Maximum volume simplices and trace-minimal graphs

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Abstract

Let (v, δ) be the set of all δ-regular graphs on v vertices. A graph $G \in (v, \delta)$ is *trace-minimal* in (v, δ) if the vector whose ith entry is the trace of the ith power of the adjacency matrix of G, is minimum under the lexicographic order among all such vectors corresponding to graphs in (v, δ). We consider the problem of maximizing the volume of an n-dimensional simplex consisting of $n+1$ vertices of the unit hypercube in ^{m}. We show that if $n \equiv -1 \pmod 4$, such a maximum can be explicitly evaluated for all m large enough whenever an appropriate trace-minimal graph is known.

Keywords: volumes of simplices, regular graph, girth, generalized polygons.

1. The problem

We consider the problem of maximizing the n-dimensional volume of a simplex S consisting of $n+1$ vertices of the unit hypercube in ^{m}. Without loss of generality we assume that the origin is a vertex of S.

Let $M_{m,n}(0,1)$ be the set of all $m \times n$ matrices all of whose entries are either 0 or 1. If X is the matrix in $M_{m,n}(0,1)$ whose columns are the coordinates of the n vertices of S distinct to the origin, then the n-dimensional volume of S is equal to $\frac{1}{n!}\sqrt{\det X^T X}$. See [1]. Let

$$G(m,n) = \max\{\det X^T X : X \in M_{m,n}(0,1)\}.$$

Hence, our problem is reduced to determine $G(m,n)$ for each pair of positive integers m, n. If $m < n$ then $\det X^T X = 0$, so we will assume throughout that $m \geq n$.

This problem also arises in a statistical setting, which dates back to 1935 [2] and the 1940s [3] [4]. In this context the rows of $X \in M_{m,n}(0,1)$ play the central role. The goal is to estimate the weights of n objects using a single-pan (spring) scale. We do not assume that the scale is accurate, its errors have a distribution. Several objects are placed on the scale at once and their total weight is noted. The information about which objects are placed on the scale is encoded as a $(0,1)$-n-tuple whose jth coordinate is 1 if object j is included in the weighing and 0 if not. The weights of n objects cannot be reasonably estimated in fewer than n weighings. With m weighings the corresponding $(0,1)$-n-tuples form the rows of an $m \times n$ *design matrix* X. Certain design matrices give better estimates of the weights of the n objects than others. Those with the property that $\det X^T X = G(m,n)$ are called *D-optimal*. Under certain assumptions about the distribution of errors of the scale, D-optimal design matrices give confidence regions for the n-tuple of weights of the objects that have minimum volume. There are other standards for evaluating the efficiency of a design matrix such as A-optimality which corresponds to a design matrix X for which $\mathrm{tr}(X^T X)^{-1}$ is smallest. See [5] and [6] for an overview, and [7], [8] for more recent work.

In general, the value of $G(m,n)$ is not known. Although there are results for some pairs m, n, the only values of n for which $G(m,n)$ is known for all $m \geq n$ are $n = 1,2,3,4,5,6$. See [1] for $n = 2,3$, [9] for $n = 4,5$, and [10] for $n = 6$. The only values of n for which $G(m,n)$ is known for all but a finite number of values of m (that is, for m sufficiently large) are $n = 7, 11, 15$. See [11] for $n = 7$, and [12] for $n = 11, 15$.

For example, the following formula for $n = 7$ was conjectured in [1] and proved in [11]:

$$G(7t + r, 7) = 4\, 2^8 (t+1)^r t^{7-r}, \tag{1}$$

for all sufficiently large integers t and $0 \leq r \leq 6$.

In this work we consider the case $n \equiv -1 \pmod 4$. Equation (1) is typical of the results known for odd n. Indeed,

Theorem 1.1 *[12] For each $n \equiv -1 \pmod 4$ and each $0 \leq r < n$, there exists a polynomial $P(n,r,t)$ in t of degree n such that*

$$G(nt + r, n) = P(n,r,t), \tag{2}$$

for all sufficiently large t.

Thus for each pair n, r, we define the polynomial $P(n,r,t)$ to be the one for which Equation (2) holds for all sufficiently large t. In some cases, this polynomial can be computed explicitly as in Equation (1). The polynomial comes from a certain regular graph that is "trace-minimal," which is described in detail in Section 2. For now, suffice it to say that the polynomial $P(n,r,t)$ can be obtained, in principle, by comparing the characteristic polynomials of the adjacency matrices of the graphs in a finite set. In the next section we give the definition of "trace-minimal graph" and its relationship to the polynomials $P(n, r, t)$. Then, in Section 3, we give sufficient conditions for a graph to be trace-minimal, and in Section 4 we list various trace-minimal graphs.

2. Trace-minimal graphs and $P(n, r, t)$

In this section we describe the results from [12] that are needed to obtain explicit expressions for the polynomials $P(n, r, t)$ from certain regular graphs.

We begin with a description of the relevant graphs. Let (v, δ) be the set of all δ-regular graphs on v vertices and let $A(G)$ be the adjacency matrix of G. We also refer to $\mathrm{ch}(G, x)$ as the characteristic polynomial of the graph G.

Let $G \in (v, \delta)$. We say G is *trace-minimal* if for all $H \in (v, \delta)$ either $\mathrm{tr}A(G)^i = \mathrm{tr}A(H)^i$ for all i or there exists a positive integer $3 \leq k \leq n$ such that $\mathrm{tr}(A(G)^i) = \mathrm{tr}(A(H)^i)$, for $i < k$ and $\mathrm{tr}(A(G)^k) < \mathrm{tr}(A(H)^k)$. We also say that a graph B is *bipartite-trace-minimal* in $(2v, \delta)$ if it is trace-minimal within the reduced class $(2v, \delta)$ of bipartite δ-regular graphs on $2v$ vertices (v vertices in each part). Since (v, δ) is finite, there always exist trace-minimal graphs in (δ, v), and clearly they all have the same characteristic polynomial. (The same applies to bipartite-trace-minimal graphs in $(2v, \delta)$.)

As we shall see from the next four theorems, the problem of finding the polynomials $P(n, r, t)$ for a particular pair n, r is reduced to that of finding a trace-minimal graph within a class (v, δ) of graphs where v and δ depend on n and r. Let $n = 4p - 1$ and $m = nt + r$, where the remainder r satisfies $0 \leq r < n$. The formulas for $P(n, r, t)$ from [12] depend on the congruence class of $r \pmod 4$. We begin with the case $r \equiv 1 \pmod 4$:

Theorem 2.1 *Let $r = 4d + 1$. Let G be a trace-minimal graph in $(2p, d)$. Then*

$$P(n, r, t) = \frac{4(t + 1)[\mathrm{ch}(G, pt + d)]^2}{t^2}. \tag{3}$$

Theorem 2.2 *Let $r = 4d + 2$. Let G be a trace-minimal graph in $(2p, p + d)$. Then*

$$P(n, r, t) = \frac{4t[\mathrm{ch}(G, pt + d)]^2}{(t - 1)^2}. \tag{4}$$

Theorem 2.3 *Let* $r = 4d - 1$*. Suppose* $p/2 \le d < p$*. Let* G *be a trace-minimal graph in* $(4p, 3p + d - 1)$*. Then*

$$P(n, r, t) = \frac{4\text{ch}(G, pt + d - 1)}{t - 3}. \tag{5}$$

Suppose $0 \le d < p/2$*. Let* B *be a bipartite-trace-minimal graph in* $(4p, d)$*. Then*

$$P(n, r, t) = \frac{4(p(t - 1) + 2d)\text{ch}(B, pt + d)}{t(pt + 2d)}. \tag{6}$$

Theorem 2.4 *Let* $r = 4d$*. Suppose* $0 \le d \le p/2$*. Let* G *be a trace-minimal graph in* $(4p, d)$*. Then*

$$P(n, r, t) = \frac{4\text{ch}(G, pt + d)}{t}. \tag{7}$$

Suppose $p/2 < d < p$*. Let* B *be a bipartite-trace-minimal graph on in* $(4p, p+d)$*. Then*

$$P(n, r, t) = \frac{4(pt + 2d)\text{ch}(B, pt + d)}{(t - 1)(p(t + 1) + 2d)}. \tag{8}$$

3. Sufficient conditions for trace-minimality

We now turn to the problem of finding sufficient conditions for a graph to be trace-minimal. It is not difficult to show that a trace-minimal graph $G \in (v, \delta)$ must have maximum girth. We establish two sufficient conditions for trace-minimality; both involve girth.

Let $\text{cyc}(G, i)$ denote the number of cycles of length i in the graph G. This first condition for trace-minimality is the following:

Theorem 3.1 *Let* G *be a graph with maximum girth* g *in* (v, δ)*. Suppose that for every graph* $H \in (v, \delta)$*, there exists an integer* $k \le 2g - 1$ *such that* $\text{cyc}(G, q) = \text{cyc}(H, q)$ *for* $q < k$ *and* $\text{cyc}(G, k) < \text{cyc}(H, k)$*. Then* G *is trace-minimal in* (v, δ)*.*

The next condition involves the number of distinct eigenvalues of the adjacency matrix of G. Suppose a graph G has girth g and its adjacency matrix $A(G)$ has $k + 1$ distinct eigenvalues. Then [[14], p88], the diameter D of G satisfies $D \le k$. It is clear that $\lfloor g/2 \rfloor \le D$. Thus $g \le 2k$ if the girth g is even and $g \le 2k + 1$ if g is odd. We analyze the case of equality in the next theorem.

Theorem 3.2 *Let G be a connected regular graph with girth g and suppose that $A(G)$ has $k+1$ distinct eigenvalues. If g is even then $g \leq 2k$ with equality only if G is trace-minimal. If g is odd then $g \leq 2k+1$ with equality only if G is trace-minimal.*

The proofs of Theorems 3.1 and 3.2 depend on an application of the Coefficient Theorem [13], [14, Theorem 1.3] to regular graphs [15], [14, Theorem 3.26].

4. Families of trace-minimal graphs

Equipped with the four theorems from Section 2, one can translate the problem of finding an explicit expression of $P(n, r, t)$ for a given $n \equiv -1 \pmod 4$ and remainder $0 \leq r < n$ into the problem of finding an appropriate trace-minimal or bipartite-trace-minimal graph. For example suppose $n = 19$ and $r = 13$ so that $p = 5$ and $r = 4d + 1$, where $d = 3$. This case falls within the scope of Theorem 2.1 and we seek a trace-minimal graph in $(10, 3)$. The Petersen graph G, which is a 3-regular graph on 10 vertices, is trace-minimal (see Theorem 4.4). Since $\mathrm{ch}(G, x) = (x-3)(x-1)^5(x+2)^4$, Theorem 2.1 gives

$$\begin{aligned} G(19t+13, t) = P(19, 13, t) &= \frac{4(t+1)[\mathrm{ch}(G, 5t+3)]^2}{t^2} \\ &= 20(5t+2)^{10}(5t+5)^9, \end{aligned}$$

for all sufficiently large t.

In a similar manner, we can get all polynomials $P(n, r, t)$ for values n and r associated to any known trace-minimal graph with an even number of vertices. In particular, using the theorems listed below, we can get all values of $G(m, 19)$ and $G(m, 23)$ for all sufficiently large m. We now list the notation used in this section:

I_v	the graph consisting of v independent vertices (no edges)
K_v	the complete graph on v vertices
$K_{v,v}$	the complete bipartite graph with v vertices in eachof the bipartition sets
C_v	the cycle with v vertices
vK_2	a matching of v edges on $2v$ vertices
$K_{2v} - vK_2$	the complete graph on $2v$ vertices with amatching of edges removed
$K_{v,v} - vK_2$	the complete bipartite graph with a matchingremoved
G'	the complement of G
$G + H$	the direct sum of graphs G and H
kG	the direct sum of k copies of G
$G \bigtriangledown H$	the complete product of graphs G and H ($G \bigtriangledown H = (G' + H')'$)
$G^{(l)}$	the complete product of l copies of the graph G
$C_v(a, b, \ldots)$	the graph on v vertices in which (i, j) isan edge if and only if $\lvert i - j\rvert \equiv a,$ or $b, \ldots \pmod v$

All graphs that are unique in their class are trace-minimal.

Theorem 4.1 *I_v, K_v, and vK_2 are trace-minimal graphs in their class. Also $K_{v,v}$ and $K_{v,v} - vK_2$ are bipartite-trace-minimal graphs in their class.*

If there is a unique graph in (v, δ) with maximum girth, then it is a trace-minimal graph.

Theorem 4.2 *C_v is a trace-minimal graphs in $(v, 2)$.*

If a graph is bipartite-trace-minimal in $(2v, \delta)$ then its bipartite complement is bipartite-trace-minimal in $(2v, v - \delta)$.

Theorem 4.3 *$K_{v,v} - C_{2v}$ is a bipartite-trace-minimal graphs in $(2v, v - 2)$.*

Since the adjacency matrix of every strongly-regular graph has only 3 distinct eigenvalues, then by Theorem 3.2 we have

Theorem 4.4 *Let G be a connected strongly regular graph with no 3-cycles. Then G is trace-minimal.*

Other regular graphs with small number of eigenvalues are obtained from a class of geometries known as generalized n-gons. (See [16, p. 5] for the definition and other details.) Generalized n-gons of order q with $n \geq 3$ exist if and only if $n = 3, 4, 6$ and q is a power of a prime integer. Generalized 3-gons are projective planes, generalized 4-gons are called generalized quadrangles, and generalized 6-gons are called generalized hexagons.

The *incidence graph* [16, p. 3] of a finite geometry is the bipartite graph whose vertices are bipartitioned into the lines and the points with an edge whenever a point and a line are incident. The adjacency matrix for the incidence graph G of a generalized n-gon has only $n+1$ distinct eigenvalues, from which it follows by Theorem 3.2 that G is trace-minimal.

Theorem 4.5 *Let G be the incidence graph for generalized n-gon of order q. Then G is trace-minimal.*

We know all trace-minimal graphs in $(2v, \delta)$ for $v-6 \leq \delta \leq v-1$.

Theorem 4.6 *The following are trace-minimal graphs in their classes.*

G	*graph class*	G	*graph class*
K_v	$(v, v-1)$	$I_5^{(l)}$	$(5l, 5l-5)$
$K_{2v} - vK_2$	$(2v, 2v-2)$	$3K_2 \bigtriangledown I_5^{(l-1)}$	$(5l+1, 5l-4)$
$I_3^{(l)}$	$(3l, 3l-3)$	$C_7 \bigtriangledown I_5^{(l-1)}$	$(5l+2, 5l-3)$
$2K_2 \bigtriangledown I_3^{(l-1)}$	$(3l+1, 3l-2)$	$C_8(1,4) \bigtriangledown I_5^{(l-1)}$	$(5l+3, 5l-2)$
$C_5 \bigtriangledown I_3^{(l-1)}$	$(3l+2, 3l-1)$	$S(9,4)_5^{(l-1)}$	$(5l+4, 5l-1)$
$I_4^{(l)}$	$(4l, 4l-4)$	$I_6^{(l)}$	$(6l, 6l-6)$
$C_6 \bigtriangledown I_4^{(l-1)}$	$(4l+2, 4l-2)$	$C_{86}^{(l-1)}$	$(6l+2, 6l-4)$
		$C_{10}(1,4) \bigtriangledown I_6^{(l-1)}$	$(6l+4, 6l-2)$

We also know most trace-minimal graphs whose degree of regularity is very close to half the number of vertices.

Theorem 4.7 *The following are trace-minimal graphs in their classes.*

G	*graph class*	
$K_{v,v}$	$(2v, v)$	$v \geq 1$
$K_{v,v} - vK_2$	$(2v, v-1)$	$v \neq 4, 5$
$K_{v,v} - C_2 v$	$(2v, v-2)$	$v \geq 11$

In addition, we know the unique trace-minimal graph for the classes $(8,3)$, $(v,4)$ for $9 \leq v \leq 14$, $(14,5)$, $(13,6)$, $(16,6)$, and $(20,8)$. Finally, note that all bipartite graphs that are trace-minimal, are also bipartite-trace-minimal graphs.

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