering H , we get dependencies as in Eq. (6) with polynomials given by the entries of H . Again, thanks to the characterization of d and the fact that the d_j 's reflect the shortest dependencies, we finally get that d' is greater than d . \square

3.1.3 Algorithm MaxIndices. Let $V \in \mathbb{F}[x]^{m \times m}$ be unimodular such that $H = TV$ is in Hermite form. The matrix $[L^\top \ H^\top]^\top = [S^\top \ T^\top]^\top V$ is also a kernel basis of $[xI - A \ -U]$, and the correctness of the algorithm follows from Lemma 3.1.

Algorithm 1 MaxIndices(A, U)

Input: $A \in \mathbb{F}^{n \times n}, U \in \mathbb{F}^{n \times m}$

Output: The tuple in \mathbb{N}^m of the maximal indices of $\text{Orb}(A, U)$

- 1: \triangleright minimal kernel basis [25, Algo. 1] \blacktriangleleft
 $[\begin{smallmatrix} S \\ T \end{smallmatrix}] \leftarrow \text{MinimalKernelBasis}([xI - A \ -U])$
 where $S \in \mathbb{F}[x]^{n \times m}$ and $T \in \mathbb{F}[x]^{m \times m}$
 - 2: \triangleright diagonal entries of the Hermite normal form \blacktriangleleft
 $(h_{11}, \dots, h_{mm}) \in \mathbb{F}[x]^m \leftarrow \text{HermiteDiagonal}(T) \triangleright$ [12, Alg. 1]
 - 3: **return** $(\deg(h_{11}), \dots, \deg(h_{mm}))$
-

For the complexity bound, the kernel basis at Line 1 is computed using $O(n^\omega)$ arithmetic operations thanks to Lemma 2.1 when $m \in O(n)$. From Lemma 3.1, the resulting matrix T is nonsingular because its Hermite form is. Using Lemma 2.1 again we also know that $|\text{cdeg}(T)| \leq n$. In combination with Lemma 2.2 we get that Line 2 can be achieved using $O(m^{\omega-1} n \log(n)^{c_1})$ operations in \mathbb{F} . In particular, as soon as the number of columns of U is in $O(n/\log(n)^{c_1/(\omega-1)})$ the complexity bound becomes $O(n^\omega)$.

3.2 Computing a Krylov matrix

Hereafter, for a column polynomial vector $v = \sum_j v_j x^j \in \mathbb{F}[x]^m$ and an integer $d \in \mathbb{N}$, we denote its truncation at order d by

$$v \text{ rem } x^d = v_0 + v_1 x + \dots + v_{d-1} x^{d-1} \in \mathbb{F}[x]^m$$

and the corresponding matrix of coefficients by

$$\text{coeffs}(v, d) = [v_0 \ v_1 \ \dots \ v_{d-1}] \in \mathbb{F}^{m \times d}.$$

We extend this column-wise for $M \in \mathbb{F}[x]^{m \times k}$ and $d = (d_j)_j \in \mathbb{N}^k$, that is, $M \text{ rem } x^d = [M_{*,1} \text{ rem } x^{d_1} \ \dots \ M_{*,k} \text{ rem } x^{d_k}]$.

Algorithm **KrylovMatrix** uses polynomial matrix subroutines at Lines 2 and 3. They are handled in detail in Sections 6.2 and 6.3.

LEMMA 3.2. *Algorithm KrylovMatrix is correct. Assuming $m \in O(n)$ and $|d| \in O(n)$, it uses $O(m^{\omega-2} n^2 \log(n)^4)$ operations in \mathbb{F} .*

PROOF. Knowing by Lemma 3.3 that $T(0)$ is invertible (hence T is nonsingular), the correctness follows from the series expansion

$$ST^{-1} = (I - xA)^{-1}U = \sum_{k \geq 0} x^k A^k U$$

mentioned in Eq. (3); here the first equality comes from the kernel relation $[I - xA \ -U] [S^\top \ T^\top]^\top = 0$, by construction in Line 1. Since $T(0)$ is invertible, Lines 2 and 3 compute $P = SQ \text{ rem } x^d = ST^{-1} \text{ rem } x^d$, according to Propositions 6.3 and 6.4. The above equation yields $\text{coeffs}(P_{*,j}, d_j) = [u_j \ Au_j \ \dots \ A^{d_j-1} u_j]$, hence the correctness of the output formed at Line 4.

We turn to the complexity analysis. We assume $m \leq |d|$ without loss of generality: the columns of U corresponding to indices j with $d_j = 0$ could simply be ignored in Algorithm **KrylovMatrix**, reducing to a case where all entries of d are positive.

Algorithm 2 KrylovMatrix(A, U, d)

Input: $A \in \mathbb{F}^{n \times n}, U \in \mathbb{F}^{n \times m}, d = (d_1, \dots, d_m) \in \mathbb{N}^m$

Output: the Krylov matrix $K_d(A, U) \in \mathbb{F}^{n \times (d_1 + \dots + d_m)}$

- 1: \triangleright minimal kernel basis [25, Algo. 1] \blacktriangleleft
 $[\begin{smallmatrix} S \\ T \end{smallmatrix}] \leftarrow \text{MinimalKernelBasis}([I - xA \ -U])$
 where $S \in \mathbb{F}[x]^{n \times m}$ and $T \in \mathbb{F}[x]^{m \times m}$
 - 2: \triangleright column-truncated inverse $T^{-1} \text{ rem } x^d$, detailed in Section 6.2 \blacktriangleleft
 $Q \in \mathbb{F}[x]^{m \times m} \leftarrow \text{TruncatedInverse}(T, d)$
 - 3: \triangleright column-truncated product $SQ \text{ rem } x^d$, detailed in Section 6.3 \blacktriangleleft
 $P \in \mathbb{F}[x]^{n \times m} \leftarrow \text{TruncatedProduct}(S, Q, d)$
 - 4: \triangleright linearize columns of P into a constant matrix and return \blacktriangleleft
return $[\text{coeffs}(P_{*,1}, d_1) \mid \dots \mid \text{coeffs}(P_{*,m}, d_m)] \in \mathbb{F}^{n \times |d|}$
-

By Lemma 2.1, Line 1 uses $O(n^\omega)$ operations in \mathbb{F} and ensures $|\text{cdeg}(K)| \leq n$. In particular, $|\text{cdeg}(S)| \leq n$ and $|\text{cdeg}(T)| \leq n$.

The latter bound ensures that the generic determinantal degree $\Delta(T)$ is in $O(n)$ (see Lemma 6.1), hence we can use the second cost bound in Proposition 6.3: Line 2 computes $Q = T^{-1} \text{ rem } x^d$ using

$$O\left(m^\omega M\left(\frac{n}{m}\right) \left(\log(n) + \left\lceil \frac{|d|}{n} \right\rceil \log(m) \log(|d|)\right)\right) \quad (7)$$

field operations. The second cost bound in Proposition 6.4 states that Line 3 computes $SQ \text{ rem } x^d$ using $O(m^{\omega-2} n M(n + |d|))$ operations in \mathbb{F} . Summing the latter bound with that in Eq. (7) yields a cost bound for Algorithm **KrylovMatrix** when the only assumption on d is $m \leq |d|$. Now, assuming further $|d| \in O(n)$, the latter bound becomes $O(m^{\omega-2} n M(n))$, whereas the one in Eq. (7) simplifies as $O(m^\omega M(\frac{n}{m}) \log(n) \log(m))$. The claimed cost bound then follows from $M(n) \in O(n \log(n) \log \log(n))$. \square

LEMMA 3.3. *For T as in Line 1 of Algorithm 2, $T(0)$ is invertible.*

PROOF. Let $B = [S^\top \ T^\top]^\top$. As a kernel basis, B can be completed into a basis of $\mathbb{F}[x]^{m+n}$ [13, Lem. 7.4, p148]: there is $C \in \mathbb{F}[x]^{(m+n) \times n}$ such that $\det([B \ C]) = \det([B(0) \ C(0)]) = 1$. We conclude by deducing that any vector $v \in \mathbb{F}^m$ such that $T(0)v = 0$ must be zero: from $[I \ -U]B(0) = 0$ we get $S(0)v = 0$, hence $B(0)v = 0$, which implies $v = 0$ since $[B(0) \ C(0)]$ is invertible. \square

4 PREPROCESSING OF SMALL INDICES

In this section we consider the case where the number m of vectors to be iterated can be large, typically $m = \Theta(n)$. In such a situation, terms with logarithmic factors of the form $O(m^{\omega-1} n \log(n)^{c_1})$ or $O(m^{\omega-2} n^2 \log(n)^4)$ in the cost of Algorithms 1 and 2 become dominant.

Algorithm **MaxKrylovBasis** computes the maximal Krylov basis of $\text{Orb}(A, U)$. It involves a preprocessing phase based on the Keller-Gehrig branching algorithm [11, Thm 5.1], which is terminated after a small number ℓ of iterations. This ensures that after this phase, no more than $m = n/2^\ell$ vectors still need to be iterated further, which can then be performed by the algorithms of the Section 3. Therefore setting $c = \max(4/(\omega-2), c_1/(\omega-1))$ ensures that with $\ell = \lceil c \log \log(n) \rceil$ and $m = n/\log(n)^c$, Algorithms 1 and 2 will run in $O(n^\omega)$.

A direct call to the algorithms of Section 3 is made if m is sufficiently small, otherwise the for-loop at Line 11 performs the preprocessing phase: ℓ loop iterations of the type used in [11, Sec. 5]. At the end of this loop, the vectors to be further iterated are identified at Line 24. Since there are at most $n/2^\ell$ such vectors, we use our polynomial matrix techniques to continue iterating on them. After merging “long” (indices in J) and “short” (indices not in J) temporary sequences of iterates, the maximal basis is finally obtained.

Algorithm 3 MaxKrylovBasis(A, U)

Input: $A \in \mathbb{F}^{n \times n}$, $U = [u_1 \ \dots \ u_m] \in \mathbb{F}^{n \times m}$
Output: the maximal Krylov basis of $\text{Orb}(A, U)$

- 1: $c \leftarrow \max(4/(\omega - 2), c_1/(\omega - 1))$
- 2: $t \leftarrow \log_2(n)^c$
- 3: **if** $m \leq n/t$ **then**
- 4: $d \leftarrow \text{MaxIndices}(A, U)$
- 5: $K \leftarrow \text{KrylovMatrix}(A, U, d)$; **return** K
- 6: **end if**
- 7: $\ell \leftarrow \lceil \log_2(t) \rceil$
- 8: $V^{(0)} \leftarrow U$; $\delta \leftarrow (1, \dots, 1) \in \mathbb{Z}^m$
- 9: $B \leftarrow A$
- 10: \triangleright Preprocessing phase in a Keller-Gehrig fashion [11] \blacktriangleleft
- 11: **for** $i \leftarrow 0, \dots, \ell - 1$ **do**
- 12: Let $V^{(i)} = [V_1^{(i)} \ V_2^{(i)} \ \dots \ V_m^{(i)}]$ where
 $V_j^{(i)} = K_{\delta_j}(A, U_{*,j}) \in \mathbb{F}^{n \times \delta_j}$.
- 13: Let $J = \{j \in \{1, \dots, m\} \mid \delta_j = 2^i\} = \{j_1 < \dots < j_s\}$
- 14: $[W_{j_1}^{(i)} \ \dots \ W_{j_s}^{(i)}] \leftarrow B [V_{j_1}^{(i)} \ \dots \ V_{j_s}^{(i)}]$
 such that $j_1 < \dots < j_s \in J$.
- 15: $W_j^{(i)} \leftarrow [] \in \mathbb{F}^{n \times 0}$ for $j \notin J$
- 16: $Z \leftarrow [V_1^{(i)} \ W_1^{(i)} \ \dots \ V_m^{(i)} \ W_m^{(i)}]$
- 17: $C \leftarrow \text{ColRankProfile}(Z)$
- 18: $\delta \leftarrow (\delta_1, \dots, \delta_m)$ s.t. δ_j is maximal with
 $K_{\delta_j}(A, u_j) = Z_{*, C \cap \{b..b+\delta_j-1\}}$ for some b .
- 19: $V^{(i+1)} \leftarrow [V_1^{(i+1)} \ \dots \ V_m^{(i+1)}]$ where
 each $V_j^{(i+1)} \leftarrow K_{\delta_j}(A, u_j)$ is copied from Z
- 20: $B \leftarrow B^2$
- 21: **end for**
- 22: \triangleright Here, $V^{(\ell)} = K_\delta(A, U)$ and $\delta = (\delta_1, \dots, \delta_m) \in \{0, \dots, 2^\ell\}^m$ is
 lexico. maximal s.t. $K_\delta(A, U)$ has full rank. \blacktriangleleft
- 23: \triangleright Further iterations for selected vectors, using polynomial matrices \blacktriangleleft
- 24: Let $J = \{j \in \{1, \dots, m\}, \delta_j = 2^\ell\}$ and $s \leftarrow \#J$
- 25: $d \leftarrow \text{MaxIndices}(A, U_{*,J})$
- 26: $[K_{j_1} \ \dots \ K_{j_s}] \leftarrow \text{KrylovMatrix}(A, U_{*,J}, d)$
- 27: \triangleright Final merge \blacktriangleleft
- 28: $K_j \leftarrow V_j^{(\ell)}$ for all $j \notin J$
- 29: $K \leftarrow [K_1 \ \dots \ K_m]$
- 30: **return** $K_{*, \text{ColRankProfile}(K)}$

THEOREM 4.1. *Algorithm MaxKrylovBasis is correct. If $m = O(n)$, it uses $O(n^\omega \log \log(n))$ operations in \mathbb{F} , and if $m = O(n/\log(n)^c)$ for the constant $c > 0$ in Line 1, it uses $O(n^\omega)$ operations in \mathbb{F} .*

PROOF. As in Keller-Gehrig’s branching algorithm [11], the loop invariant is $V^{(i)} = K_\delta(A, U)$ with $\delta \in \{0, \dots, 2^i\}^m$ lexicographically maximal such that $V^{(i)}$ has full rank. By induction, it remains valid upon exiting the loop, as stated in Line 22. At this point, $s = \#J$ is the number of vectors left to iterate. Indeed, $j \notin J$ means that a linear relation of the type

$$A^{\delta_j} u_j \in \text{Span}(u_j, Au_j, \dots, A^{\delta_j-1} u_j) + \text{Orb}(A, U_{*,1..j-1}). \quad (8)$$

has already been found.

A maximal Krylov basis for the subset of vectors given by J is then computed using the algorithms of Section 3: the maximal indices are computed and then used as input to Algorithm **KrylovMatrix**. All the Krylov iterates that form the matrix K at Line 29 are considered at higher orders than the final maximal ones, because relations of the type Eq. (8) have been detected for all j . A final column rank profile computation allows to know the maximal indices and to select the vectors for the maximal basis.

The choice for the parameter t ensures that the for-loop is executed using $O(n^\omega \log \log(n))$ field operations. On the other hand, Algorithms 1 and 2 are called with $m = s \leq n/2^\ell \leq n/\log(n)^c$, and therefore run in $O(n^\omega)$ field operations. \square

In addition, Algorithm **MaxKrylovBasis** can be adapted to compute any Krylov basis $K_d(A, U)$ where the indices d are additional input to the algorithm. This only requires the two following modifications:

(1) Lines 17 and 18 should be replaced by

```
for all  $j \in J$  do
     $\delta_j \leftarrow \min(2\delta_j, d_j)$ 
end for
```

(2) Line 30 should be replaced by

```
return  $K$ 
```

(3) remove Lines 4 and 25

COROLLARY 4.2. *Given $A \in \mathbb{F}^{n \times n}$, $U \in \mathbb{F}^{n \times m}$ and $d \in \mathbb{N}^m$ with $m, |d|$ in $O(n)$, the Krylov matrix $K_d(A, U)$ can be computed using $O(n^\omega \log \log(n))$ field operations, or $O(n^\omega)$ operations if $m = O(n/\log(n)^c)$ where c is a positive real constant.*

5 FROBENIUS AND KALMAN FORMS

In this section, as a result of our new algorithms for Krylov bases, we discuss some improved complexity bounds for problems immediately related.

5.1 Frobenius normal form

Generically, the Frobenius normal form of an $n \times n$ matrix can be computed using $O(n^\omega)$ operations in \mathbb{F} [11, Sec. 6; 17], and the approach in [17] mainly provides a Las Vegas probabilistic algorithm in $O(n^\omega)$. It is still an open question to obtain the same complexity bound with a deterministic algorithm, and to also compute an associated transformation matrix. Our results allow us to make some progress on both aspects.

Since this is often a basic operation for these problems, we can already note that from Lemma 3.1 and its proof, the minimal polynomial of a vector $u \in \mathbb{F}^m$ can be computed in $O(n^\omega)$. The minimal polynomial is actually the last entry (made monic) of the kernel basis vector of $[xI - A \quad -u]$.

Our algorithms make it possible to obtain $O(n^\omega)$ for the Frobenius form with associated transformation matrix in a special case. The general cost bound $O(n^\omega \log \log(n))$ is achieved in [18, Theorem 7.1] with a probabilistic algorithm. To have a transformation, we can first compute the Frobenius form alone using $O(n^\omega)$ operations. If it has m non-trivial blocks and $U \in \mathbb{F}^{n \times m}$ is chosen uniformly at random, then we know that a transformation matrix can be computed from the maximal Krylov basis of $\text{Orb}(A, U)$ using $O(n^\omega)$ operations [5, Thm. 2.5 & 4.3]. So we have the following.

COROLLARY 5.1. *Let $A \in \mathbb{F}^{n \times n}$ with $\#\mathbb{F} \geq n^2$, and assume that its Frobenius normal form has $m \in O(n/\log(n)^c)$ non-trivial blocks. A transformation matrix to the form can be computed by a Las Vegas probabilistic algorithm using $O(n^\omega)$ field operations.*

The fastest deterministic algorithm to compute a transformation to Frobenius form is given in [20] (see also [19, Chap. 9]), with a cost of $O(n^\omega \log(n) \log \log(n))$. This cost is essentially $O(\log \log(n))$ computations of maximal Krylov bases, plus $O(n^\omega)$ operations.

COROLLARY 5.2. *Given $A \in \mathbb{F}^{n \times n}$, a transformation matrix to Frobenius normal form can be computed using $O(n^\omega \log \log(n)^2)$ field operations.*

Finally, once the Frobenius form is known and given an integer $k \geq 0$, computing A^k costs $O(n^\omega)$ plus $O(\log(k) M(n))$ field operations (see e.g. [5, Cor. 7.4]). (As mentioned in the introduction of the paper, $d \mapsto M(d)$ is a multiplication time function for $\mathbb{F}[x]$.) So the cost is $O(n^\omega \log \log(n)^2)$ if $\log(k) \in O(n^{\omega-1-\epsilon})$. The evaluation of a polynomial $p \in \mathbb{F}[x]$ at A can also be considered in a similar way, using, for example, the analysis of [5, Thm. 7.3].

5.2 Kalman decomposition

The study of the structure of linear dynamical systems in control theory is directly related to Krylov spaces and matrix polynomial forms [9]. For example, the connection we use between maximal indices and degrees in the Hermite form originates from this correspondence.

Our work could be continued to show that the complexity bound $O(n^\omega \log \log(n))$ in Theorem 4.1 could be applied to the computation of a Kalman decomposition [10; 9, Sec. 2.4.2, p. 128]. This is beyond the scope of this paper, so we will not go into detail about it here. However, we can specify the main ingredient. Given A and U with $\dim \text{Orb}(A, U) = v$, we want to transform the system (A, U) according to [9, Sec. 2.4.2, Eq. (11), p. 130]:

$$P^{-1}AP = \begin{bmatrix} A_c & A_1 \\ 0 & A_2 \end{bmatrix}, \quad P^{-1}U = \begin{bmatrix} U_c \\ 0 \end{bmatrix},$$

where A_c is $v \times v$, U_c is $v \times m$, and P is nonsingular in $\mathbb{F}^{n \times n}$. The matrix P can be formed by a Krylov basis of $\text{Orb}(A, U)$ and a matrix with $n - v$ independent columns not in $\text{Orb}(A, U)$. The general decomposition is obtained by combining a constant number of such transformations and basic matrix operations to decompose (A, U) .

6 POLYNOMIAL MATRIX SUBROUTINES

We now detail the subroutines used in Algorithm `KrylovMatrix`. Section 6.1 introduces some convenient notation for complexity bounds. Section 6.2 combines high-order lifting [21] and partial linearization [6] to compute truncated inverse expansions, while

Section 6.3 focuses on truncated matrix products. In both cases, the difficulty towards efficiency lies in the presence of unbalanced degrees and unbalanced truncation orders.

6.1 Complexity helper functions

In this section, we briefly recall notation and assumptions about cost functions; for more details, we refer to [4, Chap. 8] for the general framework, and to [21, Sec. 2] and [15, Sec. 1.1] for polynomial matrices specifically.

In what follows, we assume fixed multiplication algorithms:

- for polynomials in $\mathbb{F}[x]$, with cost function $M(d)$ when the input polynomials have degree at most d ;
- for matrices in $\mathbb{F}^{m \times m}$, with cost $O(m^\omega)$;
- for polynomial matrices in $\mathbb{F}[x]^{m \times m}$, with cost function $\text{MM}(m, d)$ when the input matrices have degree at most d .

To simplify our analyses and the resulting bounds, we make the same assumptions as in the above references. In particular, $\omega > 2$, $M(\cdot)$ is superlinear, and $\text{MM}(m, d) \in O(m^\omega M(d))$.

We will also use the function $\text{MM}(m, d)$ from [21, Sec. 2]; as noted in this reference, the above-mentioned assumptions imply $\overline{\text{MM}}(m, d) \in O(m^\omega M(d) \log(d))$.

6.2 Polynomial matrix truncated inverse

In Algorithm `KrylovMatrix`, Line 2 asks to compute terms of the power series expansion of P^{-1} , for an $m \times m$ polynomial matrix P with $P(0)$ invertible. Customary algorithms for this task, depending on the range of parameters (m , $\deg(P)$, truncation order), include a matrix extension of Newton iteration [14; 4, Chap. 9], or matrix inversion [26] followed by Newton iteration on the individual entries.

Here, a first obstacle towards efficiency comes from the heterogeneity of truncation orders: one seeks the first d_j terms of the j th column of the expansion of P^{-1} , for some prescribed $d = (d_j)_{j \in \mathbb{N}^m}$ which may have unbalanced entries. In the extreme case $d = (d_1, 0, \dots, 0)$, the task becomes the computation of many initial terms of the expansion of $P^{-1} [1 \ 0 \ \dots \ 0]^T$, the first column of P^{-1} . This is handled efficiently via high-order lifting techniques [21, Sec. 9]. Our solution for a general tuple d is to rely on cases where the high-order lifting approach is efficient, by splitting the truncation orders into subsets of the type $\{j \in \{1, \dots, m\} \mid 2^{k-1}|d|/m < d_j \leq 2^k|d|/m\}$, for only logarithmically many values of k . Observe that this subset has cardinality less than $m/2^{k-1}$: higher truncation orders involve fewer columns of the inverse.

A second obstacle is due to the heterogeneity of the degrees in the matrix P itself. In the context of Algorithm `KrylovMatrix`, P may have unbalanced column degrees, but they are controlled to some extent: their sum is at most n (the dimension of the matrix A). Whereas such cases were not handled in the original description of high-order lifting, the partial linearization tools described in [6, Sec. 6] allow one to deal with this obstacle. For example, this was applied in [16, Lem. 3.3], yet in a way that is not efficient enough for the matrices P encountered here: this reference targets low average row degree for P , whereas here our main control is on the average column degree. Here, following this combination of [21,

Sec. 9] and [6, Sec. 6], we present an algorithm which supports a more general unbalancedness of degrees of P .

In the next two lemmas, we summarize the properties that we will use from the latter references.

LEMMA 6.1 ([6, SEC. 6]). *Let $P \in \mathbb{F}[x]^{m \times m}$ be nonsingular. Consider its so-called generic determinantal degree $\Delta(P)$,*

$$\Delta(P) = \max_{\substack{\pi \in \mathfrak{S}_m \\ 1 \leq i \leq m \\ A_{i, \pi_i} \neq 0}} \deg(A_{i, \pi_i}) \leq |\text{cdeg}(P)|.$$

One can build, without using field operations, a matrix $\bar{P} \in \mathbb{F}[x]^{\bar{m} \times \bar{m}}$ of degree $\leq \lceil \Delta(P)/m \rceil$ and size $m \leq \bar{m} < 3m$, which is such that $\det(P) = \det(\bar{P})$ and P^{-1} is the principal $m \times m$ submatrix of \bar{P}^{-1} .

LEMMA 6.2 ([21, SEC. 9]). *Algorithm SeriesSol [21, Alg. 4] takes as input $P \in \mathbb{F}[x]^{m \times m}$ of degree t with $P(0)$ invertible, $V \in \mathbb{F}[x]^{m \times n}$, and $s \in \mathbb{Z}_{>0}$, and returns the expansion $(P^{-1}V) \text{ rem } x^{st}$ using*

$$O\left(\log(s+1) \left\lceil \frac{sn}{m} \right\rceil \overline{\text{MM}}(m, t) + \overline{\text{MM}}(m, t)\right)$$

operations in \mathbb{F} . The term $\overline{\text{MM}}(m, t)$ comes from a call to [21, Alg. 1] which is independent of V , namely $\text{HighOrderComp}(P, \lceil \log_2(s) \rceil - 1)$.

PROOF. There is no operation needed when $t = 0$, i.e., for a constant matrix P . For $t > 0$, this follows from [21, Prop. 15] and the paragraph that precedes it, applied with $X = x^t$. Indeed this is a valid choice since X has degree $\deg(P)$ and is coprime with $\det(P)$. The corresponding algorithm in [21] has two requirements on s , which are easily lifted: it should be a power of 2 (one can compute with the next power of 2, i.e. $2^{\lceil \log_2(s) \rceil}$), and then truncate at the desired order) and it should be at least 4 (the case $s \in O(1)$ is handled in $O(\lceil n/m \rceil \overline{\text{MM}}(m, t))$ via a direct Newton iteration). \square

PROPOSITION 6.3. *Let $P \in \mathbb{F}[x]^{m \times m}$ with $P(0)$ invertible, and let $d = (d_j)_j \in \mathbb{N}^m$. Let t be the degree of the partially linearized matrix \bar{P} as in Lemma 6.1, thus with $t \leq \lceil \Delta(P)/m \rceil$. Algorithm TruncatedInverse uses $O(m^\omega)$ operations in \mathbb{F} if $\deg(P) = 0$, and*

$$O\left(\overline{\text{MM}}(m, t) + \left\lceil \frac{|d|}{mt} \right\rceil \overline{\text{MM}}(m, t) \log(m) \log\left(m + \frac{|d|}{t}\right)\right)$$

operations in \mathbb{F} if $\deg(P) > 0$ (which implies $t > 0$). It returns $P^{-1} \text{ rem } x^d$, the power series expansion of P^{-1} with column j truncated at order d_j . If n is a parameter such that m and $\Delta(P)$ are both in $O(n)$, the above bound is in

$$O\left(m^\omega M\left(\frac{n}{m}\right) \left(\log(n) + \left\lceil \frac{|d|}{n} \right\rceil \log(m) \log(m + |d|)\right)\right).$$

PROOF. When $d = (0, \dots, 0)$, the algorithm performs no field operations and returns the zero matrix (see Line 2). When $d \neq 0$ and $\deg(P) = 0$ (hence $t = 0$), Line 3 correctly computes $P^{-1} \text{ rem } x^d$ in complexity $O(m^\omega)$, which is within the claimed cost since $m^\omega \in O(\overline{\text{MM}}(m, 0))$. From here on, assume $d \neq 0$ and $\deg(P) > 0$.

The sets J_1, \dots, J_m built at Line 6 are disjoint and, since $\max_j d_j \leq |d| \leq 2^\ell \delta$, they are such that $J_1 \cup \dots \cup J_m = \{1, \dots, m\}$. Note also that the cardinality $n_k = \#J_k$ is less than $m/2^{k-1}$. We claim that at the end of the k th iteration of the main loop, $Q_{*,j}$ is the column j of the sought output $P^{-1} \text{ rem } x^d$ for all $j \in J_1 \cup \dots \cup J_k$, which implies the correctness of the algorithm. This claim follows from Lemma 6.1. Indeed, writing $t = \deg(\bar{P})$, since the principal $m \times m$

submatrix of \bar{P}^{-1} is P^{-1} , Line 20 computes, in the top m rows of F , all columns $j \in J_k$ of P^{-1} truncated at order $\lceil 2^k \delta/t \rceil t$, which is at least the target order d_j . The subsequent Line 21 further truncates to shave off the possible extraneous expansion terms, and also selects the relevant rows of F . Note that $t > 0$: if \bar{P} was constant, then the principal $m \times m$ submatrix of \bar{P}^{-1} would be constant, i.e. P^{-1} would be constant, which is not the case since $\deg(P) > 0$.

As noted in Lemma 6.2, the k th call to SeriesSol involves a call to HighOrderComp, which does not depend on the matrix E at this iteration and which will re-compute the same high order components as the previous iterations, plus possibly one new such component. To avoid this redundancy, we pre-compute all required high-order components before the main loop at Line 16.

As for complexity, only Lines 16 and 20 use arithmetic operations. The construction of \bar{P} in Lemma 6.1 implies $\det(\bar{P}(0)) = \det(P)(0) = \det(P)(0) \neq 0$, hence we can apply Lemma 6.2. Here, \bar{P} is $\bar{m} \times \bar{m}$ with $m \leq \bar{m} < 3m$, and $t = \deg(\bar{P}) \leq \lceil \Delta(P)/m \rceil$.

Hence, using notation $s_k = \lceil 2^k \delta/t \rceil$, the complexity is within

$$O\left(\overline{\text{MM}}(m, t) + \sum_{k=1}^{\ell} \log(s_k + 1) \left\lceil \frac{s_k n_k}{m} \right\rceil \overline{\text{MM}}(m, t)\right).$$

One can then use the upper bounds $\log_2(s_k + 1) \leq \ell + 1 + \log_2(\lceil \delta/t \rceil)$ and $\lceil s_k n_k/m \rceil \leq \lceil s_k/2^{k-1} \rceil = \lceil 2\delta/t \rceil$ to obtain

$$\sum_{k=1}^{\ell} \log(s_k + 1) \left\lceil \frac{s_k n_k}{m} \right\rceil \in O\left(\lceil \delta/t \rceil \left(\ell^2 + \ell \log(\lceil \delta/t \rceil)\right)\right).$$

To obtain the claimed general cost bound, it remains to note that

$$\ell^2 + \ell \log(\lceil \delta/t \rceil) \in O(\log(m) \log(m \lceil \delta/t \rceil)),$$

with $m \lceil \delta/t \rceil \in O(m + |d|/t)$. For the simplified bound, we first use $t \geq 1$ to bound $\log(m + |d|/t)$ by $\log(m + |d|)$. The assumptions on the introduced parameter n allow us to write $t \in O(n/m)$. In particular, $\overline{\text{MM}}(m, t)$ is in $O(m^\omega M(n/m) \log(n/m))$, which is within the claimed bound. It remains to observe that

$$\begin{aligned} \left\lceil \frac{|d|}{mt} \right\rceil \overline{\text{MM}}(m, t) &\in O\left(\left(1 + \frac{|d|}{mt}\right) m^\omega M(t)\right) \\ &\subseteq O\left(m^\omega M\left(\frac{n}{m}\right) + \frac{|d|}{m} m^\omega \frac{M(t)}{t}\right) \\ &\subseteq O\left(m^\omega M\left(\frac{n}{m}\right) + \frac{|d|}{n} m^\omega M\left(\frac{n}{m}\right)\right) \subseteq O\left(\left\lceil \frac{|d|}{n} \right\rceil m^\omega M\left(\frac{n}{m}\right)\right). \end{aligned}$$

Here we have used the superlinearity assumption on $M(\cdot)$, which gives us $\frac{M(t)}{t} \in O\left(\frac{M(n/m)}{n/m}\right)$. \square

6.3 Polynomial matrix truncated product

PROPOSITION 6.4. *Given $F \in \mathbb{F}[x]^{n \times m}$, $G \in \mathbb{F}[x]^{m \times m}$, and $d = (d_j)_j \in \mathbb{N}^m$, Algorithm TruncatedProduct uses*

$$O\left(\sum_{0 \leq k < \lceil \log_2(m) \rceil} \left\lceil 2^k \frac{n}{m} \right\rceil \overline{\text{MM}}\left(2^{-k} m, 2^k \left\lceil \frac{D}{m} \right\rceil\right)\right)$$

operations in \mathbb{F} and returns the truncated product $(FG) \text{ rem } x^d$ that is, FG with column j truncated at order d_j . Here, D is the maximum between $|d|$ and the sum of the degrees of the nonzero columns of F . If m is both in $O(n)$ and $O(D)$, this cost bound is in $O(m^{\omega-2} n M(D))$.

Algorithm 4 TruncatedInverse(P, d)

Input: $P \in \mathbb{F}[x]^{m \times m}$ with $P(0)$ invertible, $d = (d_1, \dots, d_m) \in \mathbb{N}^m$
Output: the column-truncated inverse $P^{-1} \text{ rem } x^d \in \mathbb{F}[x]^{m \times m}$

- 1: $Q \leftarrow$ zero matrix in $\mathbb{F}[x]^{m \times m}$ \triangleright stores the result
- 2: **if** $d = (0, \dots, 0)$ **then return** Q
- 3: **if** $\deg(P) = 0$ **then** \triangleright constant matrix inversion, $O(m^\omega)$
- 4: $Q \leftarrow P^{-1}$; $Q_{*,j} \leftarrow 0$ for all j with $d_j = 0$; **return** Q
- 5: **end if**
- 6: \triangleright build partition of $\{1, \dots, m\}$ based on truncation order \triangleleft
- 7: $\delta \leftarrow \lfloor d \rfloor / m$; $\ell \leftarrow \lceil \log_2(m) \rceil$
- 8: $J_1 \leftarrow \{j \in \{1, \dots, m\} \mid d_j \leq 2\delta\}$; $n_1 \leftarrow \#J_1$
- 9: **for** $k \leftarrow 2, \dots, \ell$ **do**
- 10: $J_k \leftarrow \{j \in \{1, \dots, m\} \mid 2^{k-1}\delta < d_j \leq 2^k\delta\}$; $n_k \leftarrow \#J_k$
- 11: **end for**
- 12: \triangleright partial linearization, note that $t = \deg(\bar{P}) > 0$ \triangleleft
- 13: $\bar{P} \in \mathbb{F}[x]^{\bar{m} \times \bar{m}} \leftarrow$ matrix built from P as in Lemma 6.1
- 14: $t \leftarrow \deg(\bar{P})$; **for** $k = 1, \dots, \ell$ **do** $s_k \leftarrow \lceil 2^k \delta / t \rceil$
- 15: \triangleright store high-order components to avoid redundant iterations \triangleleft
- 16: $C \leftarrow \text{HighOrderComp}[x^t](\bar{P}, \lceil \log_2(s_\ell) \rceil - 1)$ \triangleright [21, Alg. 1]
- 17: \triangleright main loop: iteration k handles $Q_{*,j}$ for j in J_k \triangleleft
- 18: **for** $k \leftarrow 1, 2, \dots, \ell$ **do**
- 19: $E \in \mathbb{F}^{\bar{m} \times n_k} \leftarrow (I_{\bar{m}})_{*,J_k}$ \triangleright columns of $\bar{m} \times \bar{m}$ identity matrix
- 20: $F \in \mathbb{F}[x]^{\bar{m} \times n_k} \leftarrow \text{SeriesSol}(\bar{P}, E, s_k)$, using the pre-computed high-order components C \triangleright Lemma 6.2
- 21: $Q_{*,J_k} \leftarrow$ first m rows of F , all truncated at order $(d_j)_{j \in J_k}$
- 22: **end for**
- 23: **return** Q

PROOF. For convenience, we denote by I_k and J_k the sets I and J defined at the iteration k of the main loop of the algorithm. Let also $R^{(k)}$ be the matrix R at the beginning of iteration k , and $R^{(\ell)}$ be the output R . Let $F^{(0:k)} = F \text{ rem } x^{2^k \delta}$ for $1 \leq k \leq \ell$, with in particular $F^{(0:\ell)} = F$ since $\max_j d_j \leq |d| \leq m\delta \leq 2^\ell \delta$.

At the beginning of the first iteration, $R^{(1)} = (F^{(0)}G) \text{ rem } x^d = (F^{(0:1)}G) \text{ rem } x^d$. Then, to prove the correctness of the algorithm, we let $k \in \{1, \dots, \ell\}$ and assume $R^{(k)} = (F^{(0:k)}G) \text{ rem } x^d$, and we show $R^{(k+1)} = (F^{(0:k+1)}G) \text{ rem } x^d$.

First, consider $j \notin J_k$. The column j of $R^{(k)}$ is not modified by iteration k , i.e. $R_{*,j}^{(k)} = R_{*,j}^{(k+1)}$. On the other hand, one has $d_j < 2^k \delta$, hence $F^{(0:k)} \text{ rem } x^{d_j} = F^{(0:k+1)} \text{ rem } x^{d_j}$. We obtain

$$R_{*,j}^{(k+1)} = R_{*,j}^{(k)} = (F^{(0:k)}G_{*,j}) \text{ rem } x^{d_j} = (F^{(0:k+1)}G_{*,j}) \text{ rem } x^{d_j}.$$

meaning that the sought equality holds for the columns $j \notin J_k$.

Now, consider $j \in J_k$. For $i \notin I_k$, one has $\text{cdeg}(F_{*,i}) < 2^k \delta$, hence $F_{*,i}^{(k)} = 0$: it follows that $F^{(k)}G_{*,j} = F_{*,I}^{(k)}G_{I,j}$. Thus Line 9 computes

$$\begin{aligned} R_{*,j}^{(k+1)} &\leftarrow R_{*,j}^{(k)} + \left((F_{*,I}^{(k)}G_{I,j}) \text{ rem } x^{d_j - 2^k \delta} \right) x^{2^k \delta} \\ &= (F^{(0:k)}G_{*,j}) \text{ rem } x^{d_j} + (x^{2^k \delta} F^{(k)}G_{*,j}) \text{ rem } x^{d_j} \\ &= (F^{(0:k+1)}G_{*,j}) \text{ rem } x^{d_j}. \end{aligned}$$

This completes the proof of correctness.

For complexity, note that the definition of D gives $\#I_k \leq 2^{-k}m$ and $\#J_k \leq 2^{-k}m$; also, only Lines 4 and 9 use arithmetic operations.

At Line 4, we first compute $F^{(0)}G$, then truncate. The left and right matrices in this product are respectively $n \times m$ of degree $< 2\delta$, and $m \times m$ with sum of column degrees $\leq m\delta$. The product can be performed by expanding the columns of G into $\leq 2m$ columns all of degree $\leq \delta$, which leads to the complexity $O(\lceil \frac{n}{m} \rceil \text{MM}(m, \delta))$.

At Line 9, the multiplication by a power of x is free. The sum consists in adding two matrices with n rows and with column degrees strictly less than $(d_j)_{j \in J_k}$ entry-wise. This costs $O(n|d|)$ operations in \mathbb{F} at each iteration, hence $O(\ell n|d|)$ in total. Using the trivial lower bound on $\text{MM}(\cdot, \cdot)$ shows that this is within the claimed overall cost bound:

$$\begin{aligned} \ell n|d| &\leq \sum_{k=0}^{\ell-1} nD \leq \sum_{k=0}^{\ell-1} \left\lceil 2^k \frac{n}{m} \right\rceil (2^{-k}m)^2 2^k \left\lceil \frac{D}{m} \right\rceil \\ &\in O\left(\sum_{k=0}^{\ell-1} \left\lceil 2^k \frac{n}{m} \right\rceil \text{MM}\left(2^{-k}m, 2^k \left\lceil \frac{D}{m} \right\rceil\right) \right). \end{aligned}$$

Finally, for the truncated product, we first multiply $F_{*,I_k}^{(k)}G_{I_k,J_k}$ and then truncate. The left matrix in this product has n rows, $\leq 2^{-k}m$ columns, and degree $< 2^k \delta$. The right matrix has row and columns dimensions both $\leq 2^{-k}m$, and sum of column degrees $\leq |d|$. The product can be performed by expanding the columns of G_{I_k,J_k} into $\leq 2^{1-k}m$ columns all of degree $\leq |d|/(2^{-k}m) \leq 2^k \delta$, which leads to the complexity $O(\lceil 2^k \frac{n}{m} \rceil \text{MM}(2^{-k}m, 2^k \delta))$. Summing the latter bound for $k \in \{1, \dots, \ell-1\}$, and adding the term $k=0$ for Line 4, yields the claimed cost bound.

The final simplified complexity bound follows from the assumptions mentioned in Section 6.1: $\text{MM}(\mu, \delta)$ is in $O(\mu^\omega \text{M}(\delta))$, $\text{M}(\cdot)$ is superlinear, and $\omega > 2$ implies that the sum $\sum_{0 \leq k < \ell} 2^{k(2-\omega)}$ is bounded by a constant. \square

Algorithm 5 TruncatedProduct(F, G, d)

Input: $F \in \mathbb{F}[x]^{n \times m}$, $G \in \mathbb{F}[x]^{m \times m}$, $d = (d_1, \dots, d_m) \in \mathbb{N}^m$
Output: the column-truncated product $(FG) \text{ rem } x^d \in \mathbb{F}[x]^{n \times m}$

- 1: $\gamma \leftarrow$ sum of the degrees of the nonzero columns of F
- 2: $D \leftarrow \max(|d|, \gamma)$; $\delta \leftarrow \lceil D/m \rceil$; $\ell \leftarrow \lceil \log_2(m) \rceil$
- 3: write $F = F^{(0)} + \sum_{1 \leq k < \ell} F^{(k)} x^{2^k \delta}$ with each $F^{(k)}$ in $\mathbb{F}[x]^{n \times m}$, $\deg(F^{(k)}) < 2^k \delta$ for $1 \leq k < \ell$, and $\deg(F^{(0)}) < 2\delta$
- 4: $R \in \mathbb{F}[x]^{n \times m} \leftarrow (F^{(0)}G) \text{ rem } x^d$ \triangleright stores the result
- 5: **for** $k \leftarrow 1, \dots, \ell-1$ **do**
- 6: $I \leftarrow \{i \in \{1, \dots, m\} \mid \text{cdeg}(F_{*,i}) \geq 2^k \delta\}$
- 7: $J \leftarrow \{j \in \{1, \dots, m\} \mid d_j \geq 2^k \delta\}$
- 8: $e \leftarrow (d_j - 2^k \delta)_{j \in J}$
- 9: $R_{*,J} \leftarrow R_{*,J} + \left((F_{*,I}^{(k)}G_{I,J}) \text{ rem } x^e \right) x^{2^k \delta}$
- 10: **end for**
- 11: **return** R

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A DECOMPOSITION OF THE SPACE \mathbb{F}^n

The following is part of the basic material when studying the behavior of a linear operator A and the decomposition of \mathbb{F}^n into cyclic subspaces [3, Chap. VII], which corresponds to the diagonal matrix form of Smith and the block diagonal form of Frobenius. The same concepts can also be used for decompositions associated with the triangular form of Hermite [22;19, Chap. 9], or more general forms such as column reduced ones [9, Sec. 6.4.6, p. 424].

Existence of a Krylov basis. Let $A \in \mathbb{F}^{n \times n}$ and $U \in \mathbb{F}^{n \times m}$, and for $1 \leq j \leq m$, let d_j is the first integer such that

$$A^{d_j} u_j \in \text{Span}(u_j, Au_j, \dots, A^{d_j-1} u_j) + \text{Orb}(A, U_{*,1..j-1}). \quad (9)$$

We prove that the columns of $K_d(A, U)$ form a basis of $\text{Orb}(A, U)$.

Given a subspace $\mathcal{E} \subseteq \mathbb{F}^n$ invariant with respect to A , we say that two vectors $u, v \in \mathbb{F}^n$ are congruent modulo \mathcal{E} if and only if $u - v \in \mathcal{E}$, and we write $u \equiv v \pmod{\mathcal{E}}$. For a fixed u , the set of polynomials $p \in \mathbb{F}[x]$ such that $p(A)u \equiv 0 \pmod{\mathcal{E}}$ is an ideal of $\mathbb{F}[x]$, generated by a monic polynomial which is the minimal polynomial of u modulo \mathcal{E} . In particular, if $p(A)u \equiv 0 \pmod{\mathcal{E}}$, then $q(A)u \equiv 0 \pmod{\mathcal{E}}$ for all multiples $q \in \mathbb{F}[x]$ of p .

The proof of Eq. (9) is by induction on m . For one vector, d_1 is the first integer such that

$$(x^{d_1})(A) = A^{d_1} u_1 \equiv 0 \pmod{\text{Span}(u_1, Au_1, \dots, A^{d_1-1} u_1)}.$$

Therefore all the subsequent vectors $(x^{d_1} x^k)(A) = A^{d_1+k} u_1$ with $k \geq 0$ are zero modulo $K_{d_1}(A, u_1)$ which then forms a basis of $\text{Orb}(A, u_1)$. Then assume that the property holds for all U of column dimension $m \geq 1$: $K_d(A, U)$ is a basis of $\text{Orb}(A, U)$. For $v \in \mathbb{F}^m$, let d_{m+1} be the smallest integer so that $A^{d_{m+1}} v$ is a combination of the previous iterates of v and the vectors in $\text{Orb}(A, U)$. By analogy to the case $m = 1$, all subsequent vectors $A^{d_{m+1}+k} v$ are also linear combinations of the vectors in $\text{Span}(v, Av, \dots, A^{d_{m+1}-1} v) + \text{Orb}(A, U)$. So the latter subspace is $\text{Orb}(A, [U, v])$, and by induction hypothesis the columns of $K_{d_{m+1}}(A, v)$ and $K_d(A, U)$ form one of its bases.

Maximal Krylov indices. The tuple d constructed this way is lexicographically maximal so that $K_d(A, U)$ is a basis of $\text{Orb}(A, U)$. The existence of an l such that (d'_1, \dots, d'_m) is another suitable tuple with $d'_l < d_l$ would indeed contradict the fact that d_l corresponds to the smallest linear dependence.

B A SLIGHTLY DIFFERENT ALGORITHM

The matrices $xI - A$ and $I - xA$ considered in Algorithm `MaxIndices` and Algorithm `KrylovMatrix` mirror each other. As we explain below, $xI - A$ could also be used to compute a Krylov matrix. Algorithm `KrylovMatrix` provides a small simplification by considering $I - xA$ instead.

Consider a minimal kernel basis $[S^T \quad T^T]^T$ of $[xI - A \quad -U]$ as in Algorithm `MaxIndices`. Since $(xI - A)^{-1}U$ is strictly proper and $S = (xI - A)^{-1}UT$, the column degrees in T are greater than those in S , and T is column reduced since the kernel basis is (Lemma 2.1). Let d_j be the degree of the j th column of T . Substituting $1/x$ for x in $(xI - A)S - UT = 0$, and multiplying on the right by the diagonal matrix $x^{\text{diag}(d_1, \dots, d_m)}$ we get

$$(I - xA)S(1/x)x^{\text{diag}(d_1-1, \dots, d_m-1)} - UT(1/x)x^{\text{diag}(d_1, \dots, d_m)}.$$

By definition of the d_j 's, the right term above is a polynomial matrix, say $U\hat{T}$. Noticing that the j th column of S is zero if $d_j = 0$, we also have that the left term is a polynomial matrix $(I - xA)\hat{S}$. It follows that the columns of $[\hat{S}^\top \quad \hat{T}^\top]^\top$ are in the kernel of $[I - xA \quad -U]$, and we can now also verify that they form a basis. Since $[S^\top \quad T^\top]^\top$ is itself a minimal basis, it is irreducible i.e. is of full rank for all finite values of x [9, Thm 6.5-10, p. 458]. Equivalently, S and T are coprime [9, Lem. 6.3-6, p. 379], so there exists V unimodular such that $V[S^\top \quad T^\top]^\top = [I \quad 0]^\top$. It follows that

$$V(1/x)x^{\text{diag}(1,\dots,1,0,\dots,0)} \begin{bmatrix} \hat{S} \\ \hat{T} \end{bmatrix} = \begin{bmatrix} I \\ 0 \end{bmatrix} x^{\text{diag}(d_1,\dots,d_m)},$$

and since V is unimodular, the rank of $[\hat{S}(x_0)^\top \quad \hat{T}(x_0)^\top]^\top$ is full for all values $x_0 \neq 0$ of x . The fact that T is column reduced adds that $\hat{T}(0)$ is nonsingular, which means that $[\hat{S}^\top \quad \hat{T}^\top]^\top$ is irreducible. By irreducibility ([9, Thm 6.5-10, p. 458] again, here after column reduction), we get as announced that $[\hat{S}^\top \quad \hat{T}^\top]^\top$ is a kernel basis of $[I - xA \quad -U]$

We see that Algorithm `KrylovMatrix` could therefore be modified using the same kernel basis as in Algorithm `MaxIndices`, and by inserting an instruction to work with \hat{T} afterwards.