# New upper bounds for nonbinary codes based on the Terwilliger algebra and semidefinite programming

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#### Abstract

We give a new upper bound on the maximum size  $A_q(n, d)$  of a code of word length nand minimum Hamming distance at least d over the alphabet of  $q \ge 3$  letters. By blockdiagonalizing the Terwilliger algebra of the nonbinary Hamming scheme, the bound can be calculated in time polynomial in n using semidefinite programming. For q = 3, 4, 5this gives several improved upper bounds for concrete values of n and d. This work is related to [6], where a similar approach is used to derive upper bounds for binary codes.

**Keywords:** codes, nonbinary codes, upper bounds, Delsarte bound, Terwilliger algebra, block-diagonalisation, semidefinite programming.

Fix integers  $n \ge 1$  and  $q \ge 2$ , and fix an alphabet  $\mathbf{q} = \{0, 1, \dots, q-1\}$ . We will consider q-ary codes of length n, that is subsets of  $\mathbf{q}^n$ . The Hamming distance  $d(\mathbf{x}, \mathbf{y})$  of two words  $\mathbf{x}$  and  $\mathbf{y}$  is defined as the number of positions in which  $\mathbf{x}$  and  $\mathbf{y}$  differ. For a word  $\mathbf{x} \in \mathbf{q}^n$ , we denote the *support* of  $\mathbf{x}$  by  $S(\mathbf{x}) := \{v \mid \mathbf{x}_v \neq 0\}$ . Note that  $|S(\mathbf{x})| = d(\mathbf{x}, \mathbf{0})$ , where  $\mathbf{0}$  is the all-zero word.

Denote by  $\operatorname{Aut}(q, n)$  the set of permutations of  $\mathbf{q}^n$  that preserve the Hamming distance. It is not hard to see that  $\operatorname{Aut}(q, n)$  consists of the permutations of  $\mathbf{q}^n$  obtained by permuting the *n* coordinates followed by independently permuting the alphabet  $\mathbf{q}$  at each of the *n* coordinates. If we consider the action of  $\operatorname{Aut}(q, n)$  on the set  $\mathbf{q}^n \times \mathbf{q}^n$ , the orbits form an association scheme known as the nonbinary Hamming scheme H(n, q), with association matrices  $A_0, A_1, \ldots, A_n$  defined by

$$(A_i)_{\mathbf{x},\mathbf{y}} := \begin{cases} 1 & \text{if } d(\mathbf{x},\mathbf{y}) = i, \\ 0 & \text{otherwise,} \end{cases}$$
(1)

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for i = 0, 1, ..., n. The association matrices span a commutative algebra called the Bose–Mesner algebra of the scheme. Diagonalizing the Bose–Mesner algebra yields the well-known linear programming bound of Delsarte [5], which gives a good upper bound on  $A_q(n, d)$ .

Here we will consider the action of  $\operatorname{Aut}(q, n)$  on ordered triples of words, which will lead to a noncommutative algebra  $\mathcal{A}_{q,n}$  containing the Bose–Mesner algebra. It turns out that the algebra coincides with the Terwilliger algebra [7] of H(n,q). In section 3 it is shown how the algebra  $\mathcal{A}_{q,n}$  can be used to obtain a new upper bound on  $A_q(n,d)$ . The bound is based on semidefinite programming and can be computed in time polynomial in n by using the block-diagonalisation constructed in section 2. The approach we follow is similar to the one in [6], which deals with binary codes. In fact we will use results from that paper to obtain our block-diagonalisation.

# 1 The Terwilliger algebra

To each ordered triple  $(\mathbf{x}, \mathbf{y}, \mathbf{z}) \in \mathbf{q}^n \times \mathbf{q}^n \times \mathbf{q}^n$  we associate the four-tuple

$$d(\mathbf{x}, \mathbf{y}, \mathbf{z}) := (i, j, t, p), \text{ where}$$

$$i := d(\mathbf{x}, \mathbf{y}),$$

$$j := d(\mathbf{x}, \mathbf{z}),$$

$$t := |\{v \mid \mathbf{x}_v \neq \mathbf{y}_v \text{ and } \mathbf{x}_v \neq \mathbf{z}_v\}|,$$

$$p := |\{v \mid \mathbf{x}_v \neq \mathbf{y}_v = \mathbf{z}_v\}|.$$

$$(2)$$

Note that  $d(\mathbf{y}, \mathbf{z}) = i + j - t - p$  and  $|\{v \mid \mathbf{x}_v \neq \mathbf{y}_v \neq \mathbf{z}_v \neq \mathbf{x}_v\}| = t - p$ . The set of four-tuples (i, j, t, p) that occur as  $d(\mathbf{x}, \mathbf{y}, \mathbf{z})$  for some  $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbf{q}^n$  is given by

$$\mathcal{I}(q,n) := \{ (i, j, t, p) \mid 0 \le p \le t \le i, j \text{ and } i+j \le n+t \},$$
(3)

and will index various objects defined below.

**Proposition 1.** For  $n \ge 1$  and  $q \ge 3$ ,  $|\mathcal{I}(q,n)| = \binom{n+4}{4}$ .

*Proof.* If we substitute p' := p, t' := t - p, i' := i - t and j' := j - t, then the integer solutions of  $0 \le p \le t \le i, j$ ,  $i + j \le n + t$  are in bijection with the integer solutions of  $0 \le p', t', i', j', p' + t' + i' + j' \le n$ .

The integers i, j, t, p parametrize the ordered triples of words up to symmetry. That is, if we define

$$X_{i,j,t,p} := \{ (\mathbf{x}, \mathbf{y}, \mathbf{z}) \in \mathbf{q}^n \times \mathbf{q}^n \times \mathbf{q}^n \mid d(\mathbf{x}, \mathbf{y}, \mathbf{z}) = (i, j, t, p) \},$$
(4)

for  $(i, j, t, p) \in \mathcal{I}(q, n)$ , we have the following.

**Proposition 2.** The sets  $X_{i,j,t,p}$ ,  $(i, j, t, p) \in \mathcal{I}(q, n)$  are the orbits of  $\mathbf{q}^n \times \mathbf{q}^n \times \mathbf{q}^n$  under the action of  $\operatorname{Aut}(q, n)$ .

*Proof.* Let  $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbf{q}^n$  and let  $(i, j, t, p) = d(\mathbf{x}, \mathbf{y}, \mathbf{z})$ . Since the Hamming distances i, j, i + j - t - p and the number  $t - p = |\{v \mid \mathbf{x}_v \neq \mathbf{y}_v \neq \mathbf{z}_v \neq \mathbf{x}_v\}|$  are unchanged when permuting the coordinates or permuting the elements of  $\mathbf{q}$  at any coordinate, we have  $d(\mathbf{x}, \mathbf{y}, \mathbf{z}) = d(\pi(\mathbf{x}), \pi(\mathbf{y}), \pi(\mathbf{z}))$  for any  $\pi \in \operatorname{Aut}(q, n)$ .

Hence it suffices to show that there is an automorphism  $\pi$  such that  $(\pi(\mathbf{x}), \pi(\mathbf{y}), \pi(\mathbf{z}))$ only depends upon i, j, t and p. By permuting  $\mathbf{q}$  at the coordinates in the support of  $\mathbf{x}$ , we may assume that  $\mathbf{x} = \mathbf{0}$ . Let  $A := \{v \mid \mathbf{y}_v \neq 0, \mathbf{z}_v = 0\}$ ,  $B := \{v \mid \mathbf{y}_v = 0, \mathbf{z}_v \neq 0\}$ ,  $C := \{v \mid \mathbf{y}_v \neq 0, \mathbf{z}_v \neq 0, \mathbf{y}_v \neq \mathbf{z}_v\}$  and  $D := \{v \mid \mathbf{y}_v = \mathbf{z}_v \neq 0\}$ . Note that |A| = i - t, |B| = j - t, |C| = t - p and |D| = p. By permuting coordinates, we may assume that  $A = \{1, 2, \dots, i - t\}$ ,  $B = \{i - t + 1, \dots, i + j - 2t\}$ ,  $C = \{i + j - 2t + 1, \dots, i + j - t - p\}$ and  $D = \{i + j - t - p + 1, \dots, i + j - t\}$ . Now by permuting  $\mathbf{q}$  at each of the points in  $A \cup B \cup C \cup D$ , we can accomplish that  $\mathbf{y}_v = 1$  for  $v \in A \cup C \cup D$  and  $\mathbf{z}_v = 2$  for  $v \in B \cup C$ and  $\mathbf{z}_v = 1$  for  $v \in D$ .

Denote the stabilizer of **0** in  $\operatorname{Aut}(q, n)$  by  $\operatorname{Aut}_0(q, n)$ . For  $(i, j, t, p) \in \mathcal{I}(q, n)$ , let  $M_{i,j}^{t,p}$  be the  $\mathbf{q}^n \times \mathbf{q}^n$  matrix defined by:

$$(M_{i,j}^{t,p})_{\mathbf{x},\mathbf{y}} := \begin{cases} 1 & \text{if } |S(\mathbf{x})| = i, \, |S(\mathbf{y})| = j, \, |S(\mathbf{x}) \cap S(\mathbf{y})| = t, \, |\{v \mid \mathbf{x}_v = \mathbf{y}_v \neq 0\}| = p, \\ 0 & \text{otherwise.} \end{cases}$$
(5)

Let  $\mathcal{A}_{q,n}$  be the set of matrices

$$\sum_{i,j,t,p)\in\mathcal{I}(q,n)} x_{i,j}^{t,p} M_{i,j}^{t,p},\tag{6}$$

where  $x_{i,j}^{t,p} \in \mathbb{C}$ . From Proposition 2 it follows that  $\mathcal{A}_{q,n}$  is the set of matrices that are stable under permutations  $\pi \in \operatorname{Aut}_0(q, n)$  of the rows and columns. Hence  $\mathcal{A}_{q,n}$  is a complex matrix algebra called the *centralizer algebra* (cf. [1]) of  $\operatorname{Aut}_0(q, n)$ . The  $M_{i,j}^{t,p}$  constitute a basis for  $\mathcal{A}_{q,n}$  and hence

$$\dim \mathcal{A}_{q,n} = \binom{n+4}{4},\tag{7}$$

by Proposition 1. Note that the algebra  $\mathcal{A}_{q,n}$  contains the Bose–Mesner algebra since

$$A_{k} = \sum_{\substack{(i,j,t,p) \in \mathcal{I}(q,n) \\ i+j-t-p=k}} M_{i,j}^{t,p}.$$
(8)

Although it is not needed for the remainder of this paper, we would like to point out here, that  $\mathcal{A}_{q,n}$  coincides with the Terwilliger algebra (see [7]) of the nonbinary Hamming scheme H(n,q) (with respect to **0**). The Terwilliger algebra  $\mathcal{T}(q,n)$  is the complex matrix algebra generated by the association matrices  $A_0, A_1, \ldots, A_n$  of the Hamming scheme and the diagonal matrices  $E_0^*, E_1^*, \ldots, E_n^*$  defined by

$$(E_i^*)_{\mathbf{x},\mathbf{x}} := \begin{cases} 1 & \text{if } |S(\mathbf{x})| = i, \\ 0 & \text{otherwise,} \end{cases}$$
(9)

for i = 0, 1, ..., n.

### **Proposition 3.** The algebras $\mathcal{A}_{q,n}$ and $\mathcal{T}_{q,n}$ coincide.

*Proof.* Since  $\mathcal{A}_{q,n}$  contains the matrices  $A_k$  and the matrices  $E_k^* = M_{k,k}^{k,k}$  for  $k = 0, 1, \ldots, n$ , it follows that  $\mathcal{T}_{q,n}$  is a subalgebra of  $\mathcal{A}_{q,n}$ . To show the reverse inclusion, define the zero-one matrices  $B_i, C_i, D_i \in \mathcal{T}_{q,n}$  by

$$B_{i} := E_{i}^{*}A_{1}E_{i}^{*},$$

$$C_{i} := E_{i}^{*}A_{1}E_{i+1}^{*},$$

$$D_{i} := E_{i}^{*}A_{1}E_{i-1}^{*}.$$
(10)

Observe that:

$$(B_i)_{\mathbf{x},\mathbf{y}} = 1 \quad \text{if and only if} \tag{11}$$
$$|S(\mathbf{x})| = i, d(\mathbf{x}, \mathbf{y}) = 1, |S(\mathbf{y})| = i, S(\mathbf{x}) = S(\mathbf{y}),$$
$$(C_i)_{\mathbf{x},\mathbf{y}} = 1 \quad \text{if and only if} \\|S(\mathbf{x})| = i, d(\mathbf{x}, \mathbf{y}) = 1, |S(\mathbf{y})| = i + 1, |S(\mathbf{x})\Delta S(\mathbf{y})| = 1,$$
$$(D_i)_{\mathbf{x},\mathbf{y}} = 1 \quad \text{if and only if} \\|S(\mathbf{x})| = i, d(\mathbf{x}, \mathbf{y}) = 1, |S(\mathbf{y})| = i - 1, |S(\mathbf{x})\Delta S(\mathbf{y})| = 1.$$

For given  $(i, j, t, p) \in \mathcal{I}(q, n)$ , let  $A_{i,j}^{t,p} \in \mathcal{T}_{q,n}$  be given by

$$A_{i,j}^{t,p} := (D_i D_{i-1} \cdots D_{t+1}) (C_t C_{t+1} \cdots C_{j-1}) (B_j)^{t-p}.$$
 (12)

Then for words  $\mathbf{x}, \mathbf{y} \in \mathbf{q}^n$ , the entry  $(A_{i,j}^{t,p})_{\mathbf{x},\mathbf{y}}$  counts the number of (i+j-t-p+3)-tuples

$$\mathbf{x} = \mathbf{d}_i, \mathbf{d}_{i-1}, \dots, \mathbf{d}_t = \mathbf{c}_t, \mathbf{c}_{t+1}, \dots, \mathbf{c}_j = \mathbf{b}_0, \dots, \mathbf{b}_{t-p} = \mathbf{y} \in \mathbf{q}^r$$

where any two consecutive words have Hamming distance 1, the  $\mathbf{b}_k$  have equal support of cardinality j, and  $|S(\mathbf{d}_k)| = k$ ,  $|S(\mathbf{c}_k)| = k$  for all k. Hence for  $\mathbf{x}, \mathbf{y} \in \mathbf{q}^n$  the following holds.

$$(A_{i,j}^{t,p})_{\mathbf{x},\mathbf{y}} = 0 \quad \text{if } d(\mathbf{x},\mathbf{y}) > i+j-t-p \text{ or } |S(\mathbf{x})\Delta S(\mathbf{y})| > i+j-2t$$
(13)

and

$$(A_{i,j}^{t,p})_{\mathbf{x},\mathbf{y}} > 0 \quad \text{if } |S(\mathbf{x})| = i, \ |S(\mathbf{y})| = j,$$

$$d(\mathbf{x},\mathbf{y}) = i + j - t - p \text{ and } |S(\mathbf{x})\Delta S(\mathbf{y})| = i + j - 2t.$$

$$(14)$$

To see (14) one may take for  $\mathbf{d}_k$  the zero-one word with support  $\{i + 1 - k, \ldots, i\}$ , for  $\mathbf{c}_k$  the zero-one word with support  $\{i + 1 - t, \ldots, i + k - t\}$  and for  $\mathbf{b}_k$  the word with support  $\{i + 1 - t, \ldots, i + j - t\}$  where the first k nonzero entries are 2 and the other nonzero entries are 1.

Now suppose that  $\mathcal{A}_{q,n}$  is not contained in  $\mathcal{T}_{q,n}$ , and let  $M_{i,j}^{t,p}$  be a matrix not in  $\mathcal{T}_{q,n}$  with t maximal and (secondly) p maximal. If we write

$$A_{i,j}^{t,p} = \sum_{t',p'} x_{i,j}^{t',p'} M_{i,j}^{t',p'},$$
(15)

then by (13)  $x_{i,j}^{t',p'} = 0$  if t' + p' < t + p or t' < t implying that  $A_{i,j}^{t,p} - x_{i,j}^{t,p}M_{i,j}^{t,p} \in \mathcal{T}_{q,n}$  by the maximality assumption. Therefore since  $x_{i,j}^{t,p} > 0$  by (14), also  $M_{i,j}^{t,p}$  belongs to  $\mathcal{T}_{q,n}$ , a contradiction.

# 2 Block-diagonalisation of the Terwilliger algebra

In this section we give an explicit block-diagonalisation of the algebra  $\mathcal{A}_{q,n}$ . The blockdiagonalisation can be seen as an extension of the block-diagonalisation in the binary case as given in [6]. In fact, we will use some results of this paper, summarized in Proposition 4 below.

For a finite set V of cardinality m and nonnegative integers i, j, define the  $2^V \times 2^V$  matrix  $C_{i,j}^V$  by

$$(C_{i,j}^V)_{I,J} := \begin{cases} 1 & \text{if } |I| = i, \, |J| = j, \, I \subseteq J \text{ or } J \subseteq I, \\ 0 & \text{otherwise.} \end{cases}$$
(16)

For  $k = 0, \ldots, \lfloor \frac{m}{2} \rfloor$  define the linear space  $L_k^V$  by

$$L_k^V := \{ x \in \mathbf{R}^{2^V} \mid C_{k-1,k}^V x = 0, \ x_I = 0 \text{ if } |I| \neq k \},$$
(17)

and let  $B_k^V$  be an orthonormal base of  $L_k^V$ .

**Proposition 4.** Let i, j, k, t, m be nonnegative integers satisfying  $k, t \leq i, j, i + j \leq m + 2t$ and  $k \leq \lfloor \frac{m}{2} \rfloor$ . Let V be a set of cardinality m and let  $b \in L_k^V$ .

i. We have

$$\dim L_k^V = \binom{m}{k} - \binom{m}{k-1}.$$
(18)

ii. For any nonnegative integer  $k' \leq \lfloor \frac{m}{2} \rfloor$  and  $b' \in L_{k'}^V$ 

$$(C_{i,k}^{V}b)^{\mathsf{T}}C_{i,k'}^{V}b' = \begin{cases} \binom{m-2k}{i-k}b^{\mathsf{T}}b' & \text{if } k = k', \\ 0 & \text{otherwise.} \end{cases}$$
(19)

*iii.* For any set  $Y \subseteq V$  of cardinality j

$$\sum_{\substack{U \subseteq V \\ |U|=i \\ |U \cap Y|=t}} (C_{i,k}^V b)_U = \beta_{i,j,k}^{m,t} {\binom{m-2k}{j-k}}^{-1} (C_{j,k}^V b)_Y,$$
(20)

where 
$$\beta_{i,j,k}^{m,t} := \sum_{u=0}^{m} (-1)^{t-u} {u \choose t} {m-2k \choose m-k-u} {m-k-u \choose i-u} {m-k-u \choose j-u}.$$

*Proof.* See [6] for a proof. Although part *iii* is not explicitly stated there, it can be derived from equations (36) and (39) in [6].  $\Box$ 

We will now describe the block-diagonalisation of  $\mathcal{A}_{q,n}$ . Let  $\phi := e^{\frac{2\pi i}{q-1}}$  be a primitive (q-1)-th root of unity. Let

$$\mathcal{V} := \{(a, k, i, \mathbf{a}, b) \mid (21) \\ a, k, i \text{ are integers satisfying } 0 \le a \le k \le i \le n + a - k, \\ \mathbf{a} \in \mathbf{q}^n \text{ satisfies } |S(\mathbf{a})| = a, \mathbf{a}_v \ne q - 1 \text{ for } v = 1, \dots, n, \\ b \in B_{k-a}^{\overline{S(\mathbf{a})}} \},$$

where  $\overline{U} := \{1, 2, \ldots, n\} \setminus U$  for any set  $U \subseteq \{1, 2, \ldots, n\}$ . For each tuple  $(a, k, i, \mathbf{a}, b)$  in  $\mathcal{V}$ , define the vector  $\Psi_{\mathbf{a}, b}^{a, k, i} \in \mathbb{C}^{\mathbf{q}^n}$  by

$$\Psi_{\mathbf{a},b}^{a,k,i}(\mathbf{x}) := \begin{cases} (q-1)^{-\frac{1}{2}i} \binom{n+a-2k}{i-k}^{-\frac{1}{2}} \phi^{\langle \mathbf{a}, \mathbf{x} \rangle} (C_{i-a,k-a}^{\overline{S(\mathbf{a})}} b) (S(\mathbf{x}) \setminus S(\mathbf{a})) & \text{if } S(\mathbf{a}) \subseteq S(\mathbf{x}), \\ 0 & \text{otherwise,} \end{cases}$$
(22)

for any  $\mathbf{x} \in \mathbf{q}^n$ . Here  $\langle \mathbf{x}, \mathbf{y} \rangle := \sum_{v=0}^n \mathbf{x}_v \mathbf{y}_v \in \mathbf{Z}_{\geq 0}$  for any  $\mathbf{x}, \mathbf{y} \in \mathbf{q}^n$ . Observe that  $\Psi_{\mathbf{a}, b}^{a, k, i}(\mathbf{x}) = 0$  if  $|S(\mathbf{x})| \neq i$ . We have:

**Proposition 5.** The vectors  $\Psi_{\mathbf{a},b}^{a,k,i}$ ,  $(a,k,i,\mathbf{a},b) \in \mathcal{V}$  form an orthonormal base of  $\mathbf{q}^n$ .

*Proof.* The number  $|\mathcal{V}|$  of vectors  $\Psi_{\mathbf{a},b}^{a,k,i}$  equals  $q^n$  since:

$$\sum_{\substack{a,k,i\\0\leq a\leq k\leq i\leq n+a-k}} \binom{n}{a} (q-2)^a \left[ \binom{n-a}{k-a} - \binom{n-a}{k-a-1} \right]$$

$$= \sum_{i=0}^n \sum_{a=0}^{i} \sum_{k=a}^{\min(i,n+a-i)} \binom{n}{a} (q-2)^a \left[ \binom{n-a}{k-a} - \binom{n-a}{k-a-1} \right]$$

$$= \sum_{i=0}^n \sum_{a=0}^{i} \binom{n}{a} (q-2)^a \binom{n-a}{i-a}$$

$$= \sum_{i=0}^n \binom{n}{i} \sum_{a=0}^{i} (q-2)^a \binom{i}{a}$$

$$= \sum_{i=0}^n \binom{n}{i} (q-1)^i = q^n.$$
(23)

We calculate the inner product of  $\Psi_{\mathbf{a},b}^{a,k,i}$  and  $\Psi_{\mathbf{a}',b'}^{a',k',i'}$ . If  $i \neq i'$  then the inner product is zero since the two vectors have disjoint support. So we may assume that i' = i. We obtain:

$$\left\langle \Psi_{\mathbf{a},b}^{a,k,i}, \Psi_{\mathbf{a}',b'}^{a',k',i} \right\rangle = (q-1)^{-i} \binom{n+a-2k}{i-k}^{-\frac{1}{2}} \binom{n+a'-2k'}{i-k'}^{-\frac{1}{2}} \cdot \sum_{\mathbf{x}} \phi^{\langle \mathbf{a},\mathbf{x}\rangle - \langle \mathbf{a}',\mathbf{x}\rangle} (C_{i-a,k-a}^{\overline{S(\mathbf{a})}} b) (S(\mathbf{x}) \setminus S(\mathbf{a})) \cdot (C_{i-a',k'-a'}^{\overline{S(\mathbf{a}')}} b') (S(\mathbf{x}) \setminus S(\mathbf{a}')),$$

$$(24)$$

where the sum ranges over all  $\mathbf{x} \in \mathbf{q}^n$  with  $|S(\mathbf{x})| = i$  and  $S(\mathbf{x}) \supseteq S(\mathbf{a}) \cup S(\mathbf{a}')$ . If  $\mathbf{a}_j \neq \mathbf{a}'_j$  for some j, then the inner product equals zero, since we can factor out  $\sum_{x_j=1}^{q-1} \phi^{x_j(\mathbf{a}_j - \mathbf{a}'_j)} = 0$ . So we may assume that  $\mathbf{a} = \mathbf{a}'$  (and hence a = a'), which simplifies the righthand side of (24) to

$$\binom{n+a-2k}{i-k}^{-\frac{1}{2}} \binom{n+a-2k'}{i-k'}^{-\frac{1}{2}} (C_{i-a,k-a}^{\overline{S(\mathbf{a})}}b)^{\mathsf{T}} C_{i-a,k'-a}^{\overline{S(\mathbf{a})}}b'.$$
(25)

Now by Proposition 4 we conclude that  $\langle \Psi_{\mathbf{a},b}^{a,k,i}, \Psi_{\mathbf{a},b'}^{a,k',i} \rangle$  is nonzero only if b = b' and k = k', in which case the inner product equals 1.

**Proposition 6.** For  $(i, j, t, p) \in \mathcal{I}(q, n)$  and  $(a, k, i', A, b) \in \mathcal{V}$  we have:

$$M_{j,i}^{t,p}\Psi_{\mathbf{a},b}^{a,k,i'} = \delta_{i,i'} \binom{n+a-2k}{i-k}^{-\frac{1}{2}} \binom{n+a-2k}{j-k}^{-\frac{1}{2}} \alpha(i,j,t,p,a,k)\Psi_{\mathbf{a},b}^{a,k,j},$$
(26)

where

$$\alpha(i,j,t,p,a,k) := \beta_{i-a,j-a,k-a}^{n-a,t-a} (q-1)^{\frac{1}{2}(i+j)-t} \sum_{g=0}^{p} (-1)^{a-g} \binom{a}{g} \binom{t-a}{p-g} (q-2)^{t-a-p+g}.$$
 (27)

*Proof.* Clearly, both sides of (26) are zero if  $i \neq i'$ , hence we may assume that i = i'. We calculate  $(M_{j,i}^{t,p} \Psi_{\mathbf{a},b}^{a,k,i})(\mathbf{y})$ . We may assume that  $|S(\mathbf{y})| = j$ , since otherwise both sides of (26) have a zero in position  $\mathbf{y}$ . We have:

$$(M_{j,i}^{t,p}\Psi_{\mathbf{a},b}^{a,k,i})(\mathbf{y}) = \sum_{\mathbf{x}\in\mathbf{q}^n} (M_{j,i}^{t,p})_{\mathbf{y},\mathbf{x}}\Psi_{\mathbf{a},b}^{a,k,i}(\mathbf{x})$$

$$= (q-1)^{-\frac{1}{2}i} \binom{n+a-2k}{i-k}^{-\frac{1}{2}} \sum_{\mathbf{x}} \phi^{\langle \mathbf{x},\mathbf{a} \rangle} (C_{i-a,k-a}^{\overline{S(\mathbf{a})}}b)(S(\mathbf{x}) \setminus S(\mathbf{a})),$$
(28)

where the last sum is over all  $\mathbf{x} \in \mathbf{q}^n$  with  $|S(\mathbf{x})| = i$ ,  $S(\mathbf{x}) \supseteq S(\mathbf{a})$ ,  $|S(\mathbf{x}) \cap S(\mathbf{y})| = t$  and  $|\{v \mid \mathbf{x}_v = \mathbf{y}_v \neq 0\}| = p$ . If  $v \in S(\mathbf{a}) \setminus S(\mathbf{y})$  we can factor out  $\sum_{l=1}^{q-1} \phi^{l\mathbf{a}_v} = 0$ , implying that both sides of (26) have a zero at position  $\mathbf{y}$ . Hence we may assume that  $S(\mathbf{y}) \supseteq S(\mathbf{a})$ . Now the support of each word  $\mathbf{x}$  in this sum can be split into five parts U, U', V, V', W, where

$$U = \{ v \in S(\mathbf{a}) \mid \mathbf{x}_v = \mathbf{y}_v \}$$

$$U' = S(\mathbf{a}) \setminus U,$$

$$V = \{ v \in S(\mathbf{y}) \setminus S(\mathbf{a}) \mid \mathbf{x}_v = \mathbf{y}_v \},$$

$$V' = ((S(\mathbf{y}) \setminus S(\mathbf{a})) \cap S(\mathbf{x})) \setminus V \text{ and}$$

$$W = S(\mathbf{x}) \setminus S(\mathbf{y}).$$

$$(29)$$

If we set g = |U|, then |U'| = a - g, |V| = p - g, |V'| = t - a - p + g and |W| = i - t. Hence splitting the sum over g, we obtain:

$$(q-1)^{-\frac{1}{2}i} \binom{n+a-2k}{i-k}^{-\frac{1}{2}} \sum_{g=0}^{p} \sum_{U,U',V,V',W} (C_{i-a,k-a}^{\overline{S(\mathbf{a})}}b)(V \cup V' \cup W) \\ \prod_{v \in U} \phi^{\mathbf{a}_v \mathbf{y}_v} \prod_{v \in U'} -\phi^{\mathbf{a}_v \mathbf{y}_v} \prod_{v \in V} \prod_{v \in V'} (q-2) \prod_{v \in W} (q-1), \quad (30)$$

where U, U', V, V', W are as indicated. Substituting  $T = V \cup V' \cup W$ , we can rewrite this as

$$(q-1)^{-\frac{1}{2}i} \binom{n+a-2k}{i-k}^{-\frac{1}{2}} \sum_{g=0}^{p} \binom{a}{g} \binom{t-a}{p-g} (-1)^{a-g} (q-2)^{t-a-p+g}.$$
$$(q-1)^{i-t} \phi^{\langle \mathbf{a}, \mathbf{y} \rangle} \sum_{T} (C_{i-a,k-a}^{\overline{S(\mathbf{a})}} b)(T), \quad (31)$$

where the sum ranges over all  $T \subseteq \overline{S(\mathbf{a})}$  with |T| = i - a and  $|T \cap S(\mathbf{y})| = t - a$ . Now by Proposition 4 this is equal to

$$(q-1)^{-\frac{1}{2}i} {\binom{n+a-2k}{i-k}}^{-\frac{1}{2}} (q-1)^{i-t} \sum_{g=0}^{p} {\binom{a}{g}} {\binom{t-a}{p-g}} (-1)^{a-g} (q-2)^{t-a-p+g}.$$
  
$$\phi^{\langle \mathbf{a}, \mathbf{y} \rangle} {\binom{n+a-2k}{j-k}}^{-1} \beta^{n-a,t-a}_{i-a,j-a,k-a} (C^{\overline{S(\mathbf{a})}}_{j-a,k-a}b) (S(\mathbf{y}) \setminus S(\mathbf{a})), \quad (32)$$

which equals

$$\Psi_{\mathbf{a},b}^{a,k,j}(\mathbf{y}) \cdot \beta_{i-a,j-a,k-a}^{n-a,t-a} \binom{n+a-2k}{i-k}^{-\frac{1}{2}} \binom{n+a-2k}{j-k}^{-\frac{1}{2}} (q-1)^{\frac{1}{2}(i+j)-t}.$$

$$\sum_{g=0}^{p} (-1)^{a-g} \binom{a}{g} \binom{t-a}{p-g} (q-2)^{t-a-p+g}.$$
(33)

If we define U to be the  $\mathbf{q}^n \times \mathcal{V}$  matrix with  $\Psi_{\mathbf{a},b}^{a,k,i}$  as the  $(a,k,i,\mathbf{a},b)$ -th column, then Proposition 6 shows that for each  $(i, j, t, p) \in \mathcal{I}(q, n)$  the matrix  $\tilde{M}_{i,j}^{t,p} := U^* M_{i,j}^{t,p} U$  has entries

$$(\tilde{M}_{i,j}^{t,p})_{(a,k,l,\mathbf{a},b),(a',k',l',\mathbf{a}',b')} = \begin{cases} \binom{n+a-2k}{i-k}^{-\frac{1}{2}} \binom{n+a-2k}{j-k}^{-\frac{1}{2}} \alpha(i,j,t,p,a,k) & \text{if } a = a', \ k = k', \ \mathbf{a} = \mathbf{a}', \ b = b' \text{ and} \\ l = i, \ l' = j, \\ 0 & \text{otherwise.} \end{cases}$$
(34)

This implies

### **Proposition 7.** The matrix U gives a block-diagonalisation of $\mathcal{A}_{q,n}$ .

Proof. Equation (34) implies that each matrix  $\tilde{M}_{i,j}^{t,p}$  has a block-diagonal form, where for each pair (a,k) there are  $\binom{n}{a}(q-2)^{a}\left[\binom{n-a}{k-a} - \binom{n-a}{n-a-1}\right]$  copies of an  $(n+a+1-2k) \times (n+a+1-2k)$  block on the diagonal. For fixed a, k the copies are indexed by the pairs  $(\mathbf{a}, b)$  such that  $\mathbf{a} \in \mathbf{q}^{n}$  satisfies  $|S(\mathbf{a})| = a$ ,  $\mathbf{a}_{v} \neq q-1$  for  $v = 1, \ldots, n$ , and  $b \in B_{k-a}^{\overline{S(a)}}$ , and in each copy the rows and columns in the block are indexed by the integers i with  $k \leq i \leq n+a-k$ . Hence we need to show that all matrices of this block-diagonal form are in  $U^*\mathcal{A}_{q,n}U$ . It suffices to show that the dimension  $\sum_{0\leq a\leq k\leq n+a-k}(n+a+1-2k)^2$  of the algebra consisting of the matrices in the given block-diagonal form equals the dimension of  $\mathcal{A}_{q,n}$ , which is  $\binom{n+4}{4}$ . This follows from

$$\sum_{0 \le a \le k \le n+a-k} (n+a+1-2k)^2$$

$$= \sum_{a=0}^n \sum_{k=a}^{\lfloor \frac{n+a}{2} \rfloor} (n+a+1-2k)^2$$

$$= \sum_{a\equiv n(2)} (1^2+3^2+\dots+(n+1-a)^2) + \sum_{a \ne n(2)} (2^2+4^2+\dots+(n+1-a)^2)$$

$$= \sum_{a\equiv n(2)} \binom{n+1-a+2}{3} + \sum_{a \ne n(2)} \binom{n+1-a+2}{3}$$

$$= \sum_{a=0}^n \binom{n-a+3}{3} = \binom{n+4}{4}.$$
(35)

## 3 Application to coding

Let  $C \subseteq \mathbf{q}^n$  be any code. For any automorphism  $\pi$ , denote the characteristic vector of  $\pi(C)$  by  $\chi^{\pi(C)}$  (taken as a columnvector). For any word  $\mathbf{x} \in \mathbf{q}^n$ , let  $\sigma_{\mathbf{x}} \in \operatorname{Aut}(q, n)$  be any automorphism with  $\sigma_{\mathbf{x}}(\mathbf{x}) = \mathbf{0}$ , and define

$$R_{\mathbf{x}} := |\operatorname{Aut}_{\mathbf{0}}(q, n)|^{-1} \sum_{\pi \in \operatorname{Aut}_{\mathbf{0}}(q, n)} \chi^{\pi(\sigma_{\mathbf{x}}(C))} (\chi^{\pi(\sigma_{\mathbf{x}}(C))})^{\mathsf{T}}.$$
(36)

Next define the matrices R and R' by:

$$R := |C|^{-1} \sum_{\mathbf{x} \in C} R_{\mathbf{x}},$$

$$R' := (q^n - |C|)^{-1} \sum_{\mathbf{x} \in \mathbf{q}^n \setminus C} R_{\mathbf{x}}.$$

$$(37)$$

As the  $R_{\mathbf{x}}$ , and hence also R and R', are convex combinations of positive semidefinite matrices, they are positive semidefinite. By construction, the matrices  $R_{\mathbf{x}}$ , and hence the matrices Rand R' are invariant under permutations  $\pi \in \operatorname{Aut}_{\mathbf{0}}(q, n)$  of the rows and columns and hence they are elements of the algebra  $\mathcal{A}_{q,n}$ . Write

$$R = \sum_{(i,j,t,p)} x_{i,j}^{t,p} M_{i,j}^{t,p}.$$
(38)

We can express the matrix R' in terms of the coefficients  $x_{i,j}^{t,p}$  as follows.

**Proposition 8.** The matrix R' is given by

$$R' = \frac{|C|}{q^n - |C|} \sum_{(i,j,t,p)} (x_{i+j-t-p,0}^{0,0} - x_{i,j}^{t,p}) M_{i,j}^{t,p}.$$
(39)

Proof. The matrix

$$S := |C|R + (q^n - |C|)R' = |\operatorname{Aut}_{\mathbf{0}}(q, n)|^{-1} \sum_{\sigma \in \operatorname{Aut}(q, n)} \chi^{\sigma(C)}(\chi^{\sigma(C)})^{\mathsf{T}}$$
(40)

is invariant under permutation of the rows and columns by permutations  $\sigma \in Aut(q, n)$  and hence is an element of the Bose–Mesner algebra, say

$$S = \sum_{k} y_k A_k. \tag{41}$$

Note that for any  $\mathbf{y} \in \mathbf{q}^n$  with  $|S(\mathbf{y})| = k$ , we have

$$y_k = (S)_{\mathbf{y},\mathbf{0}} = |C|(R)_{\mathbf{y},\mathbf{0}} = |C|x_{k,0}^{0,0},$$

since  $(R')_{\mathbf{y},\mathbf{0}} = 0$ . Hence we have

$$(q^{n} - |C|)R' = S - |C|R$$

$$= \sum_{k} |C|x_{k,0}^{0,0}A_{k} - |C| \sum_{(i,j,t,p)} x_{i,j}^{t,p}M_{i,j}^{t,p}$$

$$= |C| \sum_{k} \sum_{i+j-t-p=k} (x_{k,0}^{0,0} - x_{i,j}^{t,p})M_{i,j}^{t,p}$$

$$= |C| \sum_{(i,j,t,p)} (x_{i+j-t-p,0}^{0,0} - x_{i,j}^{t,p})M_{i,j}^{t,p},$$
(42)

which proves the proposition.

Using the block-diagonalisation of  $\mathcal{A}(n,d)$ , the positive semidefiniteness of R and R' is

equivalent to:

for all 
$$a, k$$
 with  $0 \le a \le k \le n + a - k$ , the matrices (43)  

$$\left(\sum_{t,p} \alpha(i, j, t, p, a, k) x_{i,j}^{t,p}\right)_{i,j=k}^{n+a-k}$$
and
$$\left(\sum_{t,p} \alpha(i, j, t, p, a, k) (x_{i+j-t-p,0}^{0,0} - x_{i,j}^{t,p})\right)_{i,j=k}^{n+a-k}$$
are positive semidefinite.

Define the numbers

$$\lambda_{i,j}^{t,p} := |(C \times C \times C) \cap X_{i,j,t,p}|, \tag{44}$$

for  $(i, j, t, p) \in \mathcal{I}(q, n)$ , and let

$$\gamma_{i,j}^{t,p} := |(\{\mathbf{0}\} \times \mathbf{q}^n \times \mathbf{q}^n) \cap X_{i,j,t,p}|$$
(45)

be the number of nonzero entries of  $M_{i,j}^{t,p}$ . A simple calculation yields:

$$\gamma_{i,j}^{t,p} = (q-1)^{i+j-t} (q-2)^{t-p} \binom{n}{p, t-p, i-t, j-t}.$$
(46)

The numbers  $x_{i,j}^{t,p}$  can be expressed in terms of the the numbers  $\lambda_{i,j}^{t,p}$  as follows.

**Proposition 9.**  $x_{i,j}^{t,p} = (|C|\gamma_{i,j}^{t,p})^{-1}\lambda_{i,j}^{t,p}$ .

*Proof.* Denote by  $\langle M, N \rangle := \operatorname{tr}(M^*N)$  the standard innerproduct on the space of complex  $\mathbf{q}^n \times \mathbf{q}^n$  matrices. Observe that the matrices  $M_{i,j}^{t,p}$  are pairwise orthogonal and that  $\left\langle M_{i,j}^{t,p}, M_{i,j}^{t,p} \right\rangle = \gamma_{i,j}^{t,p}$  for  $(i, j, t, p) \in \mathcal{I}(q, n)$ . Hence

$$\left\langle R, M_{i,j}^{t,p} \right\rangle = \frac{1}{|C|} \sum_{\mathbf{x} \in C} \left\langle R_{\mathbf{x}}, M_{i,j}^{t,p} \right\rangle$$

$$\tag{47}$$

$$= \frac{1}{|C|} \sum_{\mathbf{x} \in C} |(\{\mathbf{x}\} \times C \times C) \cap X_{i,j,t,p}|$$

$$= \frac{1}{|C|} \lambda_{i,p}^{t,p}$$
(48)

$$\frac{1}{|C|}\lambda_{i,j}^{t,p}$$

implies that

$$R = \frac{1}{|C|} \sum_{(i,j,t,p) \in \mathcal{I}(q,n)} \lambda_{i,j}^{t,p} (\gamma_{i,j}^{t,p})^{-1} M_{i,j}^{t,p}.$$
(49)

Comparing the coefficients of the  $M_{i,j}^{t,p}$  with those in (38) proves the proposition.

The  $x_{i,j}^{t,p}$  satisfy the following linear constraints, where (iv) holds if C has minimum distance at least d:

(i) 
$$x_{0,0}^{0,0} = 1$$
 (50)  
(ii)  $0 \le x_{i,j}^{t,p} \le x_{i,0}^{0,0}$   
(iii)  $x_{i,j}^{t,p} = x_{i',j'}^{t',p'}$  if  $t - p = t' - p'$  and  
 $(i, j, i + j - t - p)$  is a permutation of  $(i', j', i' + j' - t' - p')$   
(iv)  $x_{i,j}^{t,p} = 0$  if  $\{i, j, i + j - t - p\} \cap \{1, 2, \dots, d - 1\} \neq \emptyset$ .

Here conditions (iii) and (iv) follow from Proposition 9. Condition (ii) follows from  $x_{i,0}^{0,0} = x_{i,i}^{i,i}$ and the fact that if  $M = \chi^{\sigma(C)}(\chi^{\sigma(C)})^{\mathsf{T}}$  then  $0 \leq M_{\mathbf{x},\mathbf{y}} \leq M_{\mathbf{x},\mathbf{x}}$  for any  $\mathbf{x}, \mathbf{y} \in \mathbf{q}^n$  and  $\sigma \in \operatorname{Aut}(q, n)$ .

Since  $|C|^2 = \sum_i \lambda_{i,0}^{0,0}$ , we have  $|C| = \sum_i \gamma_{i,0}^{0,0} x_{i,0}^{0,0}$ . Hence if we view the  $x_{i,j}^{t,p}$  as variables, then maximizing  $\sum_i \gamma_{i,0}^{0,0} x_{i,0}^{0,0}$  subject to conditions (50) and (43) yields an upper bound on  $A_q(n,d)$ . This is a semidefinite programming problem with  $O(n^4)$  variables, and can be solved in time polynomial in n.

In the range  $n \leq 16$ ,  $n \leq 12$  and  $n \leq 11$ , the method gives a number of new upper bounds on  $A_3(n,d)$ ,  $A_4(n,d)$  and  $A_5(n,d)$  respectively, summarized in Table 1, 2 and 3 below (cf. the tables given by Brouwer, Hämäläinen, Östergård and Sloane [4], by Bogdanova, Brouwer, Kapralov and Östergård [2] and by Bogdanova and Östergård [3]).

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		best		best upper	
		lower	new	bound	
		bound	upper	previously	Delsarte
n	d	known	bound	known	bound
12	4	4374	6839	7029	7029
13	4	8019	19270	19682	19683
14	4	24057	54774	59046	59049
15	4	72171	149585	153527	153527
16	4	216513	424001	434815	434815
12	5	729	1557	1562	1562
13	5	2187	4078	4163	4163
14	5	6561	10624	10736	10736
15	5	6561	29213	29524	29524
13	6	729	1449	1562	1562
14	6	2187	3660	3885	4163
15	6	2187	9904	10736	10736
16	6	6561	27356	29524	29524
14	7	243	805	836	836
15	7	729	2204	2268	2268
16	7	729	6235	6643	6643
13	8	42	95	103	103
15	8	243	685	711	712
16	8	297	1923	2079	2079
14	9	31	62	66	81
15	9	81	165	166	166
16	10	54	114	117	127

Table 1: New upper bounds on  $A_3(n, d)$ 

		$\mathbf{best}$		best upper	
		lower	new	bound	
		bound	upper	previously	Delsarte
n	d	known	bound	known	bound
7	4	128	169	179	179
8	4	320	611	614	614
9	4	1024	2314	2340	2340
10	4	4096	8951	9360	9362
10	5	1024	2045	2048	2145
10	6	256	496	512	512
11	6	1024	1780	2048	2048
12	6	4096	5864	6241	6241
12	7	256	1167	1280	1280

Table 2: New upper bounds on  $A_4(n,d)$ 

Table 3: New upper bounds on  $A_5(n,d)$ 

		best		best upper	
		lower	new	bound	
		bound	upper	previously	Delsarte
n	d	known	bound	known	bound
7	4	250	545	554	625
7	5	53	108	125	125
8	5	160	485	554	625
9	5	625	2152	2291	2291
10	5	3125	9559	9672	9672
11	5	15625	44379	44642	44642
10	6	625	1855	1875	1875
11	6	3125	8840	9375	9375