

DISTANCE DISTRIBUTIONS AND ENERGY OF DESIGNS IN HAMMING SPACES

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ABSTRACT. We obtain new combinatorial upper and lower bounds for the potential energy of designs in q -ary Hamming space. Combined with results on reducing the number of all feasible distance distributions of such designs this gives reasonable good bounds. We compute and compare our lower bounds to recently obtained universal lower bounds. Some examples in the binary case are considered.

1. Introduction. Let $Q = \{0, 1, \dots, q-1\}$ be an alphabet of q symbols and $\mathbb{H}(n, q)$ be the set of all q -ary vectors $x = (x_1, x_2, \dots, x_n)$ over Q . The Hamming distance $d(x, y)$ between points $x = (x_1, x_2, \dots, x_n)$ and $y = (y_1, y_2, \dots, y_n)$ from $\mathbb{H}(n, q)$ is equal to the number of coordinates in which they differ. The use

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of q suggests that the alphabet is a finite field and most coding theory applications assume this but we will not make use of a field structure. In particular q is not necessarily a power of a prime. We refer to a finite set $C \subset \mathbb{H}(n, q)$ as a *code*.

We consider $\mathbb{H}(n, q)$ as a polynomial metric space (see, for example, [11, 9, 12]). Thus it is convenient to use the inner¹ product $\langle x, y \rangle := 1 - \frac{2d(x, y)}{n}$ instead of the Hamming distance. We denote $T = \{t_0, t_1, \dots, t_n\}$, where $t_i := 1 - \frac{2i}{n}$, $i = 0, 1, \dots, n$, are all possible values of inner products in $\mathbb{H}(n, q)$, written in decreasing order.

Definition 1.1. *For any $x \in C \subset \mathbb{H}(n, q)$ the distance distribution of C with respect to x is the ordered $(n + 1)$ -tuple $P(x) = (p_0(x), p_1(x), \dots, p_n(x))$, where $p_i(x) = |\{y \in C : \langle x, y \rangle = t_i\}|$, $i = 0, 1, \dots, n$, is the number of the points of C at distance i to x .*

It is a common approach to use distance distributions of C for investigation of the structure and properties of the code. In this paper we are interested in a special class of codes, called designs, which approximate in certain sense the whole space $\mathbb{H}(n, q)$.

Definition 1.2. *Let τ and λ be positive integers. A τ -design $C \subset \mathbb{H}(n, q)$ of strength τ and index λ is a code such that the $M \times n$ matrix obtained from the codewords of C as rows has the following property: every $M \times \tau$ submatrix contains all ordered τ -tuples of $\mathbb{H}(\tau, q)$, each one exactly $\lambda = \frac{M}{q^\tau}$ times as rows. We denote C by $(n, M; \tau)$.*

Example 1.3. The code $C_1 = \{0000, 0011, 1010, 0101, 1001, 0110, 1100, 1111\} \subset \mathbb{H}(4, 2)$ is a 3-design of cardinality 8 and index 1. The distance distributions of C_1 with respect to every point $x \in C_1$ is the same $P(x) = (1, 0, 6, 0, 1)$. The code $C_2 = \{0000, 1011, 0010, 0101, 1001, 1110, 0111, 1100\} \subset \mathbb{H}(4, 2)$ is another $(4, 8; 3)$ design with distance distributions $P(x) = (1, 1, 3, 3, 0)$ for every $x \in C_2$.

Designs of strength τ in $\mathbb{H}(n, q)$ are also called orthogonal arrays of strength τ (see [8], the book [10] and references therein) or τ -wise independent sets [1]. Defining designs by codes as in Definition 1.2. underlines that no repetition of codewords is allowed, which is not usually assumed for orthogonal arrays.

¹In fact this is not an inner product but plays for our purposes an analogous role to the standard inner product on the unit Euclidean sphere \mathbb{S}^{n-1} and we prefer to call it inner product.

For any function $h(t) : [-1, 1) \rightarrow (0, +\infty)$ we consider the h -energy (or potential energy) of $C \subset \mathbb{H}(n, q)$ defined by

$$\mathcal{E}(n, C; h) = \frac{1}{|C|} \sum_{x, y \in C, x \neq y} h(\langle x, y \rangle).$$

The function h is called potential function. Now the problems of minimizing and maximizing the potential energy provided the function h , the length n , the strength τ and the cardinality $|C| = M = \lambda q^\tau$ are fixed arise naturally. We wish to determine or estimate the quantities

$$(1) \quad \mathcal{L}(n, M; \tau; h) := \min\{\mathcal{E}(n, C; h) : C \text{ is an } (n, M; \tau) \text{ design}\},$$

and

$$(2) \quad \mathcal{U}(n, M; \tau; h) := \max\{\mathcal{E}(n, C; h) : C \text{ is an } (n, M; \tau) \text{ design}\}.$$

The quantities $\mathcal{U}(n, M; \tau; h)$ and $\mathcal{L}(n, M; \tau; h)$ depend (more or less) on the structure of the designs under consideration. Our approach looks inside the structure using a method for calculation and investigation of all possible distance distributions of designs in $\mathbb{H}(n, 2)$ proposed in [4, 5] and its generalization to the q -ary case. This allows us to obtain combinatorial-type upper bounds on $\mathcal{U}(n, M; \tau; h)$ and lower bounds on $\mathcal{L}(n, \tau, M; h)$. Our bounds are easy for calculation once the number of possible distance distributions is reduced. In the binary case we compare our bounds to recently obtained analytic bounds from [7, 3] and to the actual energies of known configurations.

2. Distance distributions and their energy. It is straightforward to connect the energy of C to its distance distributions.

Definition 2.1. If $x \in C$ has distance distribution $P(x) = (p_0(x), p_1(x), \dots, p_n(x))$ then $\mathcal{E}(x, C; h) := \frac{1}{|C|} \sum_{i=1}^n p_i(x)h(t_i)$ is called energy of the distance distribution $P(x)$ or energy of x in C .

Theorem 2.2. Let $C = (n, M; \tau)$ and $P_1(x_1), P_2(x_2), \dots, P_s(x_s)$ be all distinct distance distributions of points of C , appearing k_1, k_2, \dots, k_s times, respectively. Then the energy of C is $\mathcal{E}(n, C; h) = \sum_{i=1}^s k_i \mathcal{E}(x_i, C; h)$. In other words, we have

$$\mathcal{E}(n, C; h) \in \mathcal{E}(M) := \left\{ \sum_{k_1+k_2+\dots+k_s=M} k_i \mathcal{E}(x_i, C; h) \right\}.$$

Proof. It follows from Definition 2.1 that $\mathcal{E}(n, C; h) = \sum_{x \in C} \mathcal{E}(x, C; h)$.

Taking into account the multiplicities we obtain the desired formula. \square

Small values of the number of distinct distributions s are particularly interesting because in this case the set $\mathcal{E}(M)$ has relatively small size. Clearly, the problem of finding all possible distance distributions for fixed n , M and τ is finite but hard. However, their number can be reasonably small when τ is relatively close to n (see [4, 5] for the binary case). This is one of key motivations behind our bounds.

Example 2.3. Continuing Example 1.3 we see that $\mathcal{E}(4, C_1; h) = 8\mathcal{E}(x, C; h)$ where $x \in C_1$ and $\mathcal{E}(4, C_2; h) = 8\mathcal{E}(x, C; h)$ where $x \in C_2$. We will see below that these two energy levels give the exact values of $\mathcal{L}(4, 8; 3; h)$ and $\mathcal{U}(4, 8; 3; h)$, respectively, in $\mathbb{H}(4, 2)$.

3. Computing distance distributions. An equivalent definition of a τ -design (cf. [12]) is convenient for the so-called polynomial techniques. Let

$$K_i^{(n,q)}(d) = \sum_{j=0}^i (-1)^j (q-1)^{i-j} \binom{d}{j} \binom{n-d}{i-j}, \quad i = 0, 1, \dots, n,$$

be the Krawtchouk polynomials corresponding to $\mathbb{H}(n, q)$ and

$$Q_i^{(n,q)}(t) = \frac{1}{r_i} K_i^{(n,q)}(n(1-t)/2),$$

be a normalization of the Krawtchouk polynomials ([12, Section 6.2]) and $r_i = (q-1)^i \binom{n}{i}$.

Every real polynomial $f(t)$ of degree at most n is uniquely expanded in terms of the polynomials $Q_i^{(n,q)}(t)$, i.e.,

$$(3) \quad f(t) = \sum_{i=0}^n f_i Q_i^{(n,q)}(t)$$

for well defined coefficients f_i , $0 \leq i \leq n$.

Definition 3.1. A code $C \subset \mathbb{H}(n, q)$ is a τ -design if and only if every real polynomial $f(t)$ of degree at most τ and every point $x \in \mathbb{H}(n, q)$ satisfy

$$(4) \quad \sum_{y \in C} f(\langle x, y \rangle) = f_0 |C|,$$

where f_0 is the first coefficient in the expansion (3).

It is well known (see, for example [12, Sections 3 and 5]) that Definition 3.1 allows calculation of distance distributions with at most $\tau + 1$ non-zero entries. Indeed, for a fixed $x \in C$, Definition 3.1 easily gives a system of $\tau + 1$ linear equations for the distance distribution of C with respect to x . We can go further – it is clear that the problem is finite and for relatively small parameters this system can be resolved completely (see [4] for the binary case).

Denote $t^j = \sum_{i=0}^n f_{i,j}^{(q)} Q_i^{(n,q)}(t)$ for $j \in \{0, 1, \dots, n\}$. In fact, we are interested below only in the coefficient $f_{0,j}^{(q)}$. We have explicit formula for $q = 2$,

$$(5) \quad f_{0,i}^{(2)} = \begin{cases} 0, & \text{if } i = 2j + 1 \\ \frac{1}{2^n} \sum_{d=0}^n \left(1 - \frac{2d}{n}\right)^{2j} \binom{n}{d}, & \text{if } i = 2j \end{cases} .$$

The next assertion is folklore.

Theorem 3.2. *Let $C \subset \mathbb{H}(n, q)$ be an $(n, |C|; \tau)$ design. Then the distance distribution of C with respect to x satisfies the following system of linear equations*

$$(6) \quad \sum_{j=1}^n p_j(x) t_j^i = f_{0,i}^{(q)} |C| - 1, \quad i = 0, 1, \dots, \tau.$$

Proof. Set $f(t) = t^i, i = 0, 1, \dots, \tau$, in (4). \square

Thus we may consider the system (6) as having $\tau + 1$ equations and n non-negative integer unknowns. Then we choose $n - \tau - 1$ unknowns to be free and resolve (6) with respect to the remaining $n - (n - \tau - 1) = \tau + 1$ unknowns. Now we plug all possible values of the free unknowns and check whether the solution consists of non-negative integers. For example, in the binary case one has only two possibilities for $p_n(x)$ – it is 1 or 0 (depending on whether the antipodal point of x belongs to C or not).

The set of feasible distance distributions can be further reduced as shown in the binary case in [5]. There are many examples when we remain with several possibilities. This underlines the importance of the description of Theorem 2.2 and the bounds from Theorems 4.1 and 4.2 below.

Example 3.3. (Continuation of Examples 1.3 and 2.3) We obtain by Theorem 3.2 that every $(4, 8; 3)$ design in $\mathbb{H}(4, 2)$ can have only two distance distributions: $(1, 0, 6, 0, 1)$ and $(1, 1, 3, 3, 0)$.

4. Combinatorial upper bounds on $\mathcal{U}(n, M; \tau; h)$ and lower bounds on $\mathcal{L}(n, M; \tau; h)$. In this section we assume that the parameters n , τ and $M = |C|$ are such that all distance distributions of points of C can be effectively computed. Usually additional investigations allow further reduction of their number – many examples are given in [4, 5]. Assume that $P_1(x_1), P_2(x_2), \dots, P_s(x_s)$ are all possible (but not necessarily realized) distinct distance distributions of C with respect to its points computed from Theorem 3.2. Note that these distributions depend on n , τ and $M = |C|$ only; in other words, every τ -design in $\mathbb{H}(n, q)$ of M points can have distance distributions only from the set $\{P_i(x_i)\}$. Denote

$$w = \min\{\mathcal{E}(x_i, C; h) : i \in \{1, 2, \dots, s\}\}$$

and

$$W = \max\{\mathcal{E}(x_i, C; h) : i \in \{1, 2, \dots, s\}\}.$$

We are already in a position to state the general form of our combinatorial bounds on the energy of τ -designs of M points in $\mathbb{H}(n, q)$.

Theorem 4.1. *Let w and W be the minimum and maximum, respectively, of the possible energies of a distance distribution of τ -designs in $\mathbb{H}(n, q)$ of M points. Then*

$$Mw \leq \mathcal{L}(n, M; \tau; h) \leq \mathcal{U}(n, M; \tau; h) \leq MW.$$

Proof. Let C be a τ -design with distance distributions described as above. Then we have $\mathcal{E}(n, C; h) = \sum_{i=1}^s k_i \mathcal{E}(x_i, C; h) \geq Mw$ for the energy of C . Since the same inequality holds for every C , we conclude that $\mathcal{L}(n, M; \tau; h) \geq Mw$ as required. The estimation $\mathcal{U}(n, M; \tau; h) \leq MW$ follows similarly. \square

Theorem 4.1 defines a strip where the energies of all (n, M, τ) designs in $\mathbb{H}(n, q)$ must belong. Our continued example shows that both limits of this strip can be achieved for the same minimum distance d , length n , cardinality M and strength τ but by inequivalent designs.

Example 4.2. (Continuation of Examples 1.3, 2.3 and 3.3) Consider again the 3-designs C_1 and C_2 in $\mathbb{H}(4, 2)$ and assume that $\mathcal{E}(4, C_1; h) < \mathcal{E}(4, C_2; h)$ for some h . Then

$$\mathcal{L}(4, 8; 3; h) = \mathcal{E}(4, C_1; h) = 8P_1$$

and

$$\mathcal{U}(4, 8; 3; h) = \mathcal{E}(4, C_2; h) = 8P_2,$$

where P_1 and P_2 are the energies of the distance distributions $(1, 0, 6, 0, 1)$ and $(1, 1, 3, 3, 0)$, respectively.

We also note that two non-isomorphic $(5, 16; 4)$ designs in $\mathbb{H}(5, 2)$ provide a situation very similar to Example 4.2.

We next underline the special case where the strip becomes a point, i.e., the upper and lower bounds coincide and the corresponding designs have optimal (simultaneously minimum and maximum) energy.

Corollary 4.3. *Let the parameters q, n, M and τ be such that every $(n, M; \tau)$ design in $\mathbb{H}(n, q)$ has the same (unique) distance distribution $P = P(x)$, $x \in C$, with respect to all its points. Then, for every potential function h , these designs have optimal energy*

$$\mathcal{E}(n, C; h) = \mathcal{L}(n, M; \tau; h) = \mathcal{U}(n, M; \tau; h) = M\mathcal{E}(x, C; h).$$

There are several trivial cases where Corollary 4.3 gives optimal designs. Other, more complicated examples will be discussed elsewhere.

In the end of this section we underline the wide applicability of our combinatorial bounds. Most applications (cf. [7, 3]) require a special type of potentials h (mainly absolute monotonicity of h on $[-1, 1)$; i.e., one has $h^{(k)}(t) \geq 0$ for all $k \geq 0$ and all $t \in [-1, 1)$) in contrast to our bounds which are valid for all potential functions h . On the other hand, we are usually restricted to designs of good strength in order to obtain substantial reduction of the possible distance distributions. The evaluation of our combinatorial bounds could also be interesting if the lower bounds are close to the analytic bounds (see the next section and [7, 3]).

5. Comparison to known bounds and known designs. We compare our bounds to the actual energies of known designs and to a recently obtained universal lower bound on energy of codes in $\mathbb{H}(n, q)$ [3]. We in fact inspected the binary case $q = 2$ for strengths $\tau = 4$ and 5 in the ranges $4 \leq n \leq 17$ and $1 \leq \lambda \leq 10$.

5.1. Comparison to lower bounds for codes in $\mathbb{H}(n, q)$. We proceed with the formulation of the bound from [3]. For fixed alphabet size q , strength τ and dimension n denote

$$B(n, \tau) = \min\{|C| : \exists \tau\text{-design } C \subset \mathbb{H}(n, q)\}.$$

Then a well known bound by Rao [14] states that

$$B(n, \tau) \geq R(n, \tau) = \begin{cases} q \sum_{i=1}^{k-1} \binom{n-1}{i} (q-1)^i, & \text{if } \tau = 2k-1, \\ \sum_{i=1}^k \binom{n}{i} (q-1)^i, & \text{if } \tau = 2k. \end{cases}$$

For every $M \in (R(n, 2k-1), R(n, 2k)]$ we solve the equation

$$(7) \quad P_k(t)P_{k-1}(s) - P_k(s)P_{k-1}(t) = 0,$$

where

$$P_i(t) = \frac{K_i^{(n-1,q)}(-1 + n(1-t)/2)}{\sum_{j=0}^i \binom{n}{j} (q-1)^j}, \quad i = k, k-1$$

and s is determined from the equation $M = L_\tau(n, s)$, where $L_\tau(n, s)$ is the Levenshtein bounds on the maximal cardinality of codes of prescribed length and minimum distance, see [11, 12]. In fact, the equation (7) has the same roots as $M = L_\tau(n, s)$.

The equation (7) has simple roots $\alpha_0, \alpha_1, \dots, \alpha_{k-1} = s$ such that $-1 < \alpha_0 < \alpha_1 < \dots < \alpha_{k-1} = s < 1$. Then [3, Theorem 6] gives

$$(8) \quad \mathcal{L}(n, M; 2k-1; h) \geq M \sum_{i=0}^{k-1} \rho_i h(\alpha_i),$$

where the weights $\rho_i, i = 0, 1, \dots, k-1$, are positive. Different formulas for ρ_i can be found in [2, 11, 12].

Similarly, for every $M \in (R(n, 2k), R(n, 2k+1)]$ we have the bound

$$(9) \quad \mathcal{L}(n, M; 2k; h) \geq M \sum_{i=0}^k \gamma_i h(\beta_i),$$

where $\beta_0 = -1$ and $\beta_1, \dots, \beta_k = s$ are (in increasing order) the roots of the equation

$$(10) \quad (1+t)(P_k(t)P_{k-1}(s) - P_k(s)P_{k-1}(t)) = 0,$$

where

$$P_i(t) = \frac{K_i^{(n-2,q)}(-1 + n(1-t)/2)}{\sum_{j=0}^i \binom{n-1}{j} (q-1)^j}, \quad i = k, k-1.$$

We compared the bounds from Theorem 4.1 to the bounds from (8) and (9) for the following three potentials

$$(11) \quad h_1(t) = \frac{2}{n(1-t)},$$

$$(12) \quad h_n(t) = \left(\frac{2}{n(1-t)} \right)^{(n-2)/2},$$

$$(13) \quad h_{n,\tau}(t) = \binom{n - n(1-t)/2}{\tau + 1},$$

where $\binom{x}{k} := \frac{x(x-1)\dots(x-k+1)}{k!}$ for integer $k \geq 0$ and real x .

In all cases the computational results give lower bounds from Theorem 4.1 equal to or better than the corresponding bound from (8) and (9). We illustrate this with a description of the situation for length $n = 9$, strength $\tau = 4$ and cardinalities 96, 112 and 128.

Example 5.1. The existence/nonexistence of $(9, 96; 4)$ designs is still undecided [10, Table 12.1], [6]. There are 9 possible distance distributions with different energies. Theorem 4.1 gives the following bounds for $h_1(t)$

$$(14) \quad 23.289 < \mathcal{L}(9, 96; 4; h_1) \leq \mathcal{U}(9, 96; 4; h_1) < 23.417,$$

while the bound (9) is $\mathcal{L}(9, 96; 4; h_1) > 23.192$. Similarly, we have

$$(15) \quad 27.394 < \mathcal{L}(9, 112; 4; h_1) \leq \mathcal{U}(9, 112; 4; h_1) < 27.760,$$

and the bound (9) is $\mathcal{L}(9, 112; 4; h_1) > 27.246$.

Our comparison shows that the combinatorial lower bounds are good even in case of many possible distance distributions. This opens room for discussion whether and how far the realizations of designs tend to choose minimal energy levels. We expect that dropping the design property will allow better energies in many cases.

5.2. Comparison to actual energies. In this subsection we compare our bounds with the actual energies of designs taken from several known libraries of good orthogonal arrays (see, for example [13] and the rich connections from there).

Example 5.2. (continuation of Example 5.1) There exist $(9, 128; 4)$ designs [10, Table 12.1], [13]. The explicit versions $C = (9, 128; 4)$ have energy

$\mathcal{E}(9, C; h_1) \approx 31.644$ which is close to the lower bound from Theorem 4.1, where we have

$$(16) \quad 31.493 < \mathcal{L}(9, 128; 4; h_1) \leq \mathcal{U}(9, 128; 4; h_1) < 32.245.$$

The bound (9) in this case gives $\mathcal{L}(9, 128; 4; h_1) > 31.303$. We note that despite having many possible distance distributions the lower and upper bounds remain close.

Further bounds on the h -energy of certain designs for the potential functions (11) are given in the table below. We exhibit together cases where designs are known to exist and cases where the existence is still undecided (noted by a question mark in the table).

Table. Energy bounds for some binary $(n, M; \tau)$ -designs.

	(8, 12; 2), exists				(12, 24; 3), exists			
$h(t)$	(8) or (9)	Thm 4.1, lower	existing	Thm 4.1, upper	(8) or (9)	Thm 4.1, lower	existing	Thm 4.1, upper
h_1	2.575	2.600	2.605	2.616	3.75	3.75	3.75	3.75
h_n	0.1430	0.1594	0.1625	0.1689	0.2833	0.2833	0.2833	0.2833
$h_{n,\tau}$	33.6	37	37.333	38	330	330	330	330
	(10, 112; 4), existence undecided				(12, 128; 4), exists			
$h(t)$	(8) or (9)	Thm 4.1, lower	existing	Thm 4.1, upper	(8) or (9)	Thm 4.1, lower	existing	Thm 4.1, upper
h_1	24.153	24.233	?	24.3965	22.627	22.665	22.695, 22.705	22.727
h_n	0.389	0.433	?	0.5846	0.039	0.043	0.048, 0.050	0.054
$h_{n,\tau}$	620.869	639	?	650	2381.08	2410	2420, 2424	2429
	(11, 224; 5), existence undecided				(13, 256; 5), exists			
$h(t)$	(8) or (9)	Thm 4.1, lower	existing	Thm 4.1, upper	(8) or (9)	Thm 4.1, lower	existing	Thm 4.1, upper
h_1	24.153	44.523	?	44.632	42.2553	42.29	42.3114	42.3217
h_n	0.3215	0.3524	?	0.4625	0.0293	0.032	0.0358	0.0376
$h_{n,\tau}$	1156.47	1176	?	1186	5190.55	5236	5244	5248

6. List of programs. All calculations in this paper were performed by programs in Maple. In particular, we have developed programs for:

- (1) calculation of all feasible distance distributions via Theorem 3.2 in all spaces $\mathbb{H}(n, q)$;
- (2) reducing the number of the possible distance distributions in the binary and ternary cases for a large variety of values of n , M and τ using the algorithms from [5, 6];

(3) calculation of the universal bounds (8) and (9), the set $\mathcal{E}(M)$ from Theorem 2.2;

(4) calculation of actual energies for given designs and potential functions.

We have also developed some *ad hoc* programs for smaller concrete problems.

All programs and numerical results are available upon request.

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