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The edge-isoperimetric problem

1.1 Basic definitions

A *graph*, $G = (V, E, \partial)$, consists of a vertex-set V, edge-set E and boundary-function $\partial : E \to \binom{V}{1} + \binom{V}{2}$ which identifies the pair of vertices (not necessarily distinct) incident to each edge. Graphs are often represented by *diagrams* where vertices are points, and edges are curves connecting the pair of incident vertices. For any graph G, and $S \subseteq V$, we define

$$\Theta(S) = \{e \in E : \partial(e) = \{v, w\},\ v \in S \ \&\ w \notin S\},$$

and call it the *edge-boundary* of S. Then given a graph G, and $k \in \mathbb{Z}^+$, *the edge-isoperimetric problem* (EIP) is to minimize $|\Theta(S)|$ over all $S \subseteq V$ such that $|S| = k$. Note that $|\Theta(S)|$ is an *invariant*, i.e. if $\phi : G \to H$ is a graph isomorphism, then $\forall S \subseteq V_G$, $|\Theta(\phi(S))| = |\Theta(S)|$. Thus subsets of vertices which are equivalent under an automorphism will have the same edge-boundary.

Loops, i.e. edges incident to just one vertex, are irrelevant to the EIP so we shall ignore them. Most, but not all, of our graphs will be *ordinary graphs*, i.e. having no loops and no more than one edge incident to any pair of vertices. The representation of an ordinary graph may be shortened to (V, E), where $E \subseteq \binom{V}{2}$, and ∂ is implicitly the identity.

1.2 Examples

1.2.1 K_n, the complete graph on n vertices

K_n has n vertices with $E = \binom{V}{2}$, i.e. there is an edge between every pair of distinct vertices. For every $S \subseteq V$ such that $|S| = k$, $|\Theta(S)| = |S \times (V - S)| = k(n - k)$. So the EIP on K_n is easy: any k-set is a solution.

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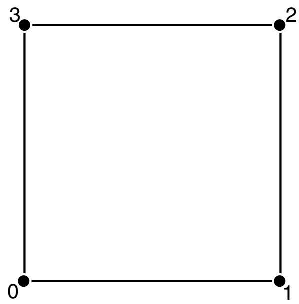

Fig. 1.1 The graph of $\mathbb{Z}_4$.

1.2.2 $\mathbb{Z}_n$, the n-cycle

For $\mathbb{Z}_n$, $V = \{0, 1, ..., n-1\}$ and $\{i, j\} \in E$ iff $i - j \equiv \pm 1 \, (\bmod\, n)$. Thus $\mathbb{Z}_3 = \mathbb{K}_3$ and $\mathbb{Z}_4$ has the diagram of Fig. 1.1.

We now deduce the solution of the EIP for $\mathbb{Z}_4$ and then $\mathbb{Z}_n$ from the following general remarks which will be useful later:

(1) (a) For $|S| = k = 0$, on any graph, there is only one subset, the empty set, $\emptyset$. Thus $\min_{|S|=0} |\Theta(S)| = |\Theta(\emptyset)| = 0$.
(b) For $k = |V| = n$, there is also only one subset, V, and $\min_{|S|=n} |\Theta(S)| = |\Theta(V)| = 0$.

(2) A graph is called *regular of degree* δ if it has exactly δ edges incident to each vertex. On a regular graph, if $|S| = k = 1$ then $|\Theta(S)| = \delta$, so any singleton is a solution set. $\mathbb{Z}_n$ is regular of degree 2; however for $n = 4$ and $k = 2$ there are two sets not equivalent under the symmetries of $\mathbb{Z}_n$: $\{0, 1\}$ and $\{0, 2\}$. All other 2-sets are equivalent to one of these two. $|\Theta(\{0, 1\})| = 2$ and $|\Theta(\{0, 2\})| = 4$, so $\min_{|S|=2} |\Theta(S)| = 2$.

(3) $\forall G$ and $\forall S \subseteq V$,

$$\Theta(V - S) = \Theta(S).$$

So for $k > \frac{1}{2}|V|$, $\min_{|S|=k} |\Theta(S)| = \min_{|S|=n-k} |\Theta(S)|$, where $n = |V|$. This completes our solution of the exterior EIP for $\mathbb{Z}_4$. It is summarized in the table

k	0	1	2	3	4
$\min_{\lvert S\rvert=k} \lvert\Theta(S)\rvert$	0	2	2	2	0

(4) Let

$$E(S) = \{e \in E : \partial(e) = \{v, w\},\ v \in S \,\&\, w \in S\}.$$

$E(S)$ is called the *induced* edges of S. The *induced edge problem* on a graph is to maximize $|E(S)|$ over all $S \subseteq V$ with $|S| = k$.

Lemma 1.1 *If $G = (V, E, \partial)$ is a regular graph of degree δ and $S \subseteq V$, then $\forall S \subseteq V$,*

$$|\Theta(S)| + 2|E(S)| = \delta |S|.$$

Proof $\delta |S|$ counts the edges incident to S but those in $E(S)$ are counted twice. □

Corollary 1.1 *If G is a regular graph, then $S \subseteq V$ is a solution of the induced edge problem iff it is a solution of the EIP. Also, $\forall k$, $\min_{|S|=k} |\Theta(S)| = \delta k - 2\max_{|S|=k} |E(S)|$.*

For regular graphs then, the EIP and induced edge problem are equivalent and we shall treat them as interchangeable. In general the EIP occurs in applications and the induced edge problem is easier to deal with in proofs. There is also a third natural variant of the EIP: for $S \subseteq V$ let

$$\partial^*(S) = \{e \in E : \partial(e) \cap S \neq \emptyset\},$$

the set of edges incident to S.

Exercise 1.1 *Show that for regular graphs, computing*

$$\min_{\substack{S \subseteq V \\ |S|=k}} \left|\partial^*(S)\right|$$

is equivalent to the EIP.

Recall that a *tree* is a graph which is connected and acyclic. An acyclic graph is also called a *forest* because it is a union of trees, its connected components.

Lemma 1.2 *The number of edges in a tree on n vertices is $n-1$. The number of induced edges in a forest is then $n-t$, t being the number of trees.*

Any proper subset, S, of $\mathbb{Z}_n$ will induce an acyclic graph so $\max_{|S|=k} |E(S)|$ will occur for a connected set, i.e. an interval. Thus if $0 < k < n$, $\min_{|S|=k} |\Theta(S)| = 2k - 2(k-1) = 2$.

1.2.3 The d-cube, Q_d

The graph of the d-dimensional cube, Q_d, has vertex-set $\{0, 1\}^d$, the d-fold Cartesian product of $\{0, 1\}$. Thus $n = \left|V_{Q_d}\right| = 2^d$. Q_d has an edge between two vertices (d-tuples of 0s and 1s) if they differ in exactly one entry.

Exercise 1.2 *Find a formula for* $m = \left|E_{Q_d}\right|$.

Q_1 is isomorphic to K_2 and Q_2 is isomorphic to $\mathbb{Z}_4$, for which the EIP has already been solved. The 3-cube has eight vertices, 12 edges and six square faces. A diagram of Q_3., actually a projection of the 3-cube, is shown in Fig. 1.2.

One can solve the EIP on Q_3 with the simple tools which we developed in the first two examples. First observe that Q_3 has *girth* (the minimum length of any cycle) 4: since the symmetry group of the 3-cube is transitive, any vertex is the same as any other. Starting from a vertex and tracing out paths, one sees that there are no closed paths of length 3. Thus for $1 \leq k \leq 3$ we have, by Lemma 1.1 and Lemma 1.2,

$$\begin{aligned} \min_{|S|=k} |\Theta(S)| &= 3k - 2 \max_{|S|=k} |E(S)| \\ &= 3k - 2(k-1) = k + 2. \end{aligned}$$

For $k = 4$ either the set induces a cycle, in which case it is a 4-cycle and has $|\Theta(S)| = 4$, or the induced graph is acyclic and by the above, $|\Theta(S)| \geq 6$. For

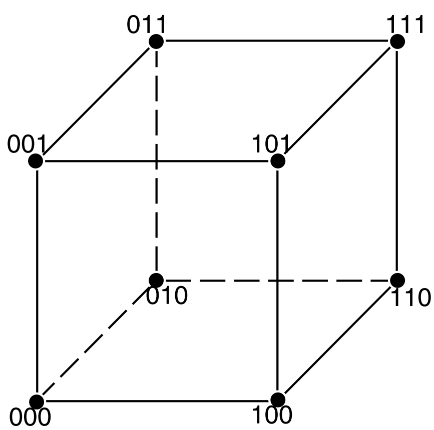

Fig. 1.2 Diagram of Q_3.

$k > 4 = \frac{8}{2}$ we complete the solution from the fact that

$$\min_{|S|=k} |\Theta(S)| = \min_{|S|=8-k} |\Theta(S)| .$$

Our solution is summarized in the table

k	0	1	2	3	4	5	6	7	8
$\min_{\vert S\vert=k} \vert\Theta(S)\vert$	0	3	4	5	4	5	4	3	0

In order to extend this solution of the EIP to $Q_d, d > 3$, we need some simple facts about cubes which we leave as exercises. A *c-subcube of the d-cube* is the subgraph of Q_d induced by the set of all vertices having the same (fixed) values in some $d - c$ coordinates.

Exercise 1.3 *Show that any c-subcube of the d-cube is isomorphic to the c-cube.*

Exercise 1.4 *How many c-subcubes of the d-cube are there*?

A *neighbor* of a c-subcube of the d-cube is any c-subcube which differs from the given one in exactly one of their $d - c$ fixed coordinates.

Exercise 1.5 *Show that all neighbors of a c-subcube are disjoint.*

Exercise 1.6 *Show that no (vertices in) two distinct neighbors of a c-subcube are connected by an edge.*

Exercise 1.7 *How many neighbors does a c-subcube of the d-cube have?*

The EIP on Q_d was originally motivated by problems in data transmission (see Chapter 2). Studies by W. H. Kautz [**59**], E. C. Posner (personal communication) and the author led to the conjecture that the initial segments of the *lexicographic numbering*,

$$lex(x) = 1 + \sum_{i=1}^{d} x_i 2^{i-1}$$

for $x \in V_{Q_d}$, were solution sets, but how was this to be proven? An obvious approach to try was induction on the dimension, d. Mathematical induction has the paradoxical property that it is often easier to prove a stronger theorem because, once the initial case has been verified, one is allowed to assume that the theorem is true for lower values of the inductive parameter in order to establish it for the next one. Thus a stronger hypothesis can produce an easier proof. In this case the strategy led to the conjecture that the following inductive procedure would produce *all* solution sets:

(1) Begin with the null set, $\emptyset$.
(2) Having constructed a set $S \subset V_{Q_d}$, augment it with any $x \in V_{Q_d} - S$ which maximizes the marginal number of induced edges,

$$|E(S + \{x\})| - |E(S)|.$$

Thus the augmentation of $\emptyset$ may be by any $x \in V_{Q_d}$ since $|E(\{x\})| - |E(\emptyset)| = 0$. The augmentation of $\{x\}$ must be by y which is a neighbor of x, etc. What kinds of k-sets are these for $k > 2$? The answer follows from the fact that if $k = 2^c$, then the set must be a c-subcube. We have just verified this for $c = 0, 1$. Assume it is true for $0, 1, ..., c-1$. In augmenting a 2^{c-1}-set, which must be a $(c-1)$-subcube, we may only choose a vertex whose marginal contribution to $|E(S)|$ is 1, i.e. any member of a neighboring $(c-1)$-subcube. Having chosen a vertex from one of those neighboring subcubes we must continue to choose vertices from the same subcube until it is exhausted, since there will always be a vertex in the chosen subcube for which $|E(S + \{x\})| - |E(S)| \geq 2$ whereas any vertex not in the subcube will have $|E(S + \{x\})| - |E(S)| \leq 1$. When we exhaust the neighboring $(c-1)$-subcube, we have completed a c-subcube.

In general, let

$$k = \sum_{i=1}^{K} 2^{c_i}, \; 0 \leq c_1 < c_2 < ... < c_K,$$

be the base 2 representation of k (note that $K = \lfloor \log_2 k \rfloor$). If $S \subseteq V_{Q_d}$ is a disjoint union of c_i-subcubes, $1 \leq i \leq K$, such that each c_i-subcube lies in a neighbor of every c_j-subcube for $j > i$, then S is called *cubal*. The cubal sets are exactly the sets constructed by successively maximizing the marginal number of interior edges. It follows that if S is cubal and $|S| = k$ then (see Exercise 1.1)

$$|E(S)| = \sum_{i=1}^{K} (K - i) 2^{c_i} + c_i 2^{c_i - 1}.$$

Note that $|E(S)|$ for a k-cubal set, $S \subseteq V_{Q_d}$, does not depend on d, just on $k = |S|$. This function is important so we denote it by $E(k)$. $E(k)$ has a fractal nature which is hinted at by the following recurrence. If $2^{d-1} \leq k < 2^d$ then

$$E(k+1) - E(k) = E\left(k - 2^{d-1} + 1\right) - E\left(k - 2^{d-1}\right) + 1.$$

This follows from the recursive structure of k-cubal sets. Subtracting the largest power of 2 from k, 2^{d-1}, corresponds to removing the largest subcube from S. That subcube provided one neighbor to every vertex in the remainder of the set.

Exercise 1.8 *Show that if $S \subseteq V_{Q_d}$ is cubal, then its complement $V_{Q_d} - S$ is cubal.*

Exercise 1.9 *Show that any two cubal k-sets are isomorphic, i.e. there is an automorphism of the d-cube which takes one to the other.*

Theorem 1.1 *$S \subseteq V_{Q_d}$ maximizes $|E(S)|$ for its cardinality, k, iff S is cubal.*

Lemma 1.3 *(Bernstein, [**13**]) $\forall d$ and $\forall k, t > 0$ such that $k + t < 2^d$,*

$$E(t) < E(k+t) - E(k) < E\left(2^d\right) - E\left(2^d - t\right).$$

Proof (of the lemma). By induction on d: It is true for $d = 2$. Assume it for $d - 1 \geq 2$ and consider the following three cases:

(1) If $k \geq 2^{d-1}$ then

$$\begin{aligned} E(k+t) - E(k) &= \sum_{i=1}^{t} E(k+i) - E(k+i-1) \\ &= \sum_{i=1}^{t} \left[E\left(k+i-2^{d-1}\right) - E\left(k+i-2^{d-1}-1\right) + 1\right] \\ &= E\left(k+t-2^{d-1}\right) - E\left(k-2^{d-1}\right) + t, \end{aligned}$$

and both inequalities follow from the inductive hypothesis.

(2) If $k + t \leq 2^{d-1}$ then the lefthand inequality follows from the inductive hypothesis and the righthand one from the above identity and then the inductive hypothesis.

(3) If $k < 2^{d-1} < k + t$ then

$$\begin{aligned} E(k+t) - E(k) &= \left[E(k+t) - E\left(2^{d-1}\right)\right] + \left[E\left(2^{d-1}\right) - E(k)\right] \\ &> \left[E\left(k+t-2^{d-1}\right)\right] + \left[E(t) - E\left(t - \left(2^{d-1} - k\right)\right)\right] \\ &\qquad \text{by Case 1 and Case 2, respectively,} \\ &= E(t). \end{aligned}$$

Exercise 1.10 *Complete the proof (the righthand inequality) of Case 3.*

□

Proof (of the theorem). We have noted that all k-cubal sets have the same number, $E(k)$, of induced edges, so we need only show that all optimal sets are cubal. We proceed by induction on d. We have already shown it to be true for $d = 1, 2$. Assume that it is true for all dimensions less than $d > 2$. Given k, $0 < k < n = 2^d$, with the representation as a sum of powers of 2 above (so

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$K < d$), let $S \subseteq V_{Q_d}$ be optimal for $|S| = k$. If we divide Q_d into two $(d-1)$-subcubes, $Q_{d,0} = \left\{x \in V_{Q_d} : x_d = 0\right\}$ and $Q_{d,1}$, by its dth coordinate, then we partition S into $S_0 = S \cap Q_{d,0}$ and $S_1 = S \cap Q_{d,1}$. Letting $|S_0| = k_0$ and $|S_1| = k_1$, we may assume that $k_0 \geq k_1$. If $k_1 = 0$ the theorem follows from the inductive hypothesis, so assume $k_1 > 0$. The edges of $E(S)$ will either have both ends in S_0, both ends in S_1 or one end in S_0 and one in S_1. Therefore

$$|E(S)| \leq \max_{|S|=k_0} |E(S)| + \max_{|S|=k_1} |E(S)| + k_1.$$

If we take S_1 to be a cubal set of cardinality k_1, by induction, $|E(S_1)| = E(k_1) = \max_{|S|=k_1} |E(S)|$. The neighbors of S_1 in $Q_{d,0}$ are isomorphic to S_1 and so are also cubal. By the recursive construction of cubal sets, $\exists S_0 \subseteq Q_{d,0}$, cubal with $|S_0| = k_0$ and containing the neighbors of S_1. Thus the upper bound can be achieved and every set which achieves it must be such a union of two cubal sets. Let $k_0 = \sum_{i=1}^{K_0} 2^{c_{i,0}}$, $0 \leq c_{1,0} < c_{2,0} < \ldots < c_{K_o,0}$ and similarly for k_1. Since $k_0 + k_1 = k$ there are just three possibilities:

(1) $c_{K_0,0} = c_K$: Then we may assume that $S_0 - Q_{c_{K_0},0}$ and S_1 are in two distinct neighbors of $Q_{c_{K_0},0}$ so S is not cubal. By Exercise 1.5 there can be no edges between a member of $S_0 - Q_{c_{K_0},0}$ and a member of S_1. With $k_0' = k_0 - 2^{c_{l_0}} > 0$ we have $k_0' + k_1 \leq 2^{c_{K_0}}$. If we alter S by removing S_1 and adding the same number of vertices to S_0, Lemma 1.3 shows that $|E(S)|$ will be increased. This contradicts the optimality of S.

(2) $c_{K_0,0} = c_K - 1$ and $c_{K_1,1} = c_K - 1$: The $(c_K - 1)$-subcubes, $Q_{c_{K_0},0}$ and $Q_{c_{K_1},1}$, are neighbors and so constitute a c_K-subcube. $S_0 - Q_{c_{K_0},0}$ and $S_1 - Q_{c_{K_1},1}$ each lie in neighboring $(c_K - 1)$-subcubes which together constitute a c_K-subcube neighboring the first. By the inductive hypothesis S must be cubal.

(3) $c_{K_0,0} = c_K - 1$ and $c_{K_1,1} < c_K - 1$: As in Case 1, we assume that $S_0 - Q_{c_{K_0},0}$ and S_1 are in two distinct neighbors of $Q_{c_{K_0},0}$ and so have no edges between them. Not only is $k_0' = k_0 - 2^{c_{K_0}} > 0$ but

$$\begin{aligned} k_0' + k_1 &= k_0 - 2^{c_{K_0}} + k_1 \\ &= k - 2^{c_K - 1} \\ &\geq 2^{c_K} - 2^{c_K - 1} \\ &= 2^{c_K - 1}. \end{aligned}$$

If we alter S by removing $2^{c_{K_0}} - k_0'$ members of S_1 and using them to complete the neighbor of $Q_{c_{K_0},0}$ which contains $S_0 - Q_{c_{K_0},0}$, Lemma 1.3 shows that this will increase $|E(S)|$, again contradicting the optimality of S.

□

1.3 Application to layout problems

Combinatorial isoperimetric problems arise frequently in communications engineering, computer science, the physical sciences and mathematics itself. We do not wish to cover all applications here but to give a representative sample. We have chosen to concentrate on layout problems. These arise in electrical engineering when one takes the wiring diagram for some electrical circuit and "lays it out" on a chassis, i.e. places each component and wire on the chassis. A wiring diagram is essentially a graph, the electrical components being the vertices and the wires connecting them being the edges. For any given placement of the vertices and edges on the chassis, there will be certain costs or measurements of performance which we wish to optimize.

1.3.1 The wirelength problem

Suppose that we wish to place components (vertices of the graph $G = (V, E, \partial)$) on a linear chassis, each a unit distance from the preceding one, in such a way as to minimize the total length of all the wires connecting them. To make this precise, we define a *vertex-numbering* of G to be a function

$$\eta : V \to \{1, 2, ..., n\}, \text{ where } n = |V|,$$

which is one-to-one (and therefore onto). The integers in the range of η may be identified with positions on the linear chassis. The *(total) wirelength of* η is then

$$wl(\eta) = \sum_{\substack{e \in E \\ \partial(e) = \{v, w\}}} |\eta(v) - \eta(w)|.$$

For a graph, $G = (V, E, \partial)$,

$$wl(G) = \min\{wl(\eta) : \eta \text{ is a vertex-numbering of } G\}.$$

Remember that a graph on n vertices has $n!$ vertex-numberings.

1.3.1.1 Example

The graph of the square has $4! = 24$ vertex-numberings, but it also has eight symmetries. Any two numberings symmetric to each other have the same wirelength. The three numberings in Fig. 1.3 are representative of the $24/8 = 3$ equivalence classes of numberings. Thus the first two numberings minimize the wirelength, wl, and the third maximizes it. Therefore $wl(Q_2) = 6$. $wl(Q_3)$ is not so easily determined since Q_3 has $8! = 40\,320$

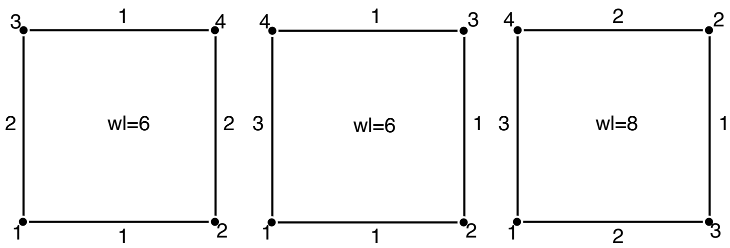

Fig. 1.3 Numberings of Q_2.

numberings and 48 symmetries. $40\,320/48 = 840$ is not all that large, but how does one systematically generate representatives of those 840 equivalence classes of numberings? We now show how to get around these apparent difficulties.

In seeking to minimize a sum like wl, an obvious strategy is to minimize each summand separately. The sum of those minima is a lower bound on the minimum of the sum and one could hope that it would be a good lower bound, even sharp. That is not the case for the definition of $wl(\eta)$, however, since for every edge $e \in E$ with $\partial(e) = \{v, w\}$

$$\min_{\eta} |\eta(v) - \eta(w)| = 1.$$

1.3.1.2 Another representation of *wl*

Given a numbering, η, and an integer k, $0 \leq k \leq n$, let

$$S_k(\eta) = \eta^{-1}(\{1, 2, \ldots, k\}) = \{v \in V : \eta(v) \leq k\},$$

the set of the first k vertices numbered by η. Then we have the following alternative representation of the wirelength.

Lemma 1.4

$$wl(\eta) = \sum_{k=0}^{n} |\Theta(S_k(\eta))|$$

Proof Note that $S_0(\eta) = \eta^{-1}(\emptyset) = \emptyset$. Let

$$\chi(e, k) = \begin{cases} 1 & \text{if } \partial(e) = \{v, w\}, \eta(v) \leq k < \eta(w) \\ 0 & \text{otherwise.} \end{cases}$$