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ON HIGMAN'S CONJECTURE*

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Abstract. Let \mathcal{G}_n be the subgroup of $\text{GL}_n(q)$ consisting of the $n \times n$ upper unitriangular matrices over the field \mathbb{F}_q with q elements. Higman [G. Higman. Enumerating p -groups. I. Inequalities. *Proc. London Math. Soc.* (3), 10:24–30, 1960.] conjectured that the number of conjugacy classes of \mathcal{G}_n , denoted by $r(\mathcal{G}_n)$, is a polynomial in q with integer coefficients. This has been verified for $n \leq 13$ by A. Vera-López and J.M. Arregi [A. Vera-López and J.M. Arregi. Conjugacy classes in unitriangular matrices. *Linear Algebra Appl.*, 370:85–124, 2003.]. The main purpose of this paper is to prove that for every n , $r(\mathcal{G}_n)$ can be expressed in terms of $r(\mathcal{G}_i)$, with $i < n$, and $r(\mathcal{T}_n)$, where \mathcal{T}_n is the subset of primitive canonical matrices of \mathcal{G}_n . Moreover, the expression of $r(\mathcal{T}_n)$ modulo $(q-1)^{\lfloor \frac{n+1}{2} \rfloor + 3}$ is determined and, consequently, it is deduced that $r(\mathcal{T}_n) \bmod (q-1)^{\lfloor \frac{n+1}{2} \rfloor + 3}$ is a polynomial in q with integer coefficients.

Key words. Unitriangular matrices, Higman's conjecture.

AMS subject classifications. 20D15.

1. Introduction. Let q be a power of a prime p . Let \mathcal{G}_n be the subgroup of $\text{GL}_n(q)$ consisting of the $n \times n$ upper unitriangular matrices over the field \mathbb{F}_q with q elements. A longstanding conjecture, attributed to Higman [5], states that the number of conjugacy classes of \mathcal{G}_n , denoted by $r(\mathcal{G}_n)$, is a polynomial in q with integer coefficients. This has been verified by Vera-López and Arregi [10] for $n \leq 13$. This conjecture has generated a great deal of interest. See, for example, Robinson [6], Alperin [1], Goodwin and Röhrle [3, 4], and Evseev [2].

One way to study the conjugacy classes of \mathcal{G}_n is to determine canonical representatives that share the main characteristics of their conjugacy classes. Vera-López and Arregi [8] provided such canonical representatives. We call these *canonical matrices*, and denote the set of $n \times n$ canonical matrices by \mathcal{C}_n . Obviously, the number $r(\mathcal{G}_n)$ of conjugacy classes of \mathcal{G}_n is the cardinality of \mathcal{C}_n .

To describe the structure of canonical matrices, we need a few definitions. The lexicographical order of the indices (i, j) is defined by

$$(i, j) \prec (k, l) \iff (i > k) \text{ or } (i = k \text{ and } j < l).$$

Let x_{ij} , with $1 \leq i < j \leq n$ be distinct indeterminates and let X be the strictly upper triangular matrix whose (i, j) -entry is x_{ij} for all i, j with $1 \leq i < j \leq n$. Given $A \in \mathcal{G}_n$, we set $L_{ij}(A)$ to be the linear form given by the (i, j) -entry of $AX - XA$, that is,

$$L_{ij}(A) = \sum_{i < k < j} (a_{ik}x_{kj} - a_{kj}x_{ik}).$$

Position (i, j) of A is an *inert point* of A (respectively *ramification point* of A), if $L_{i,j}(A)$ is linearly independent (respectively linearly dependent) from the sets of forms $L_{u,v}(A)$, where $(u, v) \prec (i, j)$. Vera-López and

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Arregi [8] showed that a necessary and sufficient condition for a matrix A to be canonical is that $a_{ij} = 0$ for every inert point (i, j) . Obviously, if $A \in \mathcal{G}_n$ is a canonical matrix and a_{ij} , with $i < j$, is non-zero, then (i, j) is a ramification point. We remember that the *pivot points* of a canonical matrix $A \in \mathcal{G}_n$ are the entries corresponding to the first non-zero off-diagonal entry in each row.

Let $A \in \mathcal{G}_n$ be. Then the *graph* of A , denoted by $\Gamma_A = (V_A, E_A)$, is the undirected graph defined as follows:

1. The vertex set V_A is $\{1, 2, \dots, n\}$.
2. The edge set E_A is $\{(i, j) \mid i < j \text{ and } a_{ij} \neq 0\}$.

For $A \in \mathcal{G}_n$ with graph $\Gamma_A = (V_A, E_A)$ and $v \in V_A$, the degree of the vertex v , denoted by $d(v)$, is the number of edges at v and $\Delta(\Gamma_A) = \max\{d(v) \mid v \in V_A\}$.

Let $A \in \mathcal{G}_n$ be. Then,

1. A is *connected*, if its graph Γ_A is connected.
2. A is *primitive*, if its graph Γ_A has no isolated vertices, that is, $d(v) \geq 1$, for all $v \in V_A$.
3. A is a *forest matrix*, if its graph Γ_A contains no cycles.

A maximal connected subgraph of a graph (i.e. one where the addition of any more vertices would make it disconnected) is called *connected component*. If we denote by d_A the number of connected components of Γ_A , then $A \in \mathcal{G}_n$ is connected if and, only if, $d_A = 1$. A matrix $A \in \mathcal{G}_n$ is said to be a *tree matrix*, if it is a forest matrix with one connected component.

If $A \in \mathcal{C}_n$ is a canonical matrix and $i \in \{1, \dots, n\}$, the set of elements in the i -th row or i -th column and not on the diagonal is called the *i -th broken line* and it is denoted by X_i . We note that there exists $i \in \{1, \dots, n\}$ such that $X_i = \{0\}$ if and only if A is not a primitive matrix. That is, if $A \in \mathcal{G}_n$ is a primitive canonical matrix, then $X_i \neq \{0\}$ for all i .

The primitive canonical matrices will enable us to establish in Section 2 the following relationship between $r(\mathcal{G}_n)$ and $r(\mathcal{G}_i)$, with $i < n$:

THEOREM 1.1. *Let \mathcal{T}_n be the subset of the primitive canonical matrices of \mathcal{G}_n . Then,*

$$r(\mathcal{G}_n) = r(\mathcal{T}_n) + \sum_{k=1}^{n-1} (-1)^{k-1} \binom{n}{k} r(\mathcal{G}_{n-k}) + (-1)^{n-1}.$$

Vera-López et al. [11] found an expression of $r(\mathcal{G}_n)$ in terms of the number of conjugacy classes of \mathcal{G}_n whose canonical matrices have spanning connected graphs. Theorem 1.1 connects $r(\mathcal{G}_n)$ with $r(\mathcal{G}_i)$, with $i < n$ and $r(\mathcal{T}_n)$.

Since we know $r(\mathcal{G}_n)$ for $n \leq 13$ (see Vera-López and Arregi, [10]), Theorem 1.1 suggests to us that it is interesting to study $r(\mathcal{T}_n)$. Indeed, Theorem 1.1 implies that to prove Higman's conjecture is equivalent to show that $r(\mathcal{T}_n)$ is a polynomial in q with integer coefficients. Towards this end, in Section 3, we study $r(\mathcal{T}_n)$ and prove if it is an integer multiple of $(q-1)^{\lfloor \frac{n+1}{2} \rfloor}$.

Finally, in Section 4, we show that for every n , there exist integer numbers $\mathbf{a}_{i,n}$ (non-dependent of q) with $i = 0, 1, 2$ such that

$$r(\mathcal{T}_n) = \left(\sum_{i=0}^2 \mathbf{a}_{i,n} (q-1)^{\lfloor \frac{n+1}{2} \rfloor + i} \right) \text{mod } (q-1)^{\lfloor \frac{n+1}{2} \rfloor + 3}.$$

That is, we find $r(\mathcal{T}_n)$ modulo $(q-1)^{\lfloor \frac{n+1}{2} \rfloor + 3}$. For this, we consider the subset \mathcal{PC}_n of \mathcal{C}_n formed by the primitive connected canonical matrices of \mathcal{G}_n and we classify the canonical matrices of \mathcal{PC}_n according to the zero-nonzero pattern of their entries. Thus, given $A, B \in \mathcal{PC}_n$, we say that A is *graph-equivalent* with B (and we write $A \approx B$), if for all $i, j \in \{1, \dots, n\}$, $a_{ij} \neq 0$ if and only if $b_{ij} \neq 0$. Clearly to be graph-equivalent is an equivalence relation on \mathcal{PC}_n and if we consider an equivalence class $[A] \in \mathcal{PC}_n / \approx$, then $\Gamma_B = \Gamma_A$, for all $B \in [A]$. So, we denote this graph by $\Gamma_{[A]}$. Furthermore, in Section 4, we also prove that the search of $\mathbf{a}_{i,n}$, with $i = 0, 1, 2$ is closely related to the number of equivalence classes of \mathcal{PC}_j / \approx such that their graphs are trees and $j \leq 7$. Because of this, we have found the quotient set \mathcal{PC}_j / \approx for $j \leq 7$. In order to obtain \mathcal{PC}_j / \approx for $j \leq 7$, we have considered all possible zero-nonzero patterns that give a primitive connected matrix and between these, we have selected the canonical matrices, by checking that all positions (i, j) with non-zero entry are ramification points. For $[A] \in \mathcal{PC}_j / \approx$, we note:

1. If $j \leq 5$, the graph $\Gamma_{[A]}$ is a tree.
2. If $j \leq 4$, then $j - 2$ vertices of $\Gamma_{[A]}$ have degree 2 and the rest vertices have degree 1.
3. If $j = 5, 6$, then $\Delta(\Gamma_{[A]}) \leq 3$.
4. If $j = 6$, then there exists exactly one $[A] \in \mathcal{PC}_6 / \approx$ such that its graph contains a cycle.

Moreover, direct calculation shows that the number of $[A] \in \mathcal{PC}_j / \approx$ such that $\Gamma_{[A]}$ is a tree, for $j \leq 7$ are:

j	$\#\{[A] \in \mathcal{PC}_j / \approx \mid \Gamma_{[A]} \text{ is a tree}\}$
2	1
3	1
4	2
5	5
6	18
7	77

We will use them to calculate $\mathbf{a}_{i,n}$, for $i = 0, 1, 2$.

2. The relationship between $r(\mathcal{G}_n)$ and $r(\mathcal{G}_i)$, with $i < n$. As noted in Section 1, we are interested in finding a relation between $r(\mathcal{G}_n)$ and $r(\mathcal{G}_i)$, with $i < n$. First, we need to relate the canonical matrices of \mathcal{C}_n with canonical matrices of \mathcal{C}_{n-1} . We begin by describing how to construct matrices of \mathcal{C}_n from canonical matrices of \mathcal{C}_{n-1} .

Let A be a matrix of \mathcal{G}_n . Suppose that $X_i = \{0\}$. Then, A is given by

$$A = \begin{bmatrix} A_{[1..i-1]}^{[1..i-1]} & 0 & A_{[1..i-1]}^{[i+1..n]} \\ & 1 & 0 \\ & & A_{[i+1..n]}^{[i+1..n]} \end{bmatrix}$$

where $A_{[k_1..k_2]}^{[l_1..l_2]}$ is the submatrix of A whose rows are the rows $k_1, k_1 + 1, \dots, k_2$ of A and whose columns are the columns $l_1, l_1 + 1, \dots, l_2$ of A and 0 represents the zero matrix of appropriated size. We notice that

$A_{[1..i-1]}^{[1..i-1]}$ and $A_{[i+1..n]}^{[i+1..n]}$ are unitriangular matrices. Then, we can determine from A a unique unitriangular matrix $B \in \mathcal{G}_{n-1}$ given by

$$B = \begin{bmatrix} A_{[1..i-1]}^{[1..i-1]} & A_{[1..i-1]}^{[i+1..n]} \\ & A_{[i+1..n]}^{[i+1..n]} \end{bmatrix}$$

and conversely, given $B = \begin{bmatrix} B_{[1..i-1]}^{[1..i-1]} & B_{[1..i-1]}^{[i..n-1]} \\ & B_{[i..n-1]}^{[i..n-1]} \end{bmatrix} \in \mathcal{G}_{n-1}$, we can always determine

$$A = \begin{bmatrix} B_{[1..i-1]}^{[1..i-1]} & 0 & B_{[1..i-1]}^{[i..n-1]} \\ & 1 & 0 \\ & & B_{[i..n-1]}^{[i..n-1]} \end{bmatrix} \in \mathcal{G}_n$$

with $X_i = \{0\}$. That is, we can define a one to one correspondence between the indices of the entries of the matrices of \mathcal{G}_{n-1} and the indices of entries of the matrices of \mathcal{G}_n which are not in the i -th broken line as follows:

$$(u, v) \mapsto (u, v) \uparrow = \begin{cases} (u, v), & \text{if } u < v < i, \\ (u, v + 1), & \text{if } u < i \leq v, \\ (u + 1, v + 1), & \text{if } i \leq u < v. \end{cases}$$

and its inverse map is

$$(r, s) \mapsto (r, s) \downarrow = \begin{cases} (r, s) & \text{if } r < s < i, \\ (r, s - 1) & \text{if } r < i < s, \\ (r - 1, s - 1) & \text{if } i < r < s. \end{cases}$$

PROPOSITION 2.1. *Let A be a matrix of \mathcal{G}_n such that $X_i = \{0\}$, that is,*

$$A = \begin{bmatrix} A_{[1..i-1]}^{[1..i-1]} & 0 & A_{[1..i-1]}^{[i+1..n]} \\ & 1 & 0 \\ & & A_{[i+1..n]}^{[i+1..n]} \end{bmatrix}.$$

Then, A is a canonical matrix for \mathcal{G}_n if and only if the matrix

$$B = \begin{bmatrix} A_{[1..i-1]}^{[1..i-1]} & A_{[1..i-1]}^{[i+1..n]} \\ & A_{[i+1..n]}^{[i+1..n]} \end{bmatrix}$$

is a canonical matrix of \mathcal{G}_{n-1} . Moreover, the type of position (r, s) of A is:

1. *The same one as position $(r, s) \downarrow$ in the matrix B , provided $r \neq i \neq s$;*
2. *If $s = i$, then it is an inert point if and only if it is preceded by the pivot point of its row.*
3. *If $r = i$, then it is an inert point if and only if it is above a pivot point of its column.*

Proof. Let

$$A = \begin{bmatrix} A_{[1..i-1]}^{[1..i-1]} & 0 & A_{[1..i-1]}^{[i+1..n]} \\ & 1 & 0 \\ & & A_{[i+1..n]}^{[i+1..n]} \end{bmatrix}, \quad B = \begin{bmatrix} A_{[1..i-1]}^{[1..i-1]} & A_{[1..i-1]}^{[i+1..n]} \\ & A_{[i+1..n]}^{[i+1..n]} \end{bmatrix}$$

$$X = \begin{bmatrix} u & v & w \\ 0 & 0 & x \\ 0 & 0 & y \end{bmatrix} \quad \text{and} \quad \hat{X} = \begin{bmatrix} u & w \\ 0 & y \end{bmatrix}.$$

Then,

$$AX - XA = \left[\begin{array}{c|c|c} A_{[1..i-1]}^{[1..i-1]}x - xA_{[1..i-1]}^{[1..i-1]} & A_{[1..i-1]}^{[1..i-1]}v - v & Y \\ \hline 0 & 0 & x - xA_{[i+1..n]}^{[i+1..n]} \\ \hline 0 & 0 & A_{[i+1..n]}^{[i+1..n]}y - yA_{[i+1..n]}^{[i+1..n]} \end{array} \right],$$

and

$$B\hat{X} - \hat{X}B = \left[\begin{array}{c|c} A_{[1..i-1]}^{[1..i-1]}x - xA_{[1..i-1]}^{[1..i-1]} & Y \\ \hline 0 & A_{[i+1..n]}^{[i+1..n]}y - yA_{[i+1..n]}^{[i+1..n]} \end{array} \right],$$

where $Y = A_{[1..i-1]}^{[1..i-1]}w + A_{[1..i-1]}^{[i+1..n]}y - uA_{[1..i-1]}^{[i+1..n]} - wA_{[i+1..n]}^{[i+1..n]}$. One can now easily show that an entry of A is inert if and only if the corresponding entry of B is inert. All off-diagonal entries in row and column i of A are 0, and hence A is canonical if and only if B is. \square

By Proposition 2.1, we can conclude that the study of the character of an entry can be reduced to the study of the character of an entry in the matrix obtained after eliminating all indices i such that $X_i = \{0\}$. This fact and an application of the principle of inclusion exclusion are enough to prove Theorem 1.1.

REMARK 2.2. We notice that each canonical matrix of \mathcal{G}_n with $n - k$ null broken lines fixes and is fixed by a canonical primitive matrix of \mathcal{G}_k and a combination $1 \leq i_1 < \dots < i_k \leq n$. Therefore, we obtain

$$r(\mathcal{G}_n) = 1 + \sum_{k=2}^n \binom{n}{k} r(\mathcal{T}_k).$$

From this equality jointly with the agreement

$$r(\mathcal{T}_0) = 1, \quad r(\mathcal{T}_1) = 0, \quad r(\mathcal{G}_0) = 1, \quad r(\mathcal{G}_1) = 1,$$

the following relation is established,

$$r(\mathcal{T}_n) = (-1)^{n-1}(n-1) + \sum_{k=2}^n (-1)^{n-k} \binom{n}{k} r(\mathcal{G}_k).$$

3. On the number of primitive canonical matrices of \mathcal{G}_n . As we know, the number of conjugacy classes of \mathcal{G}_n , with $n \leq 13$ is given (see Vera-López and Arregi, [7, 9, 10]). Now, we have calculated $r(\mathcal{T}_n)$ for $n = 4, \dots, 13$. These are:

$$\begin{aligned} r(\mathcal{T}_4) &= 3(q-1)^2 + 2(q-1)^3, \\ r(\mathcal{T}_5) &= 10(q-1)^3 + 5(q-1)^4, \\ r(\mathcal{T}_6) &= 15(q-1)^3 + 40(q-1)^4 + 18(q-1)^5 + (q-1)^6, \\ r(\mathcal{T}_7) &= 105(q-1)^4 + 175(q-1)^5 + 77(q-1)^6 + 8(q-1)^7, \end{aligned}$$

$$\begin{aligned}
 r(\mathcal{T}_8) &= 105(q-1)^4 + 700(q-1)^5 + 924(q-1)^6 + 432(q-1)^7 \\
 &\quad + 74(q-1)^8 + 4(q-1)^9, \\
 r(\mathcal{T}_9) &= 1260(q-1)^5 + 4690(q-1)^6 + 5544(q-1)^7 + 2823(q-1)^8 \\
 &\quad + 665(q-1)^9 + 72(q-1)^{10} + 3(q-1)^{11}, \\
 r(\mathcal{T}_{10}) &= 945(q-1)^5 + 12600(q-1)^6 + 34440(q-1)^7 + 38760(q-1)^8 \\
 &\quad + 21810(q-1)^9 + 6642(q-1)^{10} + 1140(q-1)^{11} \\
 &\quad + 110(q-1)^{12} + 5(q-1)^{13}, \\
 r(\mathcal{T}_{11}) &= 17325(q-1)^6 + 119350(q-1)^7 + 274890(q-1)^8 \\
 &\quad + 306405(q-1)^9 + 190520(q-1)^{10} + 71204(q-1)^{11} \\
 &\quad + 16797(q-1)^{12} + 2563(q-1)^{13} + 242(q-1)^{14} + 11(q-1)^{15}, \\
 r(\mathcal{T}_{12}) &= 10395(q-1)^6 + 242550(q-1)^7 + 1165780(q-1)^8 \\
 &\quad + 2420220(q-1)^9 + 2732598(q-1)^{10} + 1872834(q-1)^{11} \\
 &\quad + 833357(q-1)^{12} + 253023(q-1)^{13} + 54352(q-1)^{14} + 8352(q-1)^{15} \\
 &\quad + 890(q-1)^{16} + 60(q-1)^{17} + 2(q-1)^{18}, \\
 r(\mathcal{T}_{13}) &= 270270(q-1)^7 + 3078075(q-1)^8 + 11931920(q-1)^9 \\
 &\quad + 23335455(q-1)^{10} + 27065181(q-1)^{11} + 20340047(q-1)^{12} \\
 &\quad + 10509852(q-1)^{13} + 3909673(q-1)^{14} + 1085682(q-1)^{15} \\
 &\quad + 229866(q-1)^{16} + 36998(q-1)^{17} + 4355(q-1)^{18} \\
 &\quad + 338(q-1)^{19} + 13(q-1)^{20}.
 \end{aligned}$$

We notice that for $n \leq 13$, $r(\mathcal{T}_n)$ is a multiple of $(q-1)^{\lfloor \frac{n+1}{2} \rfloor}$ and we are interested in extending this result for every $n \in \mathbb{N}$. We remember that since the matrices of \mathcal{T}_n are canonical, two different matrices of \mathcal{T}_n are not in the same conjugacy class. Therefore, in order to find $r(\mathcal{T}_n)$ it is enough to calculate the cardinality of \mathcal{T}_n .

First, we consider \mathcal{PC}_n , the subset of \mathcal{C}_n (and also of \mathcal{T}_n) formed by primitive connected canonical matrices of \mathcal{G}_n . In order to find its cardinality, we need the following Lemma.

LEMMA 3.1. *Let $A \in \mathcal{PC}_n$ be and \mathcal{R} be the group of triangular matrices of $\text{GL}_n(q)$. Then, the conjugacy class of A by \mathcal{R} is formed by $(q-1)^{n-1}$ different conjugacy classes by \mathcal{G}_n .*

Proof. We note that $\mathcal{R} = \mathcal{D}_n \mathcal{G}_n$, where $\mathcal{D}_n = \{\text{diag}(d_1, \dots, d_n) \mid d_i \in \mathbb{F}_q^*\}$. So, given $Y \in \mathcal{R}$, there exist $D \in \mathcal{D}_n$ and $T \in \mathcal{G}_n$ such that $Y = DT$. Then, for $A \in \mathcal{PC}_n$, if

$$C_{\mathcal{R}}(A) = \{DT \in \mathcal{R} \mid T^{-1}D^{-1}ADT = A\},$$

we have

$$C_{\mathcal{R}}(A) = \mathcal{E}C_{\mathcal{G}_n}(A),$$

where $\mathcal{E} = \{\lambda I_n \mid \lambda \in \mathbb{F}_q^*\}$, that is, \mathcal{E} is the group of scalar matrices over \mathbb{F}_q . Thus, from the fundamental

counting principle, we can deduce the cardinality of the $\text{Cl}_{\mathcal{R}}(A)$:

$$\begin{aligned} |\text{Cl}_{\mathcal{R}}(A)| &= |\mathcal{R} : C_{\mathcal{R}}(A)| = |\mathcal{D}_n \mathcal{G}_n : \mathcal{E} C_{\mathcal{G}_n}(A)| = \frac{|\mathcal{D}_n|}{|\mathcal{E}|} |\mathcal{G}_n : C_{\mathcal{G}_n}(A)| \\ &= (q-1)^{n-1} |\text{Cl}_{\mathcal{G}_n}(A)|, \end{aligned}$$

since $|\mathcal{D}_n| = (q-1)^n$ and $|\mathcal{E}| = (q-1)$. □

REMARK 3.2. If we consider a diagonal matrix $D \in \mathcal{D}_n$ such that $D^{-1}AD = A$, it follows that whenever $a_{ij} \neq 0$, then $d_i = d_j$. But if $A \in \mathcal{PC}_n$, its graph is connected, so D is a scalar matrix.

Now, by applying Lemma 3.1, it is immediate to show the following Proposition.

PROPOSITION 3.3. *The number of primitive connected canonical matrices of \mathcal{G}_n is a multiple of $(q-1)^{n-1}$.*

By using an argument similar to Lemma 3.1, we can extend Lemma 3.1 to primitive canonical matrices.

LEMMA 3.4. *Let $A \in \mathcal{T}_n$ be a primitive canonical matrix, with d_A connected components and let \mathcal{R} be the subgroup of triangular matrices of $\text{GL}_n(q)$. Then, the conjugacy class of A by \mathcal{R} consists of $(q-1)^{n-d_A}$ different \mathcal{G}_n -classes.*

REMARK 3.5. We notice that if $d_A = 1$, then A is connected and Lemma 3.1 is a particular case of Lemma 3.4.

REMARK 3.6. It is easy to check that

$$\text{Cl}_{\mathcal{R}}(A) = \cup_{D \in \mathcal{D}_n} \text{Cl}_{\mathcal{G}_n}(A^D),$$

where $\mathcal{D}_n = \{\text{diag}(d_1, \dots, d_n) \mid d_i \in \mathbb{F}_q^*\}$ is the diagonal group.

As a consequence of Lemma 3.4, it follows:

PROPOSITION 3.7. *The number of primitive canonical matrices of \mathcal{G}_n with d_A connected components is a multiple of $(q-1)^{n-d_A}$.*

Proof. If Γ_A is primitive but non-connected, let $\Gamma_1, \dots, \Gamma_{d_A}$ be its connected components of sizes n_1, \dots, n_{d_A} . The action of the diagonal group \mathcal{D}_n on these components is equivalent to the action of d_A diagonal groups of sizes n_i , corresponding to each connected component the factor $(q-1)^{n_i-1}$. The product of all factors is $\prod_{i=1}^{d_A} (q-1)^{n_i-1} = (q-1)^{n-d_A}$ because $(n_1-1) + \dots + (n_{d_A}-1) = n-d_A$. □

If $A \in \mathcal{T}_n$ is a primitive canonical matrix, then the maximum number of connected components of its graph is $\lfloor \frac{n}{2} \rfloor$. Besides, the matrices of \mathcal{T}_n can be classified according to the number of connected components in their graphs and this is a partition of \mathcal{T}_n . Then there is the next corollary.

COROLLARY 3.8. *The cardinality of \mathcal{T}_n , and consequently $r(\mathcal{T}_n)$, is a multiple of $(q-1)^{\lfloor \frac{n+1}{2} \rfloor}$.*

4. Primitive canonical matrices of \mathcal{G}_n with exactly $\lfloor \frac{n+1}{2} \rfloor + \lambda$, $\lambda = 0, 1, 2$, non-zero entries.

We can classify the matrices of \mathcal{T}_n according to the number of non-zero off-diagonal entries. If $A \in \mathcal{T}_n$ is a primitive canonical matrix, we know that $\Gamma_A = (V_A, E_A)$ has no isolated vertices, so $|E_A| \geq \lfloor \frac{n+1}{2} \rfloor$ and A has, at least, $\lfloor \frac{n+1}{2} \rfloor$ non-zero off-diagonal entries. For $\lambda \geq 0$, we define $\mathcal{A}_{\lambda, n}$ as the subset of primitive canonical matrices of \mathcal{G}_n with exactly $\lfloor \frac{n+1}{2} \rfloor + \lambda$ non-zero off-diagonal entries. We are interested in calculating the cardinality of $\mathcal{A}_{\lambda, n}$, for $\lambda = 0, 1, 2$. In order to do this, the primitive canonical matrices such that they are forest matrices play a main role.

LEMMA 4.1. *If $A \in \mathcal{A}_{\lambda,n}$, with $\lambda = 0, 1, 2$, then A is a forest matrix. Moreover, the number of connected components of Γ_A is $\lfloor \frac{n}{2} \rfloor - \lambda$.*

Proof. We write Γ_A as the union of its d_A connected components:

$$\Gamma_A = (V_A, E_A) = \Gamma_1 \cup \dots \cup \Gamma_{d_A}, \quad \Gamma_i = (V_i, E_i),$$

$$v_i = |V_i|, \quad l_i = |E_i|, \quad v = |V_A| = \sum_i v_i, \quad l = |E_A| = \sum_i l_i,$$

where V_i and E_i are the set of vertices and the set of edges of Γ_i , respectively.

For each connected component, we have the relation

$$l_i = v_i - 1 + e_i, \quad e_i \geq 0,$$

where the values $e_i = 0$ correspond to the connected components without cycles. From the preliminary relations, if $e = \sum_i e_i$, it follows

$$(4.1) \quad l = v - d_A + e.$$

Moreover, each connected component has, at least, two vertices (without considering the singletons), that is, $v_i \geq 2$ and, therefore, $v = \sum_i v_i \geq 2d_A$. The condition that A is primitive implies $d_A \leq \frac{n}{2}$. We write

$$(4.2) \quad l = \left\lfloor \frac{n+1}{2} \right\rfloor + \lambda.$$

Then, from the equalities (4.1) and (4.2), it follows

$$\left\lfloor \frac{n+1}{2} \right\rfloor + \lambda = n - d_A + e,$$

hence

$$(4.3) \quad \lambda = \left\lfloor \frac{n}{2} \right\rfloor - d_A + e, \quad \left\lfloor \frac{n}{2} \right\rfloor - d_A \geq 0, \quad e \geq 0.$$

Suppose that $e > 0$. If we look for canonical matrices of \mathcal{G}_j , for $j \leq 6$, we notice that for $j = 2, 3, 4, 5$ the graphs of the primitive canonical matrices are trees and the first graph that contains a cycle appears for $j = 6$. Hence, if $e_i \geq 1$ for some connected component Γ_i , then $v_i \geq 6$. This fact jointly with $v_j \geq 2$, for $j = 1, \dots, d_A$ gives $n = v_i + \sum_{j \neq i} v_j \geq 6 + 2(d_A - 1) = 2d_A + 4$, hence $\lfloor \frac{n}{2} \rfloor - d_A \geq 2$ and

$$\lambda = \left\lfloor \frac{n}{2} \right\rfloor - d_A + e \geq 2 + 1 = 3.$$

Consequently, for $\lambda = 0, 1, 2$, it follows $e = 0$ and, hence, $e_i = 0$ for all connected components. Then, by substitution in (4.3), we can conclude $d_A = \lfloor \frac{n}{2} \rfloor - \lambda$. \square

It is easy to prove the following lemma (see Vera-López and Arregi, [10][Lemma 2 and Theorem 4]):

LEMMA 4.2. *Let $A \in \mathcal{A}_{\lambda,n}$ be. If $B \in \mathcal{G}_n$ has all non-zero entries in the same indices as A , then $B \in \mathcal{A}_{\lambda,n}$. Therefore,*

$$|\mathcal{A}_{\lambda,n}| = a_{\lambda,n}(q-1)^{\lfloor \frac{n+1}{2} \rfloor + \lambda},$$

where $a_{\lambda,n}$ is the number of arrangement of primitive canonical matrices of $\mathcal{A}_{\lambda,n}$.

Now, we find the value of $a_{\lambda,n}$, for $\lambda = 0, 1, 2$. In the following, we consider $\frac{1}{(k-u)!} = 0$, if $k < u$ and we denote for every n nonnegative integer by $n!!$ to

$$n!! = \begin{cases} n(n-2) \dots 5.3.1, & \text{if } n \geq 1 \text{ is odd;} \\ n(n-2) \dots 6.4.2, & \text{if } n \geq 2 \text{ is even;} \\ 1, & \text{if } n = 0. \end{cases}$$

PROPOSITION 4.3. $|\mathcal{A}_{0,n}| = \mathbf{a}_{0,n}(q-1)^{\lfloor \frac{n+1}{2} \rfloor}$, where

$$\mathbf{a}_{0,n} = \begin{cases} \binom{2k}{2 \dots 2} \frac{1}{k!} = (2k-1)!!, & \text{if } n = 2k; \\ \binom{2k+1}{3 \ 2 \dots 2} \frac{1}{(k-1)!} = \binom{2k+1}{3} (2k-3)!!, & \text{if } n = 2k+1. \end{cases}$$

Proof. By applying Lemma 4.2, we know that

$$|\mathcal{A}_{0,n}| = \mathbf{a}_{0,n}(q-1)^{\lfloor \frac{n+1}{2} \rfloor},$$

where $\mathbf{a}_{0,n}$ is the number of different zero-nonzero patterns of their entries for primitive canonical matrices of $\mathcal{A}_{0,n}$. Let $A \in \mathcal{A}_{0,n}$ be. Then, Γ_A has order n with no isolated vertices and exactly $\lfloor \frac{n+1}{2} \rfloor$ edges. Consequently, all vertices of Γ_A have degree 1 or all but one vertex have degree one and that vertex has degree 2. If all vertices have degree 1, then $n = 2k$ and

$$a_{0,n} = a_{0,2k} = \binom{2k}{2 \dots 2} \frac{1}{k!} = (2k-1)!!.$$

If all vertices but one have degree 1 and that vertex has degree 2, then $n = 2k+1$ and

$$a_{0,n} = a_{0,2k+1} = \binom{2k+1}{3 \ 2 \dots 2} \frac{1}{(k-1)!} = \binom{2k+1}{3} (2k-3)!! \quad \square$$

REMARK 4.4. We can also express $\mathbf{a}_{0,n}$ by

$$\mathbf{a}_{0,n} = \left(2 \left\lfloor \frac{n+1}{2} \right\rfloor - 1 \right)!! \left(\frac{\lfloor \frac{n+1}{2} \rfloor - 4}{3} \cdot \epsilon + 1 \right),$$

with $\epsilon = 0$, if n is even or $\epsilon = 1$, if n is odd.

PROPOSITION 4.5. $|\mathcal{A}_{1,n}| = \mathbf{a}_{1,n}(q-1)^{\lfloor \frac{n+1}{2} \rfloor + 1}$, where

$$\mathbf{a}_{1,n} = \begin{cases} 2 \cdot \binom{2k}{4 \ 2 \dots 2} \frac{1}{(k-2)!} + \binom{2k}{3 \ 3 \ 2 \dots 2} \frac{1}{2!} \frac{1}{(k-3)!}, & \text{if } n = 2k; \\ 5 \cdot \binom{2k+1}{5 \ 2 \dots 2} \frac{1}{(k-2)!} + 2 \cdot \binom{2k+1}{4 \ 3 \ 2 \dots 2} \frac{1}{(k-3)!} \\ + \binom{2k+1}{3 \ 3 \ 3 \ 2 \dots 2} \frac{1}{3!} \frac{1}{(k-4)!}, & \text{if } n = 2k+1. \end{cases}$$

Proof. From Lemma 4.1, we know that the number of connected components of $A \in \mathcal{A}_{1,n}$ is $d_A = \lfloor \frac{n}{2} \rfloor - 1$. Furthermore, by applying Lemma 4.2, we know that

$$|\mathcal{A}_{1,n}| = \mathbf{a}_{1,n}(q-1)^{\lfloor \frac{n+1}{2} \rfloor + 1},$$

where $\mathbf{a}_{1,n}$ is the number of different zero-nonzero patterns of their entries for primitive canonical matrices of $\mathcal{A}_{1,n}$. Now all that remains is to calculate $\mathbf{a}_{1,n}$.

If $A \in \mathcal{A}_{1,n}$, then A is a forest matrix and Γ_A is a graph of order n with no isolated vertices and exactly $\lfloor \frac{n+1}{2} \rfloor + 1$ edges. Thus,

1. If $n = 2k$, then $\sum_{v \in V_A} d(v) = 2k + 2$. Obviously, it follows that $\Delta(\Gamma_A) > 1$. We assert that $\Delta(\Gamma_A) = 2$. In fact, if there was a vertex of degree 3, this would mean that one connected component of Γ_A has 4 vertices and the rest only 2. But the submatrix corresponding to the connected component with 4 vertices, one of which is of degree 3, is not a canonical submatrix. So, $\Delta(\Gamma_A) = 2$. The two vertices of degree 2 can belong to the same connected component or not. If they belong to the same connected component, it implies that there is a connected component with 4 vertices, two of them with degree 2. But this connected component corresponds to a primitive connected canonical submatrix of order 4 and there are 2 different zero-nonzero patterns for this. If the vertices of degree 2 belong to different components, then there are two connected components with 3 vertices. Consequently,

$$\mathbf{a}_{1,2k} = 2 \cdot \binom{2k}{4 \ 2 \ \dots \ 2} \frac{1}{(k-2)!} + \binom{2k}{3 \ 3 \ 2 \ \dots \ 2} \frac{1}{2!} \frac{1}{(k-3)!}.$$

2. If $n = 2k + 1$, then $\sum_{v \in V_A} d(v) = 2k + 4$. Again, by considering the canonical character of the matrices, it is easy to check that $\Delta(\Gamma_A) = 2$. So, there are three vertices with degree 2 and $n - 3$ with degree 1. The vertices of degree 2 can belong to the same connected component or not. If they belong to the same connected component, then there is one connected component with 5 vertices and the others have 2 vertices in Γ_A . If two vertices of degree 2 belong to the same component and the other one to a different component, then Γ_A has one connected component with 4 vertices, another one with 3 vertices and the rest ones with 2 vertices. If the vertices of degree 2 belong to different connected components, then Γ_A has three connected components with 3 vertices and the rest ones of size 2. Thus, bearing in mind the zero-nonzero patterns for canonical matrices of size 5, 4, 3 and 2, we conclude that

$$\mathbf{a}_{1,2k+1} = 5 \cdot \binom{2k+1}{5 \ 2 \ \dots \ 2} \frac{1}{(k-2)!} + 2 \cdot \binom{2k+1}{4 \ 3 \ 2 \ \dots \ 2} \frac{1}{(k-3)!} + \binom{2k+1}{3 \ 3 \ 3 \ 2 \ \dots \ 2} \frac{1}{3!} \frac{1}{(k-4)!}. \quad \square$$

REMARK 4.6. Another expression for $\mathbf{a}_{1,n}$ is

$$\mathbf{a}_{1,n} = \left(2 \left\lfloor \frac{n+1}{2} \right\rfloor - 1 \right)!! \frac{\lfloor \frac{n}{2} \rfloor (\lfloor \frac{n}{2} \rfloor - 1) q_1(n)}{27 \cdot 6},$$

where $q_1(n) = (2 \lfloor \frac{n}{2} \rfloor^2 + 5 \lfloor \frac{n}{2} \rfloor) \cdot \epsilon + 3(\lfloor \frac{n}{2} \rfloor + 1)(5(1 - \epsilon) + 1)$ and $\epsilon = 0$, if n is even or $\epsilon = 1$, if n is odd.

Finally, by using similar argument, we calculate $\mathbf{a}_{2,n}$:

PROPOSITION 4.7. $|\mathcal{A}_{2,n}| = \mathbf{a}_{2,n}(q-1)^{\lfloor \frac{n+1}{2} \rfloor + 2}$, where

$$\mathbf{a}_{2,n} = \begin{cases} \begin{aligned} &18 \cdot \binom{2k}{6 \ 2 \ \dots \ 2} \frac{1}{(k-3)!} + 5 \cdot \binom{2k}{5 \ 3 \ 2 \ \dots \ 2} \frac{1}{(k-4)!} \\ &+ 2 \cdot 2 \cdot \binom{2k}{4 \ 4 \ 2 \ \dots \ 2} \frac{1}{2!} \frac{1}{(k-4)!} + 2 \cdot \binom{2k}{4 \ 3 \ 3 \ 2 \ \dots \ 2} \frac{1}{2!} \frac{1}{(k-5)!} \\ &+ \binom{2k}{3 \ 3 \ 3 \ 3 \ 2 \ \dots \ 2} \frac{1}{4!} \frac{1}{(k-6)!}, \end{aligned} & \text{if } n = 2k; \\ \begin{aligned} &77 \cdot \binom{2k+1}{7 \ 2 \ \dots \ 2} \frac{1}{(k-3)!} + 18 \cdot \binom{2k+1}{6 \ 3 \ 2 \ \dots \ 2} \frac{1}{(k-4)!} \\ &+ 5 \cdot 2 \cdot \binom{2k+1}{5 \ 4 \ 2 \ \dots \ 2} \frac{1}{(k-4)!} + 5 \cdot \binom{2k+1}{5 \ 3 \ 3 \ 2 \ \dots \ 2} \frac{1}{2!} \frac{1}{(k-5)!} \\ &+ 2 \cdot 2 \cdot \binom{2k+1}{4 \ 4 \ 3 \ 2 \ \dots \ 2} \frac{1}{2!} \frac{1}{(k-5)!} \\ &+ 2 \cdot \binom{2k+1}{4 \ 3 \ 3 \ 3 \ 2 \ \dots \ 2} \frac{1}{3!} \frac{1}{(k-6)!} \\ &+ \binom{2k+1}{3 \ 3 \ 3 \ 3 \ 3 \ 2 \ \dots \ 2} \frac{1}{5!} \frac{1}{(k-7)!}, \end{aligned} & \text{if } n = 2k + 1. \end{cases}$$

Proof. By Lemma 4.1, we know that the number of connected components of $A \in \mathcal{A}_{2,n}$ is $d_A = \lfloor \frac{n}{2} \rfloor - 2$. Furthermore, by Lemma 4.2, we know that

$$|\mathcal{A}_{2,n}| = \mathbf{a}_{2,n}(q-1)^{\lfloor \frac{n+1}{2} \rfloor + 2},$$

where $\mathbf{a}_{2,n}$ is the number of different zero-nonzero patterns of the entries for primitive canonical matrices of $\mathcal{A}_{2,n}$. A similar argument of Proposition 4.3 and Proposition 4.5 yields that the maximum order of a connected component of Γ_A is 6, if n is even, or 7, if n is odd and by considering the zero-nonzero patterns of canonical tree matrices of size 2 to 7, we conclude the expression of $\mathbf{a}_{2,n}$. \square

REMARK 4.8. Another expression for $\mathbf{a}_{2,n}$ is

$$\mathbf{a}_{2,n} = \frac{\lfloor \frac{n}{2} \rfloor \left(\lfloor \frac{n}{2} \rfloor - 1 \right) \left(\lfloor \frac{n}{2} \rfloor - 2 \right) q_2(n)}{2 \cdot 3^6 \cdot 5} \left(2 \left\lfloor \frac{n+1}{2} \right\rfloor - 1 \right)!!,$$

with

$$q_2(n) = \left\lfloor \frac{n}{2} \right\rfloor^4 \epsilon + 12 \left\lfloor \frac{n}{2} \right\rfloor^3 + 29 \left\lfloor \frac{n}{2} \right\rfloor^2 + 69 \left\lfloor \frac{n}{2} \right\rfloor + 18 + \left(3 \left\lfloor \frac{n}{2} \right\rfloor^3 + 61 \left\lfloor \frac{n}{2} \right\rfloor^2 - 39 \left\lfloor \frac{n}{2} \right\rfloor + 135 \right) (1 - \epsilon)$$

and $\epsilon = 0$, if n is even, or $\epsilon = 1$, if n is odd.

If we write $\mathcal{T}_n = \cup_{\lambda} \mathcal{A}_{\lambda,n}$ and bearing in mind that $r(\mathcal{T}_n) = \mathcal{T}_n$ and Lemma 4.2 and Propositions 4.3, 4.5 and 4.7, it follows:

COROLLARY 4.9.

$$r(\mathcal{T}_n) \equiv \sum_{i=0}^2 \mathbf{a}_{i,n}(q-1)^{\lfloor \frac{n+1}{2} \rfloor + i} \text{mod}(q-1)^{\lfloor \frac{n+1}{2} \rfloor + 3}.$$

It is clear that if we know $\mathbf{a}_{i,n}$ for $i = 0, 1, \dots, l$, then we can determine $r(\mathcal{G}_n)$ modulus $(q-1)^{8+l}$.

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