Exhaustive Search for Small Dimension Recursive MDS Diffusion Layers for Block Ciphers and Hash Functions

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Abstract—This article presents a new algorithm to find MDS matrices that are well suited for use as a diffusion layer in lightweight block ciphers. Using an recursive construction, it is possible to obtain matrices with a very compact description. Classical field multiplications can also be replaced by simple \mathbb{F}_2 -linear transformations (combinations of XORs and shifts) which are much lighter. Using this algorithm, it was possible to design a 16×16 matrix on a 5-bit alphabet, yielding an efficient 80-bit diffusion layer with maximal branch number.

Index Terms—Block ciphers, Generalised Feistel, Branch number, Singleton bound, MDS codes, MDS conjecture, Companion matrices.

I. INTRODUCTION

There are many ways to construct Maximum Distance Separable (MDS) codes and, depending on the target application, some are better than others. One application of MDS codes is the design of linear diffusion layers in block ciphers (or cryptographic hash functions). The linear code consisting of words formed by the concatenation of inputs and outputs of a linear diffusion layer should have the best possible minimum distance to ensure optimal diffusion. Hence, MDS codes having the largest possible minimal distance, they are a good choice from a security point of view. However, they also require a dense matrix to be used, leading to a large description and somewhat slow evaluation.

In 2011, Guo et al. introduced the LED block cipher [1] and the PHOTON hash function family [2] where they use a 4 × 4 MDS diffusion matrix constructed as a power of a companion matrix. LED and PHOTON being lightweight designs, this structure allows for a much more compact description of the diffusion layer, which is crucial in this context. In the beginning of 2012, Sajadieh et al. [3] used a similar construction, and presented it as a Feistel-like recursive construction to design efficient and compact (in terms of code size or gate usage) MDS diffusion matrices for block ciphers. In addition, they also replaced the finite field operations present in PHOTON by simpler \mathbb{F}_2 -linear operations, again improving the efficiency and compactness of the construction. The same design strategy was then used by Wu et al. [4] to obtain optimal diffusion layers using the smallest possible number of XOR gates when specifically targeting hardware implementation. These constructions are probably not the best choice for a software implementation running on a computer,

but they are perfect for lightweight designs where MDS diffusion was usually not considered an option.

In this article, we continue this idea and propose an algorithm to build even larger MDS matrices, using the same recursive construction. Our main target is to obtain full statewide optimal diffusion, as opposed to designs like the AES where the MDS diffusion is only applied to a small part of the state, offering optimal diffusion in this part, but sub-optimal diffusion in the state as a whole.

This article is structured as followed. After presenting the notations we will use throughout the paper, we start by recalling the works of Sajadieh et~al. and of Wu et~al. and the results they were able to obtain. We then present the new approach we used for our construction and a series of theoretical results supporting it. Eventually, we expose the results we obtained for 8×8 diffusion matrices with symbols of 4 bits and 16×16 matrices with symbols of 5 bits.

A. Notation

The final result we aim at is a square matrix operating on ℓ symbols in \mathbb{F}_{q^s} . For any ring R, we denote $M_\ell(R)$ the set of $\ell \times \ell$ matrices with coefficients in R. We will term symbolic a polynomial $p(X) \in \mathbb{F}_q[X]$ or $\mathbb{F}_{q^s}[X]$, or an $\ell \times \ell$ square polynomial matrix $M(X) \in M_\ell(\mathbb{F}_q[X])$, where X is an indeterminate. Given values $\alpha \in \mathbb{F}_{q^s}$, or L an $s \times s$ square matrix in \mathbb{F}_q , we will get values by substituting α or L in the symbolic polynomial p(X), or in the symbolic matrix M(X). Using the standard computer science notation, we will denote such substitutions

$$p(X \leftarrow a) \in \mathbb{F}_{q^s}, \qquad p(X \leftarrow L) \in M_{\ell}(\mathbb{F}_q) M(X \leftarrow a) \in M_{\ell}(\mathbb{F}_{q^s}), \qquad M(X \leftarrow L) \in M_{\ell}(M_s(\mathbb{F}_q))$$

The aim is to find an $\ell \times \ell$ symbolic matrix M(X) and an $s \times s$ matrix L in \mathbb{F}_q such that the mapping $M_L := M(X \leftarrow L)$:

$$\begin{array}{ccc} M_L: & (\mathbb{F}_{q^s})^\ell & \to & (\mathbb{F}_{q^s})^\ell \\ v & \mapsto & M_L \cdot v \end{array}$$

has maximum branch number $\ell+1$, i.e. such that, denoting w(v) the Hamming weight of v:

$$\min_{v \neq 0} \{ w(v) + w(M_L \cdot v) \} = \ell + 1.$$

Let C_{M_L} be the code of length 2ℓ over the alphabet \mathbb{F}_{q^s} , whose codewords are $(v||M_L\cdot v)$ for all $v\in (\mathbb{F}_{q^s})^\ell$, or

equivalently, whose generating matrix is

$$[I | M_L]$$

Requiring that M_L has maximum branch number is equivalent to asking that the code C_{M_L} has minimum distance $\ell+1$. Note that, L being \mathbb{F}_q -linear, C_{M_L} is linear over \mathbb{F}_q , but non-linear over the field \mathbb{F}_{q^s} . Still, the Singleton bound also holds for non linear codes.

Theorem 1 (Singleton bound[5]): Consider a Q-ary unspecified alphabet. Let C be a Q-ary code of length n, minimal distance d. Then $|C| \leq Q^{n-d+1}$.

A code is called Maximum Distance Separable (MDS) if the equality d=n-k+1 holds. In our case $n=2\ell$ and $k=\ell$, so being MDS requires $d=\ell+1$. We briefly recall the MDS conjecture for linear codes, when Q is a prime power, the alphabet is given a field structure, and the code is linear: except for particular or degenerate cases, if there exists a Q-ary linear MDS code of length n, then $n \leq Q+1$. Which translates to $2\ell \leq q^s+1$. The mentioned degenerate cases above do not cover the cases $n=2\ell$, $k=\ell$ we are interested in.

Given an $s \times s$ matrix L in \mathbb{F}_q , we denote $\mathrm{Min}_L(X)$ the minimal polynomial of L, which is the smallest degree non zero polynomial $p(X) \in \mathbb{F}_q[X]$ such that $p(X \leftarrow L) = 0$.

II. PREVIOUS WORK

Sajadieh, Dakhilalian, Mala and Sepehrdad [3] describe their diffusion layer as a Feistel-like recursive structure. One application of such a diffusion layer to an ℓ symbol state S_0 consists in ℓ successive applications of a sub-layer which adds to one symbol a linear combination of the others, and circularly shifts the state (as in a generalised Feistel cipher). This sub-layer can be represented as the multiplication by a companion matrix C:

$$S_{i+1} = C \cdot S_i, \text{ with } C = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 1 \\ 1 & c_1 & c_2 & \dots & c_{\ell-1} \end{bmatrix}.$$

Where each c_i represents an \mathbb{F}_q -linear transformation and a 1 the identity function. c_0 is chosen equal to 1, making the inverse transformation almost identical. The output S_ℓ of the full diffusion layer can thus be expressed as $S_\ell = C^\ell \cdot S_0$.

Before presenting the construction they propose, we need to recall a few facts about MDS codes over rings, as the matrices M and C no longer have coefficients in a field.

A. MDS Codes over Commutative Rings

Over a finite field, the criterion for an $\ell \times \ell$ matrix to have maximum branch number (and define an MDS code) is that all its minors (of any size $\leq \ell$) should be non-zero. Over a commutative ring, this criterion simply translates to minors being *invertible*.

Proposition 1: Let $M \in M_{\ell}(R)$ be a matrix over a finite commutative ring R. Then M has maximum branch number if and only if all the minors of M are invertible in R.

Proof: For any square matrix A over a commutative ring, denoting A' the adjugate matrix of A, we have the following relation:

$$A' \cdot A = A \cdot A' = \det(A) \cdot I \tag{1}$$

We first prove that if M is non MDS, then there is a minor of M which is not invertible. Since M is not MDS and does not have maximum branch number, there exists $v \in R^\ell$, of weight say w, such that $M \cdot v$ has weight strictly less than $\ell+1-w$, i.e. it has at least w zero coordinates. Consider $J=\{j_1,...,j_w\}\subset\{1,...,\ell\}$ a set of non zero coordinates of v and $I=\{i_1,...,i_w\}\subset\{1,...,\ell\}$ a subset of the zero coordinates of $M \cdot v$. Then the submatrix $M_{|I,J}$ sends $v_{|J}$ to 0. Using Eq. 1, we get

$$\det(M_{|I,J}) \cdot v = 0,$$

meaning that the $\det(M_{|I,J})$ is non invertible, since v has at least one non zero coordinate.

Suppose now that M has maximum branch number, then for any integer w and any v of weight w, with non zero positions located in I, |I| = w, we have $w(M \cdot v) \geq \ell + 1 - w$. In particular for any subset $J \subset \{1, \ldots, \ell\}$ of size w, $(M \cdot v)|_J \neq 0$. Considering the matrix $M_{|I,J}$, the mapping $x \mapsto M_{|I,J} \cdot x$ thus has a kernel equal to $\{0\}$. It is thus invertible, and using Eq. 1, $\det(M_{|I,J})$ is invertible in R.

B. The Method

Going back to the Sajadieh $et\ al.$ construction, they propose to choose an $s\times s$ binary matrix L and have each c_i be a non zero polynomial $c_i(X)\in F_2[X]$ evaluated in L. In practice, they restrict to $c_i(X)$ of degree 1 or 2. Wu $et\ al.$ [4] use the same construction but restrict to $c_i(X)$ which are monomials in L. Restricting to such polynomials in L makes products of c_i commutative. Thanks to the previous proposition, the search for an efficient diffusion matrix with maximum branch number can be done in two steps:

- 1) exhaustively search for a good symbolic matrix $M(X) = C(X)^{\ell}$ (where C(X) is an $\ell \times \ell$ symbolic companion matrix). Here, good means that the set m(X) of all the minors of M(X) does not contain the null polynomial.
- 2) find a suitable \mathbb{F}_2 -linear operator $L: \mathbb{F}_2^s \to \mathbb{F}_2^s$, such that all the matrices in m(L) (the set obtained when applying $X \leftarrow L$ to the minors in m(X)) are invertible.

The first part of the search outputs a set of symbolic matrices, each one with a set of constraints associated to it. Each of these constraints is a polynomial that has to be invertible when evaluated in L, so fewer distinct polynomials is usually better. Sajadieh $et\ al.$ also focus on having low degree polynomials: this way, picking an L matrix that has a minimal polynomial $\min_L(X)$ irreducible and of higher degree than all the minors in m(X) will always give an MDS matrix. Wu $et\ al.$ rather focus on some specific matrices L with a single XOR gate and directly check whether they verify each constraint.

$\ell = 5$	$[1, L^2, L^{-1}, L^{-1}, L^2]$
$\ell = 6$	$[1, L^{-2}, L^{-1}, L^2, L^{-1}, L^{-2}]$
$\ell = 7$	$[1, L, L^{-5}, 1, 1, L^{-5}, L]$
$\ell = 8$	$[1, L^{-3}, L, L^3, L^2, L^3, L, L^{-3}]$

TABLE I COMPANION MATRICES FOUND BY WU et al. [4]

C. Obtained Results

Using the previous method, Sajadieh et~al. were able to exhaustively search all $M(X) = C(X)^{\ell}$ with polynomials $c_i(X)$ of degree 1 for values of ℓ up to 8. No results were found for $\ell > 4$ and only very few solutions exist for $\ell = 2, 3$ or 4, with different sets of constraints. They propose various matrices L verifying these constraints for sizes s ranging from 4 bits to 64 bits. They also present some solutions for C when $\ell \in \{5,6,7,8\}$ using polynomials c_i of degree 2.

We were able to run the full exhaustive search for $\ell=8$ with polynomials c_i of degree 2 looking for constraints m(X) of the smallest possible degree. We found 12 solutions where all minors can be decomposed into factors of degree at most 14. It is thus possible to use any of these 12 solutions with a matrix L having a minimal polynomial $\mathrm{Min}_L(X)$ of degree 15 or more and get a matrix with maximum branch number. However, a $\mathrm{Min}_L(X)$ of degree 15 requires L to operate on at least s=15 bits. This is much more than the MDS bound which implies that the number of possible symbols 2^s should be at least 2ℓ . For $\ell=8$, symbols of s=4 bits could be possible.

Indeed, as shown by Wu et al., symbols of s=4 bits are possible. Instead of searching for m(X) with only low degree factors, they search for m(X) containing no multiples of an irreducible polynomial p(X) of given degree. This way, any L such that $\operatorname{Min}_L(X) = p(X)$ will yield an M(L) with maximum branch number. Using $p(X) = X^4 + X + 1$, they found the companion matrices listed in Table I.

III. NEW APPROACH

A. Changing the Ordering of the Searches

The first thing we noted when performing our experiments on 8×8 matrices using degree 2 polynomials c_i is that the symbolic computation of minors are very expensive, especially as the obtained polynomials are of rather high degree (even if they decompose in small factors). In order to make the search more efficient, and thus be able to explore larger parameters, we needed to get rid of symbolic computation. This is what we did by reordering the search:

- 1) instead of considering any \mathbb{F}_2 -linear operator L, focus only on operators having a given minimal polynomial $\operatorname{Min}_L(X)$ of degree d,
- 2) exhaustively search for a good symbolic matrix $M(X) \in \mathbb{F}_2[X]$ whose symbolic minors are all invertible under $X \leftarrow L$.

The crucial remark is that requiring that some minor m(X) is invertible under $m(X \leftarrow L)$ is the same as requiring that m(X) is invertible in $\mathbb{F}_2[X]/\min_L(X)$. The minors can thus

all be computed directly in $\mathbb{F}_2[X]/\operatorname{Min}_L(X)$. In particular, when $\operatorname{Min}_L(X)$ is irreducible, $\mathbb{F}_2[X]/\operatorname{Min}_L(X)$ is a field, and all computations can be done directly in \mathbb{F}_{2^d} .

If we define α as a root of $\mathrm{Min}_L(X)$ in \mathbb{F}_{2^d} , requiring that $M(X \leftarrow L)$ has maximal branch number is the same as requiring that $M(X \leftarrow \alpha)$ has maximal branch number in the classical sense. This paves the way to theorems, see below, and to much faster computations, enabling exhaustive searches which were out of reach.

B. Case of General Symbolic Matrices

We state the theorems for arbitrary finite fields, but our primary target remains \mathbb{F}_2 only.

Proposition 2: Let \mathbb{F}_q be a finite field. Let M(X) be an $\ell \times \ell$ matrix with coefficients in $\mathbb{F}_q[X]$. Let L be an $s \times s$ matrix with coefficients in \mathbb{F}_q , such that its minimal polynomial $p(X) = \mathrm{Min}_L(X)$ is irreducible of degree d. Then $M(X \leftarrow L)$ has maximum branch number if and only if $M(X \leftarrow \alpha)$ is an MDS matrix over the field

$$\mathbb{F}_q[\alpha] = \mathbb{F}_q[X]/p(X) \simeq \mathbb{F}_{q^d}$$

where α is a root of $\operatorname{Min}_L(X)$ in \mathbb{F}_{q^d} .

Proof: Matrix $M(X \leftarrow L)$ has maximal branch number if and only if all the minors of all sizes of M(X) are invertible after $X \leftarrow L$, which is the same as saying that they are coprime with $\mathrm{Min}_L(X) = p(X)$. Since p(X) is irreducible, minors of M(X) should simply not be multiples of p(X), which is equivalent to saying that $\alpha \in \mathbb{F}_{q^d}$ should not be a root of any minor. This will be the case if and only if $M(X \leftarrow \alpha)$ is an MDS matrix over \mathbb{F}_{q^d} .

Assuming that the MDS conjecture holds true, we get directly a bound on ℓ in terms of s. Since we are dealing with codes of even length 2ℓ , the conjecture gives $2\ell \leq Q$ where Q is the size of the field of symbols.

Corollary 1: Suppose that the minimal polynomial of L is irreducible of degree d, then $\ell \leq \frac{1}{2}q^d$ is a necessary condition for $M(X \leftarrow L)$ to be MDS. Also, if L operates on elements of \mathbb{F}_q^s , the degree of its minimal polynomial is at most s, so $d \leq s$. In the case q=2, we have the bound $s \geq 1+\lceil \log_2(\ell) \rceil$.

Next proposition shows that for the case of a matrix L with irreducible minimal polynomial p(X), the computation needs to be done only once, and that will encompass all matrices L with any irreducible minimal polynomial p(X) of the same degree d, since all finite fields of the same extension degree over the ground field are isomorphic.

Proposition 3: Consider $p_1(X), p_2(X) \in \mathbb{F}_q[X]$ two irreducible polynomials of same degree d. Consider $\alpha_1 \in \mathbb{F}_q[X]/p_1(X)$, and $\alpha_2 \in \mathbb{F}_q[X]/p_2(X)$ such that $p_1(\alpha_1) = p_2(\alpha_2) = 0$. Now choose $\alpha_1' \in \mathbb{F}_q[X]/p_2(X)$ such that $p_1(\alpha_1') = 0$. There exists a polynomial $K(X) \in \mathbb{F}_q[X]$ such that $\alpha_1' = K(\alpha_2)$. We have an \mathbb{F}_q -isomorphism:

$$\sigma: \begin{tabular}{lll} $\sigma:$ & $\mathbb{F}_q[X]/p_1(X)$ & \to & $\mathbb{F}_q[X]/p_2(X)$ \\ & α_1 & \mapsto & α_1' \\ \end{tabular}$$

Suppose that $M_1(X)$ is such that $M_1(X \leftarrow \alpha_1)$ is MDS. Then, any matrix $M_2(X)$ such that $M_2(X \leftarrow \alpha_2) = \sigma(M_1(X \leftarrow \alpha_2))$

 $lpha_1)$) is such that $M_2(X\leftarrow lpha_2)$ is MDS. Any \mathbb{F}_q -linear operator L with minimal polynomial $\mathrm{Min}_L(X)=p_2(X)$ will then define a matrix $M_2(X\leftarrow L)$ with maximum branch number. Such a matrix $M_2(X)$ will have the same recursive structure as $M_1(X)$ and can be computed as:

$$M_2(X) = M_1(X \leftarrow K(X)).$$

Proof: Elements α_1 and α'_1 have the same minimal polynomial, so there exists a field isomorphism σ sending one onto the other. This field isomorphism preserves the invertibility of matrices and also preserves the MDS property of a matrix, so $\sigma(M_1(X\leftarrow\alpha_1))$ is MDS over the field $\mathbb{F}_q[X]/p_2(X)$.

If $M_2(X \leftarrow \alpha_2) = \sigma(M_1(X \leftarrow \alpha_1))$ it is MDS, and we know from Proposition 2 that any L with the same minimal polynomial $p_2(X)$ as α_2 will define a matrix $M_2(X \leftarrow L)$ with maximum branch number.

The field isomorphism σ commutes with any polynomial operation, so $\sigma(M_1(X\leftarrow\alpha_1))=M_1(X\leftarrow\alpha_1')$. So $M_2(X\leftarrow\alpha_2)=M_1(X\leftarrow K(\alpha_2))$. Substituting X by K(X) in M_1 thus gives a valid matrix $M_2(X)$.

Concerning the recursive structure of M_1 and M_2 , if $M_1(X) = C_1(X)^\ell$ one can define $C_2(X) = C_1(X \leftarrow K(X))$ and matrix $M_2(X) = C_2(X)^\ell$ to get $M_2(X \leftarrow \alpha_2) = \sigma(M_1(X \leftarrow \alpha_1))$ as expected.

Finally, matrix $M_1(X)$ will usually be computed as $C_1(X)^\ell \mod p_1(X)$ so as to keep the degree of the polynomials bounded. As $M_1(X)$ is only evaluated on elements of minimal polynomial $p_1(X)$ this does not change anything. This reduction modulo $p_1(X)$ is compatible with the substitution $X \leftarrow K(X)$ if matrix $M_2(X)$ is reduced modulo $p_2(X)$: $M_2(X) = M_1(X \leftarrow K(X)) \mod p_2(X)$. This comes from the equality $p_1(K(X)) = 0 \mod p_2(X)$, which in turn is true because α_2 is a root of $p_1(K(X))$.

As we have seen, when $\operatorname{Min}_L(X)$ is irreducible, everything happens exactly as in the finite field MDS case. The following results show that when $\operatorname{Min}_L(X)$ is not irreducible, similar results can apply.

Corollary 2: Let \mathbb{F}_q be a finite field. Let M be a $\ell \times \ell$ matrix with coefficients in $\mathbb{F}_q[X]$. Let L be a $s \times s$ matrix with coefficients in \mathbb{F}_q , with minimal polynomial $p(X) = p_1(X)p_2(X)$, where $p_1(X)$ and $p_2(X)$ are co-prime. Then $M(X \leftarrow L)$ has maximum branch number if and only if both matrices

$$M_1 = M(X \leftarrow \alpha_1), \quad M_2 = M(X \leftarrow \alpha_2)$$

have maximum branch number over the rings

$$\mathbb{F}_q[\alpha_1] = \mathbb{F}_q[X]/p_1(X), \quad \mathbb{F}_q[\alpha_1] = \mathbb{F}_q[X]/p_2(X)$$

where $\alpha_1 = X \mod p_1(X)$, and $\alpha_2 = X \mod p_2(X)$.

Proof: From the Chinese Remainder Theorem, a minor m(X) is invertible mod p(X) if and only if it is invertible both mod $p_1(X)$ and mod $p_2(X)$. Extending this to all minors implies that M_1 and M_2 have maximum branch number.

Next we study the case $Min_L(X)$ is a power of an irreducible polynomial.

Corollary 3: Let \mathbb{F}_q be a finite field. Let M be a $\ell \times \ell$ matrix with coefficients in $\mathbb{F}_q[X]$. Let L be a $s \times s$ matrix with coefficients in \mathbb{F}_q , with minimal polynomial $p(X) = p_1(X)^e$, where $p_1(X)$ is irreducible. Then $M(X \leftarrow L)$ has maximal branch number if and only if

$$M_1 = M(X \leftarrow \alpha)$$

is an MDS matrix over the field

$$\mathbb{F}_q[\alpha] = \mathbb{F}_q[X]/p_1(X)$$

where $\alpha = X \mod p_1(X)$.

Proof: As in the proof of Corollary 2, it is enough to remark that a minor m(X) is invertible mod $p_1(X)^e$ if and only it is non zero mod $p_1(X)$.

We can now extend these results to the most general case for $\mathrm{Min}_L(X)$.

Corollary 4: Let \mathbb{F}_q be a finite field. Let M be an $\ell \times \ell$ matrix with coefficients in $\mathbb{F}_q[X]$. Let L be a $s \times s$ matrix with coefficients in \mathbb{F}_q , with minimal polynomial

$$p(X) = p_1(X)^{e_1} \dots p_k(X)^{e_k},$$

where $p_1(X), \ldots, p_k(X)$ are irreducible. Then $M(X \leftarrow L)$ is MDS if and only if $\forall i \leq k, M(X \leftarrow \alpha_i)$ is MDS over $\mathbb{F}_q[\alpha_i]$ (with $\alpha_i = X \mod p_i(X)$). As a consequence, $\ell \leq \frac{q^d}{2}$, where $d = \min\{\deg p_i(X), i = 1, \ldots, k\}$.

These theorems clearly indicate that to get a large maximal diffusion matrix, it is always preferable to use an operator L with irreducible minimal polynomial.

IV. EXPERIMENTAL RESULTS

Even though all the results from the previous section hold over \mathbb{F}_q , our primary focus being lightweight block ciphers, we only ran experiments on extensions of \mathbb{F}_2 .

A. Operating on 4 bit Blocks

To test our algorithm, our first targets were the results of Wu et~al. [4]. We wanted to go through all recursive matrices with $\ell=8$ and s=4 and see how many 8×8 MDS matrices we could obtain. There are 3 irreducible polynomials of degree 4 on \mathbb{F}_2 , but as stated in Proposition 3, performing the search for only one of them is enough. We chose the minimal polynomial $p(X)=X^4+X+1$. We then simply ran an exhaustive search through the 15^7 companion matrices C with $c_0=1$ and coefficients c_i in $\mathbb{F}_{2^4}^*$. For each of these C we computed $M=C^8$ and checked whether all the minors of M (computed in \mathbb{F}_{2^4}) were non zero. Noting $\alpha\in\mathbb{F}_{2^4}$ a root of p(X), we found the following solutions for $[c_0,\ldots,c_7]$:

$$\begin{split} S_0 &= \begin{bmatrix} 1, \ \alpha^3, \ \alpha^4, \ \alpha^{12}, \ \alpha^8, \ \alpha^{12}, \ \alpha^4, \ \alpha^3 \ \end{bmatrix} \\ S_1 &= \begin{bmatrix} 1, \ \alpha^6, \ \alpha^8, \ \alpha^9, \ \alpha, \ \alpha^9, \ \alpha^8, \ \alpha^6 \ \end{bmatrix} \\ S_2 &= \begin{bmatrix} 1, \ \alpha^{12}, \ \alpha, \ \alpha^3, \ \alpha^2, \ \alpha^3, \ \alpha, \ \alpha^{12} \ \end{bmatrix} \\ S_3 &= \begin{bmatrix} 1, \ \alpha^9, \ \alpha^2, \ \alpha^6, \ \alpha^4, \ \alpha^6, \ \alpha^2, \ \alpha^9 \ \end{bmatrix} \\ S_4 &= \begin{bmatrix} 1, \ \alpha^7, \ \alpha^2, \ \alpha^{11}, \ \alpha^{13}, \ \alpha^{11}, \ \alpha^2, \ \alpha^7 \ \end{bmatrix} \\ S_5 &= \begin{bmatrix} 1, \ \alpha^{14}, \ \alpha^4, \ \alpha^7, \ \alpha^{11}, \ \alpha^7, \ \alpha^4, \ \alpha^{14} \ \end{bmatrix} \\ S_6 &= \begin{bmatrix} 1, \ \alpha^{13}, \ \alpha^8, \ \alpha^{14}, \ \alpha^7, \ \alpha^{14}, \ \alpha^8, \ \alpha^{13} \ \end{bmatrix} \\ S_7 &= \begin{bmatrix} 1, \ \alpha^{11}, \ \alpha, \ \alpha^{13}, \ \alpha^{14}, \ \alpha^{13}, \ \alpha, \ \alpha^{11} \ \end{bmatrix} \end{split}$$

The solution presented by Wu *et al.* (last line of Table I) corresponds to our solution S_2 . The mapping $\alpha \to \alpha^2$ is a morphism in \mathbb{F}_{2^4} , so it transforms an MDS matrix into another MDS matrix. It allows to group the 8 solutions in two classes of equivalent solutions $\{S_0, S_1, S_2, S_3\}$ and $\{S_4, S_5, S_6, S_7\}$.

The whole exhaustive search (about $2^{27.3}$ matrices) took 2 days on a single core using Magma [6]. The same computation using symbolic polynomials would probably have taken a few months.

Any of these solution can then be used with a matrix L having minimal polynomial $\mathrm{Min}_L(X) = X^4 + X + 1$. This L matrix can be a binary 4×4 matrix, yielding a 32 bit diffusion layer, but an 8×8 matrix with suitable minimal polynomial can also be used to obtain a 64 bit diffusion layer.

One thing that can be noted about these solutions is their symmetry: in every solution, $c_1 = c_7$, $c_2 = c_6$, and $c_3 = c_5$. The same symmetry can be observed in the solutions found by Wu et al. (see Table I). We also ran the full exhaustive search for $\ell = 4$ and s = 3 and found a single class of solutions (3) equivalent solutions) which is also symmetric $[1, \alpha^3, \alpha, \alpha^3]$. For $\ell = 5$ and s = 4, we found 60 solutions in 15 classes among which only 3 classes are symmetric. For $\ell=6$ and s=4, we found 36 solutions in 9 classes among which only 3 classes are symmetric. This symmetry can thus be observed both for odd and even values of ℓ . One thing we proved is that for a given MDS solution, its symmetric is also MDS. This is due to the fact that the inverse of a recursive layer can be expressed as a recursive layer using the symmetric coefficients, and the inverse of an MDS matrix is also MDS. However, this property does not explain why symmetric solutions exist, or why when the MDS bound is "tight", that is, when $2\ell = 2^s$, only symmetric solutions exist.

B. Operating on 5 bit Blocks

With symbols of s=5 bits, the MDS conjecture indicates that matrices of size 16×16 can have maximal branch number. There are 6 irreducible polynomials of degree 5 over \mathbb{F}_2 and we used Magma's choice $p(X)=X^5+X^2+1$ for our search.

In our previous experiment with s=4, the full exhaustive search required to test $15^7 \simeq 2^{27.3}$ matrices. Here, the full search would require to test $31^{15} \simeq 2^{74.3}$ matrices, which is not feasible. However, all solutions we found for small instances seem to display a nice symmetry. Instead of exhaustively searching all companion matrices, we only search "symmetric" companion matrices. This reduces the number of matrices to test to $31^8 \simeq 2^{39.6}$. The number of tests can be reduced even further by taking into account the equivalence classes with respect to $\alpha \to \alpha^2$. For c_9 (the middle coefficient) we only tested the values $\left\{1,\alpha,\alpha^3,\alpha^5,\alpha^7,\alpha^{11},\alpha^{15}\right\}$, reducing the tests to $7\cdot 31^7 \simeq 2^{37.4}$.

Testing if a 16×16 matrix is MDS also requires to compute much more minors than for an 8×8 matrix. However, most candidate matrices possess null coefficients, or null minors of size 2, and computations can be interrupted early. The total exhaustive search took about 80 days of CPU time, and was

run in about two weeks on a single quad-core computer. In the end, only two solutions were found (each one representing a class of 5 solutions):

$$S_{0} = \begin{bmatrix} 1, \ \alpha^{17}, \ \alpha, & \alpha^{9}, \ \alpha^{12}, \ \alpha, & \alpha^{27}, \ \alpha^{25}, \ \alpha^{7}, \\ & \alpha^{25}, \ \alpha^{27}, \ \alpha, & \alpha^{12}, \ \alpha^{9}, \ \alpha, & \alpha^{17} \end{bmatrix}$$

$$S_{1} = \begin{bmatrix} 1, \ \alpha^{20}, \ \alpha^{25}, \ \alpha^{3}, \ \alpha^{27}, \ \alpha^{19}, \ \alpha^{9}, \ \alpha^{27}, \ \alpha^{15}, \\ & \alpha^{27}, \ \alpha^{9}, \ \alpha^{19}, \ \alpha^{27}, \ \alpha^{3}, \ \alpha^{25}, \ \alpha^{20} \end{bmatrix}$$

There might be other "non-symmetric" solutions as we have not searched for them, but we conjecture there are none. Each of the solutions we found can be used with a 5×5 binary matrix L with $\mathrm{Min}_L(X)=X^5+X^2+1$ to obtain an optimal 80 bit diffusion layer. For example, the simple transformation $x\to (x\ll 2)\oplus (x\ggg 1)$ can be used.

Any other size L can also be used as long as it has a minimal polynomial $\mathrm{Min}_L(X) = X^5 + X^2 + 1$, or any other degree 5 minimal polynomial using the transformation described in Proposition 3. Unfortunately, not any matrix can have a minimal polynomial of degree 5. Typically, if one wants to design a 128 bit diffusion layer, using a 16×16 matrix acting on 8 bit symbols, it will not be possible to use our solutions as an 8×8 binary matrix L cannot have an irreducible minimal polynomial of degree 5. A new search using a 16×16 companion matrices in \mathbb{F}_{2^8} has to be done, but it will be much more expensive than on \mathbb{F}_{2^5} , probably even out of reach.

C. Going Further

The next step is s=6 allowing to build a 32×32 matrix for a 192 bit diffusion layer. Such a diffusion would have a branch number of 33, which is way above anything usual in symmetric cryptography. In this sense, finding one such matrix would be of interest, especially as it would still have a somehow compact description (compared to a traditional 32×32 MDS matrix).

The exhaustive search is however completely out of reach, with a number of "symmetric" companion matrices to explore around 2^{93} . Building such a matrix will thus require a direct construction. The first step to getting this direct construction is probably to understand what additional structure the solutions we found possess.

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