Isoperimetric Graph Partitioning for Data Clustering and Image Segmentation

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Abstract

Spectral methods of graph partitioning have been shown to provide a powerful approach to the image segmentation problem. In this paper, we adopt a different approach, based on finding partitions with a small isoperimetric constant in an image graph. Our algorithm produces the high quality segmentations and data clustering of spectral methods, but with improved speed and stability.

Index Terms

I.4.6.b, E.1.d, G.2.2.a, I.4.10, I.5.5.c, I.5.3.a, I.5.4.b, G.2.3

I. Introduction

THE application of graph theoretic methods to spatial pattern analysis has a long history, including the pioneering work of Zahn [1] on minimal spanning tree clustering, the development of connectivity graph algorithms for space-variant sensors by Wallace et al. [2], and the seminal work on image segmentation, termed "Ncuts" by Shi and Malik [3]. One reason for this interest is that the segmentation quality of Ncuts and other graph-based segmentation methods [4], [5], [6] is very good. However, there are several other important advantages of graph-based sensor strategies.

1) *Local-global interactions* are well expressed by graph theoretic algorithms. As Zahn [1] originally pointed out, the important notion of Gestalt in image processing— the relationship of the whole to the part—seems to be an important ingredient in both biological and machine image processing.
2) *New algorithms* for image processing may be crafted from the large corpus of well-explored algorithms which have been developed by graph theorists. For example, spectral graph partitioning was developed to aid in design automation of computers [7] and has provided the foundation for the development of the Ncuts algorithm [3]. Similarly, graph theoretic methods for solving lumped,

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Ohmic electrical circuits based on Kirchhoff's voltage and current law [8], [9], [10], [11], form the basis for the method proposed in this paper for solving the isoperimetric problem.

3) *Adaptive sampling* and space-variant vision require a "connectivity graph" approach to allow image processing on sensor architectures with space-variant visual sampling. Space-variant architectures have been intensively investigated for application to computer vision for several decades [2], [12] partly because they offer extraordinary data compression.
4) *New architectures for image processing* may be defined that generalize the traditional Cartesian design. Just as in the spatial case, the temporal domain can (and does, in animals) exploit an adaptive, variable sampling strategy. In a computational context, this suggests the use of graph theoretic data structures, rather than pixels and clocks. Some applications based on graphs have no counterpart in quasi-continuous, pixel based applications. For example, the *small world* property of graphs, which allows the introduction of sparse global connectivity at little computational cost, has been applied to image processing with good results [13]. In general, the flexible nature of data structures based on graphs provides a natural language for space-time adaptive sensors.

A. Overview of Graph partitioning

The graph partitioning problem is to choose subsets of the vertex set such that the sets share a minimal number of spanning edges while satisfying a specified cardinality constraint. Graph partitioning appears in such diverse fields as parallel processing [14], solving sparse linear systems [15], VLSI circuit design [16] and image segmentation.

The paradigm of use for graph partitioning in image segmentation is to view the image as a lattice with pixels representing nodes and neighboring pixels connected with an edge, weighted to reflect the similarity of the pixels. Therefore, finding a good graph partition corresponds to finding a segmentation such that the boundary between segments has a small number of (weighted) edges cut, i.e., the boundary threads between as many "dissimilar" pixels as possible.

There are two major approaches used to apply graph partitioning to image segmentation, depending on whether or not the "indicator function" on the nodes has values confined to the real line or binary/integers (see (8) for a formal definition of an indicator function). A binary constraint has the advantage that a computed indicator function defines a partition. The disadvantage of binary constraints is that combinatorial optimization is often more difficult, or completely impractical, for minimization of many functionals.

The canonical example of an algorithm employing a binary-valued indicator function is the set of algorithms based on the Potts model or *max-flow/min-cut* [17]. Wu and Leahy [18] initiated this application to automatic image segmentation by taking many pairs of source/sink nodes and finding the partition with the smallest cut. As many have pointed out [3], minimization of this functional leads to small partitions. Alternately, one may employ this approach as a seeded, semi-automatic algorithm [19], where the user is

able to supply enough terminal nodes to overcome the small partition problem. The interpretation of this algorithm in terms of a Markov random field [20], [21], [22] allows the max-flow/min-cut algorithm to be used to produce a binary segmentation if priors are available that indicate the probability with which each pixel will belong to one segment or another (e.g., calculated from intensity). The second major approach to using a binary-valued function defined on the node set is to establish a probability space of partitions based on a Gibbs probability measure, such that cuts with small partition have greater probability [23], [24]. By an appropriate sampling regime, one can determine which edges are likely to be cut and convert these probabilities into a partition or to use this probability space to grow and/or modify an existing partition.

In contrast, several algorithms relax the binary constraint on the indicator function and achieve different methods of producing a cut, based on the functional in question or the chosen method of regularization. The main disadvantage to relaxing the binary constraint on the indicator function is that the solution to the optimization problem must then be converted to a "hard" segmentation. However, the main advantage to relaxing the binary constraint is that many optimization problems become tractable. The most celebrated approach in this context is the normalized cuts algorithm [25] and the related approaches of [5], [4]. All of these algorithms are related to the spectrum of an image graph and ultimately require the solution to an eigenvector problem. By adopting a different method of regularization, it is also possible to frame a real-valued optimization as a semidefinite programming problem [26]. One may also find a real-valued minimization of the minimum-cut functional, allowing an exact, polynomial-time optimization for an arbitrary number of labels (i.e., terminals). This approach leads to an algorithm best interpreted in terms of random walks on a graph [27].

The present paper describes an algorithm in the second class — solution for a real-valued indicator function. Although the functional qualitatively favors partitions similar to those favored by the NCuts, etc. criteria (i.e., large, loosely connected regions), the formulation permits a solution in terms of a system of linear equations, resulting in a faster, more stable algorithm. In addition to the unsupervised segmentation approach promoted in this paper, it is also natural to run this algorithm in a supervised manner, since an "attention" point is explicitly defined.

Methods of graph partitioning may take different forms, depending on the number of partitions required, whether or not the nodes have coordinates, and the cardinality constraints of the sets. In this paper, we use the term **partition** to refer to the assignment of each node in the vertex set into two (not necessarily equal) parts. We propose a partitioning algorithm termed **isoperimetric partitioning**, since it is derived and motivated by the equations defining the isoperimetric constant (to be defined later). Isoperimetric partitioning does not require coordinate information about the graph and allows one to find partitions of an "optimal" cardinality instead of a predefined cardinality. The isoperimetric algorithm most closely

resembles spectral partitioning in its use and ability to create hybrids with other algorithms (e.g., multilevel spectral partitioning [28], geometric-spectral partitioning [29]), but requires the solution to a large, sparse system of equations, rather than solving the eigenvector problem for a large, sparse matrix. In this paper we will develop the isoperimetric algorithm, prove some of its properties, and apply it to problems in data clustering and image segmentation.

B. The Isoperimetric Problem

Graph partitioning has been strongly influenced by properties of a combinatorial formulation of the classic isoperimetric problem: *For a fixed area, find the region with minimum perimeter.*

Define the **isoperimetric constant** h of a manifold as [30]

$$h = \inf_S \frac{|\partial S|}{\mathrm{Vol}_S}, \tag{1}$$

where S is a region in the manifold, Vol_S denotes the volume of region S, $|\partial S|$ is the area of the boundary of region S, and h is the infimum of the ratio over all possible S. For a compact manifold, $\mathrm{Vol}_S \leq \frac{1}{2}\mathrm{Vol}_{\mathrm{Total}}$, and for a noncompact manifold, $\mathrm{Vol}_S < \infty$ (see [31], [32]).

We show in this paper that the set (and its complement) for which h takes a minimum value defines a good heuristic for data clustering and image segmentation. In other words, finding a region of an image that is simultaneously both large (i.e., high volume) and that shares a small perimeter with its surroundings (i.e., small boundary) is intuitively appealing as a "good" image segment. Therefore, we will proceed by defining the isoperimetric constant on a graph, proposing a new algorithm for approaching the sets that minimize h, and demonstrate applications to data clustering and image segmentation.

II. The Isoperimetric Partitioning Algorithm

A **graph** is a pair $G = (V, E)$ with vertices (nodes) $v \in V$ and edges $e \in E \subseteq V \times V$. An edge, e, spanning two vertices, v_i and v_j, is denoted by e_{ij}. Let $n = |V|$ and $m = |E|$ where $|\cdot|$ denotes cardinality. A **weighted graph** has a value (typically nonnegative and real) assigned to each edge called a **weight**. The weight of edge e_{ij}, is denoted by $w(e_{ij})$ or w_{ij}. Since weighted graphs are more general than unweighted graphs (i.e., $w(e_{ij}) = 1$ for all $e_{ij} \in E$ in the unweighted case), we will develop all our results for weighted graphs. The **degree** of a vertex v_i, denoted d_i is

$$d_i = \sum_{e_{ij}} w(e_{ij}) \;\; \forall\, e_{ij} \in E. \tag{2}$$

For a graph, G, the **isoperimetric constant** [31], h_G is

$$h_G = \inf_S \frac{|\partial S|}{\mathrm{Vol}_S}, \tag{3}$$

where $S \subset V$ and

$$\mathrm{Vol}_S \leq \frac{1}{2}\mathrm{Vol}_V. \tag{4}$$

In graphs with a finite node set, the infimum in (3) becomes a minimum. Since we will be computing only with finite graphs, we will henceforth use a minimum in place of an infimum. The boundary of a set, S, is defined as $\partial S = \{e_{ij} | i \in S, j \in \overline{S}\}$, where $\overline{S}$ denotes the set complement, and

$$|\partial S| = \sum_{e_{ij} \in \partial S} w(e_{ij}). \tag{5}$$

In order to determine a notion of volume for a graph, a metric must be defined. Different choices of a metric lead to different definitions of volume and even different definitions of a combinatorial Laplacian operator (see [32], [33]). Dodziuk suggested [34], [35] two different notions of combinatorial volume,

$$\mathrm{Vol}_S = |S|, \tag{6}$$

and

$$\mathrm{Vol}_S = \sum_i d_i \;\; \forall\, v_i \in S. \tag{7}$$

One may view the difference between the definition of volume in (6) and that in (7) as the difference between what Shi and Malik term the "Average Cut" versus their "Normalized Cut" [3], although the isoperimetric ratio (with either definition of volume) corresponds to neither criterion. The matrix used in the Ncuts algorithm to find image segments corresponds to the combinatorial Laplacian matrix under the metric defined by (7). Traditional spectral partitioning [36] employs the same algorithm as Ncuts, except that it uses the combinatorial Laplacian matrix defined by the metric associated with (6). In agreement with [3], we find that the second metric (and hence, volume definition) is more suited for image segmentation since regions of uniform intensity are given preference over regions that simply possess a large number of pixels. Therefore, we will use Dodziuk's second metric definition and employ volume as defined in equation (7).

For a given set, S, we term the ratio of its boundary to its volume the **isoperimetric ratio**, denoted by $h(S)$ (i.e., the argument of $\inf$ in (3)). The **isoperimetric sets** for a graph, G, are any sets S and $\overline{S}$ for which $h(S) = h_G$ (note that the isoperimetric sets may not be unique for a given graph). The specification of a set satisfying equation (4), together with its complement may be considered as a *partition* and therefore we will use the term interchangeably with the specification of a set satisfying equation (4). Throughout this paper, we consider a good partition as one with a low isoperimetric ratio (i.e., the optimal partition is represented by the isoperimetric sets themselves). Therefore, our goal is to maximize Vol_S while minimizing $|\partial S|$. Unfortunately, finding isoperimetric sets is an NP-hard problem [31]. Our algorithm

is may be considered a heuristic for finding a set with a low isoperimetric ratio that runs in low-order polynomial time.

A. Derivation of Isoperimetric Algorithm

Define an indicator vector, x, that takes a binary value at each node

$$x_i = \begin{cases} 0 & \text{if } v_i \in \overline{S}, \\ 1 & \text{if } v_i \in S. \end{cases} \tag{8}$$

Note that a specification of x may be considered a partition.

Define the $n \times n$ matrix, L, of a graph as

$$L_{v_i v_j} = \begin{cases} d_i & \text{if } i = j, \\ -w(e_{ij}) & \text{if } e_{ij} \in E, \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

The notation $L_{v_i v_j}$ is used to indicate that the matrix L is being indexed by vertices v_i and v_j. This matrix is also known as the **admittance matrix** in the context of circuit theory or the **Laplacian matrix** (see, [37] for a review) in the context of finite difference methods (and in the context of [34]).

By definition of L,

$$|\partial S| = x^T L x, \tag{10}$$

and $\mathrm{Vol}_S = x^T d$, where d is the vector of node degrees. If r indicates the vector of all ones, minimizing (10) subject to the constraint that the set, S, has fixed volume may be accomplished by asserting

$$\mathrm{Vol}_S = x^T d = k, \tag{11}$$

where $0 < k < \frac{1}{2} r^T d$ is an arbitrary constant and r represents the vector of all ones. We shall see that the choice of k becomes irrelevant to the final formulation. Thus, the isoperimetric constant (3) of a graph, G, may be rewritten in terms of the indicator vector as

$$h_G = \min_x \frac{x^T L x}{x^T d}, \tag{12}$$

subject to (11). Given an indicator vector, x, then $h(x)$ is used to denote the isoperimetric ratio associated with the partition specified by x. Note that the ratio given by (12) is different from both the "ratio cut" of [38], [39] and the "average cut" of [3]. Although the criterion in (12) rewards similar partitions to the normalized cut, average cut and ratio cut (i.e., large segments with small boundaries), what appears as a minor difference in the formulation allows us to use a solution to a system of linear equations instead of

solving an eigenvector problem. Note that the ratio cut technique of [38], [39] is distinct (in algorithm and pertinent ratio) from the ratio cut of [6], which applies only to planar graphs. The advantages of a system of linear equations over an eigenvector problem will be discussed below.

The constrained optimization of the isoperimetric ratio is made into a free variation via the introduction of a Lagrange multiplier Λ [40] and relaxation of the binary definition of x to take nonnegative real values by minimizing the cost function

$$Q(x) = x^T L x - \Lambda(x^T d - k). \tag{13}$$

Since L is positive semi-definite (see, [41], [42]) and $x^T d$ is nonnegative, $Q(x)$ will be at a minimum for any critical point. Differentiating $Q(x)$ with respect to x yields

$$\frac{dQ(x)}{dx} = 2Lx - \Lambda d. \tag{14}$$

Thus, the problem of finding the x that minimizes $Q(x)$ (minimal partition) reduces to solving the linear system

$$2Lx = \Lambda d. \tag{15}$$

Henceforth, we ignore the scalar multiplier 2 and the scalar Λ since, as we will see later, we are only concerned with the relative values of the solution.

Unfortunately, the matrix L is singular: all rows and columns sum to zero (i.e., the vector r spans its nullspace), so finding a unique solution to equation (15) requires an additional constraint.

We assume that the graph is connected, since the optimal partitions are clearly each connected component if the graph is disconnected (i.e., $h(x) = h_G = 0$). Note that in general, a graph with c connected components will correspond to a matrix L with rank $(n - c)$ [41]. If we arbitrarily designate a node, v_g, to include in S (i.e., fix $x_g = 0$), this is reflected in (15) by removing the gth row and column of L, denoted by L_0, and the gth row of x and d, denoted by x_0 and d_0, such that

$$L_0 x_0 = d_0, \tag{16}$$

which is a nonsingular system of equations.

Solving equation (16) for x_0 yields a real-valued solution that may be converted into a partition by setting a threshold (see below for a discussion of different methods). In order to generate a clustering or segmentation with more than two parts, the algorithm may be recursively applied to each partition separately, generating subpartitions and stopping the recursion if the isoperimetric ratio of the cut fails to meet a predetermined threshold. We term this predetermined threshold the **`stop`** parameter and note that since $0 \leq h(x) \leq 1$, the `stop` parameter should be in the interval $(0, 1)$. Since lower values of $h(x)$ correspond to more desirable partitions, a stringent value for the `stop` parameter is small, while a

large value permits lower quality partitions (as measured by the isoperimetric ratio). In Appendix I we prove that the partition containing the node corresponding to the removed row and column of L must be connected, for any chosen threshold i.e., the nodes corresponding to x_0 values less than the chosen threshold form a connected component.

B. Circuit analogy

Equation (15) also occurs in circuit theory when solving for the electrical potentials of an ungrounded circuit in the presence of current sources [10]. After grounding a node in the circuit (i.e., fixing its potential to zero), determination of the remaining potentials requires a solution of (16). Therefore, we refer to the node, v_g, for which we set $x_g = 0$ as the **ground node**. Likewise, the solution, x_i, obtained from equation (16) at node v_i, will be referred to as the **potential** for node v_i. The need for fixing an $x_g = 0$ to constrain equation (15) may be seen not only from the necessity of grounding a circuit powered only by current sources in order to find unique potentials, but also from the need to provide a boundary condition in order to find a solution to Poisson's equation, of which (15) is a combinatorial analog. In our case, the "boundary condition" is that the grounded node is fixed to zero.

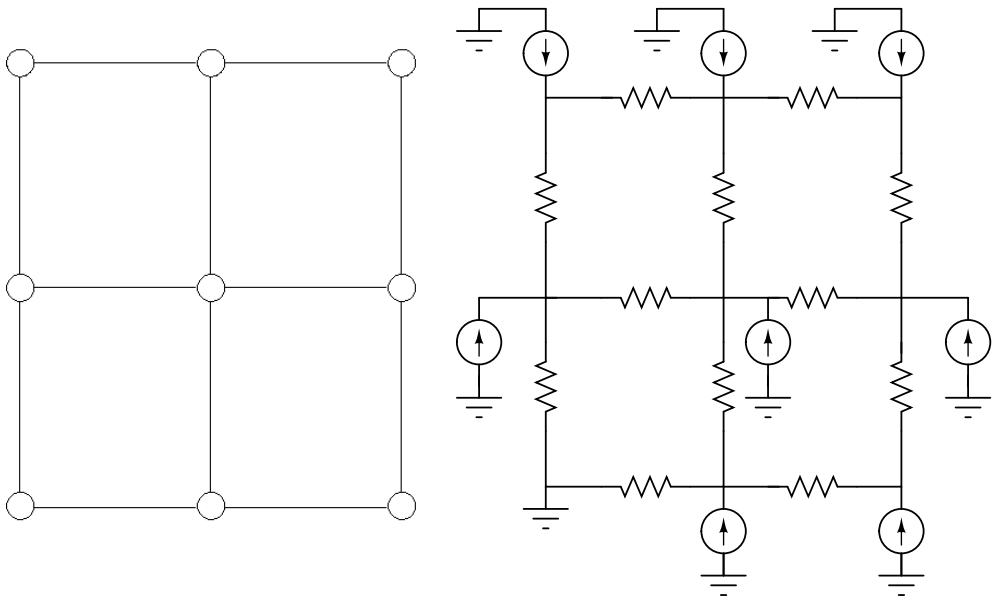
Define the $m \times n$ edge-node **incidence matrix** as

$$A_{e_{ij}v_k} = \begin{cases} +1 & \text{if } i = k, \\ -1 & \text{if } j = k, \\ 0 & \text{otherwise,} \end{cases} \tag{17}$$

for every vertex v_k and edge e_{ij}, where e_{ij} has been arbitrarily assigned an orientation. As with the Laplacian matrix, $A_{e_{ij}v_k}$ is used to indicate that the incidence matrix is indexed by edge e_{ij} and node v_k. As an operator, A may be interpreted as a combinatorial gradient operator and A^T as a combinatorial divergence [43], [11]. Define the $m \times m$ **constitutive matrix**, C, as the diagonal matrix with the weights of each edge along the diagonal.

As in the familiar continuous setting, the combinatorial Laplacian is equal to the composition of the combinatorial divergence operator with the combinatorial gradient operator, $L = A^T A$. The constitutive matrix defines a weighted inner product of edge values i.e., $\langle y, Cy \rangle$ for a vector of edge values, y [11], [10]. Therefore, the combinatorial Laplacian operator generalizes to the combinatorial Laplace-Beltrami operator via $L = A^T C A$. The case of a uniform (unit) metric, (i.e., equally weighted edges) reduces to $C = I$ and $L = A^T A$. Removing a column of the incidence matrix produces what is known as the **reduced incidence matrix**, A_0 [44].

With this interpretation of the notation used above, the three fundamental equations of circuit theory



(a) (b)

Fig. 1. An example of a simple graph and its equivalent circuit. Solving equation (16) (using the node in the lower left as ground) for the graph in (a) is equivalent to connecting the circuit in (b) and reading off the potential values at each node.

(Kirchhoff's current and voltage law and Ohm's law) may be written for a grounded circuit as

$$A_0^T y = f \quad \text{(Kirchhoff's Current Law)}, \tag{18}$$

$$Cp = y \quad \text{(Ohm's Law)}, \tag{19}$$

$$p = A_0 x \quad \text{(Kirchhoff's Voltage Law)}, \tag{20}$$

for a vector of branch currents, y, current sources, f, and potential drops (voltages), p. Note that there are no voltage sources present in this formulation. These three equations may be combined into the linear system

$$A_0^T C A_0 x = L_0 x = f, \tag{21}$$

since $A^T C A = L$ [41].

In summary, the solution to equation (16) in the isoperimetric algorithm is provided by the steady state of a circuit where each edge has a conductance equal to the edge weight and each node is attached to a current source of magnitude equal to the degree (i.e., the sum of the conductances of incident edges) of the node. The potentials that are established on the nodes of this circuit are exactly those which are being solved for in equation (16). An example of this equivalent circuit is displayed in Figure 1.

One final remark on the circuit analogy to (16) follows from recalling Maxwell's principle of least dissipation of power: A circuit with minimal power dissipation provides a solution to Kirchhoff's current

and voltage laws [45]. Explicitly, solving equation (16) for x is equivalent to solving the dual equation for $y = CAx$. The power of the equivalent circuit is $P = I^2R = y^TC^{-1}y$ subject to the constraint from Kirchhoff's law that $A^Ty = f$. Therefore, the y found by $y = CAx$ also minimizes the above expression for y [11], [46]. Thus, our approach to minimizing the combinatorial isoperimetric ratio is identical to minimizing the power of the equivalent electrical circuit with the specified current sources and ground [11].

There is a deep connection between electric circuits and random walks on graphs [47], which suggests the analysis of this algorithm in terms of a random walk on a graph. The electric potential calculated above for each node admits interpretation as the expected number of steps a random walker starting from that node would take in order to reach the ground, if his probability of walking from node v_i to v_j is equal to $\frac{w_{ij}}{d_i}$. In this interpretation, the threshold is in units of expected steps of a random walker to ground, chosen to partition the graph into subsets possessing the smallest isoperimetric ratio (see [48] for justification of this interpretation).

C. Algorithmic details

1) Summary of the algorithm: Applying the isoperimetric algorithm to data clustering or image segmentation may be described in the following steps:

1) Find weights for all edges using equation (22).
2) Build the L matrix (9) and $d = \mathrm{diag}(L)$ vector.
3) Choose the node of largest degree as the ground node, v_g, and determine L_0 and d_0 by eliminating the row/column corresponding to v_g.
4) Solve equation (16) for x_0.
5) Threshold the potentials x at the value that gives partitions corresponding to the lowest isoperimetric ratio.
6) Continue recursion on each segment until the isoperimetric ratio of the subpartitions is larger than the `stop` parameter.

2) Choosing edge weights: In order to apply the isoperimetric algorithm to partition a graph, the position values (for data clustering) or the image values (for image segmentation) must be encoded on the graph via edge weights. We employ the standard [3], [19], [49] weighting function

$$w_{ij} = \exp\left(-\beta(I_i - I_j)^2\right), \tag{22}$$

where β represents a parameter we call **`scale`** and I_i indicates the intensity value at node v_i. Note that $(I_i - I_j)^2$ may be replaced by the squared norm of a Euclidean distance in the case of vector valued data or coordinates, in the case of a clustering problem. In order to make one choice of β applicable to a wide

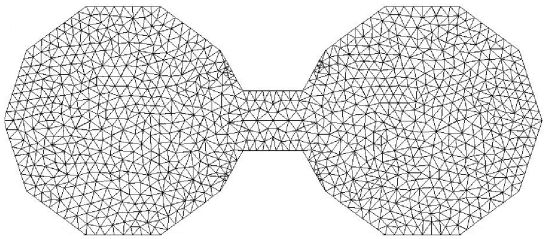


Fig. 2. Dumbbell graph with uniform weights

range of data sets, we have found it helpful to normalize the intensity differences for an image before applying (22).

3) Choosing Partitions from the Solution: The binary definition of x was extended to the real numbers in order to solve (16). Therefore, in order to convert the solution, x, to a partition, a subsequent step must be applied (as with spectral partitioning). Conversion of a potential vector to a partition may be accomplished using a threshold. A **cut value** is a value, α, such that $S = \{v_i | x_i \leq \alpha\}$ and $\overline{S} = \{v_i | x_i > \alpha\}$. The partitioning of S and $\overline{S}$ in this way may be referred to as a **cut**. This thresholding operation creates a partition from the potential vector, x. Note that since a connected graph corresponds to an L_0 that is an M-matrix [42], and is therefore monotone, $L_0^{-1} \geq 0$. This result then implies that $x_0 = L_0^{-1} d_0 \geq 0$.

Employing the terminology of [50], the standard approaches to cutting the indicator vector in spectral partitioning are to cut based on the median value (the **median cut**) or to choose a threshold such that the resulting partitions have the lowest available isoperimetric ratio (the **ratio cut**). Note that in the remainder of this paper, we use "ratio cut" in the sense of [50] (which describes a method for binarizing a real-valued solution) and not in [38], [39] or [6] (which describe complete partitioning/segmentation algorithms). The ratio cut method will clearly produce partitions with a lower isoperimetric ratio than the median cut. Unfortunately, because of the required sorting of x, the ratio cut method requires $\mathcal{O}(n \log(n))$ operations (assuming a bounded degree). The median cut method runs in $\mathcal{O}(n)$ time, but forces the algorithm to produce equal sized partitions, even if a better cut could be realized elsewhere. Despite the required sorting operation for the ratio cut, the operation is still very inexpensive relative to the solution of equation (16) for the range of n we focus on (typically 128×128 to 512×512 images). Therefore, we have chosen to employ the ratio cut method.

4) Ground node: We will demonstrate that, in the image processing context, the ground node may be viewed from an attentional standpoint. However, in the more general graph partitioning context it remains unclear how to choose the ground. Anderson and Morley [51] proved that the spectral radius of L, $\rho(L)$, satisfies $\rho(L) \leq 2d_{\max}$, suggesting that grounding the node of highest degree may have the most beneficial effect on the conditioning of equation (16). Empirically, we have found that as long as the ground is not along the ideal cut, a partition with a low isoperimetric ratio is produced.

Figure 3 illustrates this principle using the dumbbell shape (in Figure 2) discussed in Cheeger's seminal

paper [30] on the relationship of the isoperimetric constant and the eigenvalues of the Laplacian on continuous manifolds. The left column (i.e., (a), (c), (e), and (g) in Figure 3) shows the potentials, x, solved for using (16). The brightest node on the graph represents the ground node. For the rest of the nodes, bright nodes are closer to ground (i.e., have lower potentials) and dark nodes are further from ground. The right column (i.e., (b), (d), (f), and (h) in Figure 3) shows the post-threshold function where the ratio cut method has been employed. The top two rows indicate a random selection of ground nodes and the bottom two represent pathological choices of ground nodes. Of the two pathological cases, the third row example (i.e., (e) and (f) in Figure 3) uses a ground in the exact center of the neck, while the last row takes ground to be one node over from the center. Although the grounding in the exact center produces a partition that does not resemble the known ideal partition, grounding one node over produces a partition that is nearly the same as the ideal, as shown in the fourth row example (i.e., (g) and (h) in Figure 3). This illustrates that the solution is largely independent of the choice of ground node, except in the pathological case where the ground is on the ideal cut. Moreover, it is clear that choosing a ground node in the interior of the balls is better than choosing a point on the neck, which corresponds in some sense to our above rule of choosing the point with maximum degree since a node of high degree will be in the "interior" of a region, or in an area of uniform intensity in the context of image processing.

5) Solving the System of Equations: Solving equation (16) is the computational core of the algorithm. It requires the solution to a large sparse system of symmetric equations where the number of nonzero entries in L will equal $2m$.

Methods for solving a system of equation fall generally into two categories: direct and iterative methods [52], [53], [42]. The former are generally based on Gaussian elimination with partial pivoting while for the latter, the method of conjugate gradients is arguably the best approach. Iterative procedures have the advantage that a partial answer may be obtained at intermediate stages of the solution by specifying a limit on the number of iterations allowed. This feature allows one to trade speed for accuracy in finding a solution. An additional feature of using the method of conjugate gradients to solve equation (16) is that it lends itself to efficient parallelization [54], [55]. In this work, we used the sparse matrix package in ™MATLAB [56] to find direct solutions.

6) Time Complexity: Running time depends mainly on the solution to equation (16). A sparse matrix-vector operation depends on the number of nonzero values, which is, in this case, $\mathcal{O}(m)$. If we may assume a constant number of iterations is required for the convergence of the conjugate gradients method, the time complexity of solving (16) is $\mathcal{O}(m)$. Cutting the potential vector with the ratio cut requires a $\mathcal{O}(n\log(n))$ sort. Combined, the time complexity is $\mathcal{O}(m + n\log n)$. In cases of graphs with bounded degree, then $m \leq nd_{\max}$ and the time complexity reduces to $\mathcal{O}(n\log(n))$. If a constant recursion depth may be assumed (i.e., a consistent number of "objects" in the scene), the time complexity is unchanged.

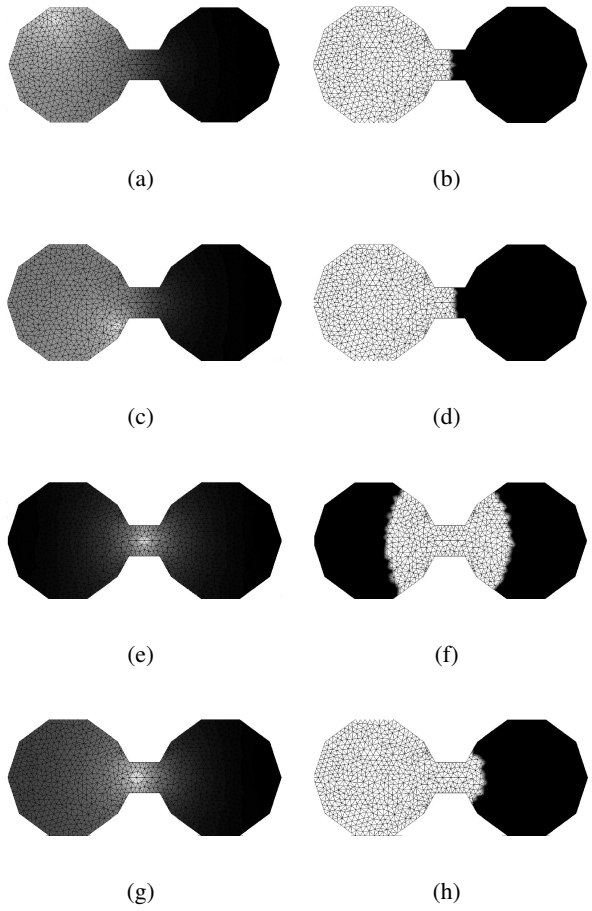


Fig. 3. An example of the effects on the solution with different choices of ground node for a problem with a trivial optimal partition. The left column shows the potential function (brightest point is ground) for several choices of ground while the right column shows thresholded partitions. Uniform weights ($\beta = 0$) were employed.

D. Relationship to Spectral Partitioning

Building on the early work of Fiedler [57], [58], [59], Alon [60], [61] and Cheeger [30], who demonstrated the relationship between the second smallest eigenvalue of the Laplacian matrix (the **Fiedler value**) for a graph and its isoperimetric constant, spectral partitioning was one of the first successful graph partitioning algorithms [7], [36]. The algorithm partitions a graph by finding the eigenvector corresponding to the Fiedler value, termed the **Fiedler vector**, and cutting the graph based on the value in the Fiedler vector associated with each node. Like isoperimetric partitioning, the output of the spectral partitioning algorithm is a set of values assigned to each node, which require cutting in order to generate partitions.

Spectral partitioning may be used [36] to minimize the isoperimetric ratio of a partition by solving

$$Lz = \lambda z, \tag{23}$$

with L defined as above and λ representing the Fiedler value. Since the vector of all ones, r, is an eigenvector corresponding to the smallest eigenvalue (zero) of L, the goal is to find the eigenvector

associated with the second smallest eigenvalue of L. Requiring $z^T r = 0$ and $z^T z = n$ may be viewed as additional constraints employed in the derivation of spectral partitioning to circumvent the singularity of L (see, [62] for an explicit formulation of spectral partitioning from this viewpoint). Therefore, one way of viewing the difference between the isoperimetric and the spectral methods is in terms of the choice of an additional constraint that allows one to circumvent the singular nature of the Laplacian L.

In the context of spectral partitioning, the indicator vector z is usually defined as

$$z_i = \begin{cases} -1 & \text{if } v_i \in \overline{S}, \\ +1 & \text{if } v_i \in S, \end{cases} \tag{24}$$

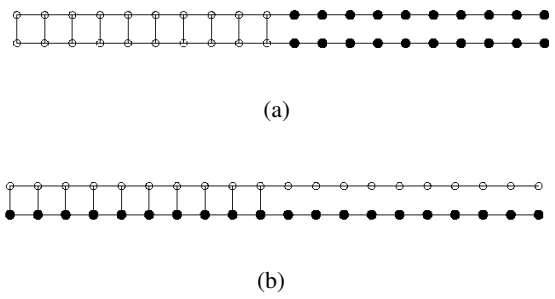
such that z is orthogonal to r, for $|S| = \frac{1}{2}|V|$. The two definitions of the indicator vector (equations (8) and (24)) are related through $x = \frac{1}{2}(z + r)$. Since r is in the nullspace of L, the definitions are equivalent up to a scaling.

The Ncuts algorithm of Shi and Malik [3] is essentially the spectral partitioning algorithm, except that the authors implicitly choose the metric of [35] to define a combinatorial Laplacian matrix rather than the metric of [34] typically used to define the Laplacian in spectral partitioning. Specifically, the Ncuts algorithm requires the solution of

$$D^{-\frac{1}{2}} L D^{-\frac{1}{2}} z = \lambda z, \tag{25}$$

where $D = \text{diag}(d)$. Therefore, although the spectral and Ncuts algorithms produce different results when applied to a specific graph, they share many theoretical properties.

Despite the remarkable success of spectral partitioning [36], it has been pointed out that there are some significant problems. Guattery and Miller [63] proposed families of graphs for which spectral partitioning fails to produce the best partition. One of these is the "roach" graph shown in Figure 4. This graph will always be partitioned by the spectral method into two symmetrical halves (using the median cut), which yields a suboptimal partition relative to the minimum isoperimetric ratio criterion. For a roach with an equal number of "body" and "antennae" segments, the spectral algorithm will always produce a partition with $|\partial S| = \Theta(n)$ (where $\Theta()$ is the function of [64]) instead of the constant cut set of two edges obtained by cutting the antennae from the body. Teng and Spielman [50] demonstrated that the spectral approach may be made to correctly partition the roach graph if additional processing is performed. The partitions obtained from the spectral and isoperimetric algorithms when applied to the roach graph are compared in Figure 4. The solution for the spectral method was obtained from the MESHPART toolbox written by Gilbert, Miller and Teng [65]. This simple example demonstrates that the isoperimetric algorithm performs in a fundamentally different manner from the spectral method and, at least in this case, outperforms it significantly. We note that the failure of the spectral algorithm to produce a good partition of the roach graph is not a function of a difference in criterion (i.e., the partition given by the isoperimetric algorithm



(a)

(b)

Fig. 4. The "roach" graph (n = 20) illustrated here is a member of a family of graphs for which spectral partitioning is known to fail to produce a partition with low isoperimetric ratio. Uniform weights were used for both algorithms. (a) Solution using isoperimetric algorithm. Ratio = 0.1. (b) Solution using spectral algorithm. Ratio = 0.5.

is favored by both criteria over the spectral result) but rather lies in the fact that each approach employs a different heuristic to find a reasonable solution to an NP-Hard problem.

A second difference is that the isoperimetric method requires the solution of a sparse linear system rather than the solution to the eigenvector problem required by spectral methods of image segmentation [3], [5], [4]. The Lanczos algorithm provides an excellent method for approximating the eigenvectors corresponding to the smallest or largest eigenvalues of a matrix with a time complexity comparable to the conjugate gradient method of solving a sparse system of linear equations [52]. However, solution to the eigenvector problem is less stable to minor perturbations of the matrix than the solution to a system of linear equations, if the desired eigenvector corresponds to an eigenvalue that is very close to other eigenvalues (see, [52]). In fact, the eigenvector problem is degenerate for graphs in which the Fiedler value has algebraic multiplicity greater than one, allowing the Lanczos algorithm to converge to any vector in the subspace spanned by the Fiedler *vectors* (if it converges at all). A square lattice with uniform weights is an example of a graph for which the Fiedler value has algebraic multiplicity greater than unity, as is the fully connected graph with uniform weights (see Appendix III). The authors of [66] raise additional concerns about the Lanczos method. Appendix II formally compares the sensitivity of the isoperimetric, spectral and Ncuts algorithms to a changing edge weight. We note that most graph partitioning-based image segmentation algorithms rely on the solution to an eigenvector problem. In contrast, the isoperimetric algorithm requires the solution of a linear system, and is therefore robust to the previous criticism.

III. Applications

A. Clustering applied to examples used by Zahn

When humans view a point cluster, certain groupings immediately emerge. The properties that define this grouping have been described by the Gestalt school of psychology . Unfortunately, these descriptions are not precisely defined and therefore finding an algorithm that can group clusters in the same way has proven very difficult. Zahn used his minimal spanning tree idea to try to capture these Gestalt clusters

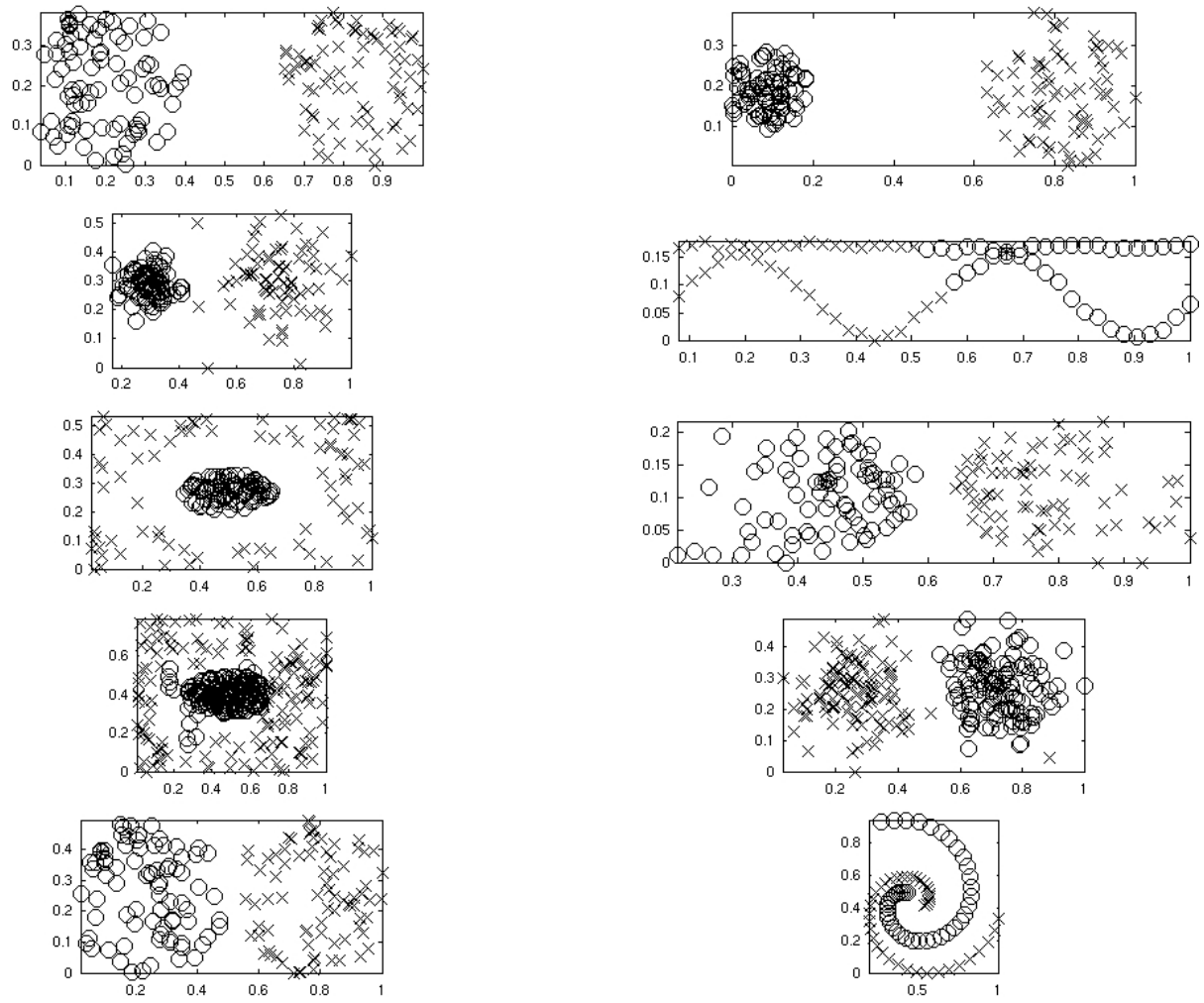
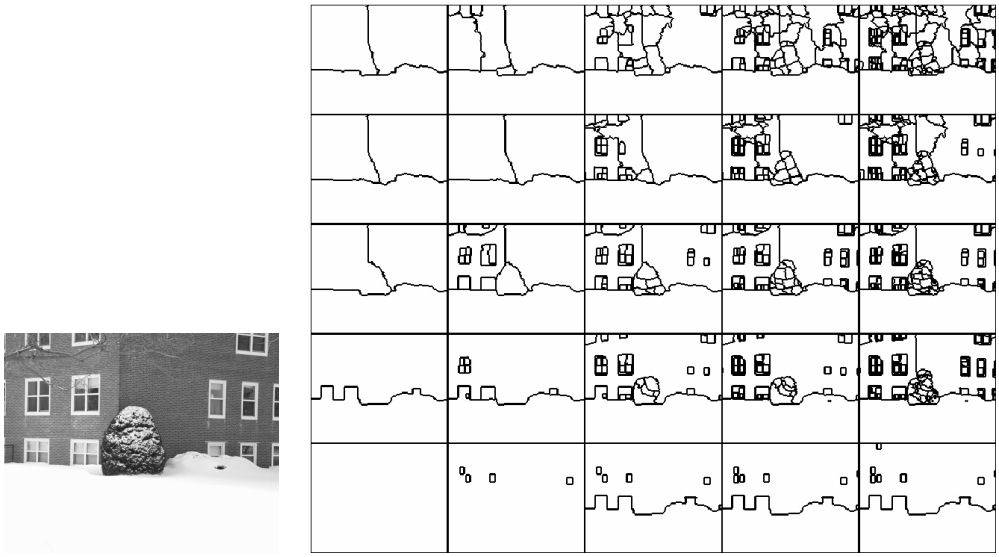


Fig. 5. An example of partitioning the Gestalt-inspired point set challenges of Zahn using the isoperimetric algorithm. The x's and o's represent points in different partitions. $\beta = 50$.

[1]. To this end, he established a collection of point sets with clear cluster structure (to a human), but which are difficult for a single algorithm to group.

We stochastically generated point clusters to mimic the challenges Zahn issues to automatic clustering algorithms. For a set of points, it is not immediately clear how to choose which nodes are connected by edges. In order to guarantee a connected graph, but still make use of local connections, we generated an edge set from the Delaunay triangulation of the points. Edge weights were generated as a function of Euclidean geometric distance, as in equation (22).

The clusters and partitions are shown below in Figure 5. Each partition is represented by a symbol, with the 'x's and 'o's indicating the points belonging to the same partition. Partitions were generated using the median cut on a single solution to (16). Ground nodes were chosen using the maximum degree rule discussed above. Of these clusters, it is shown in Figure 5 that the algorithm performs as desired on all groups, failing only on the problem in the second row of the second column that appears to require a more cognitive grouping.



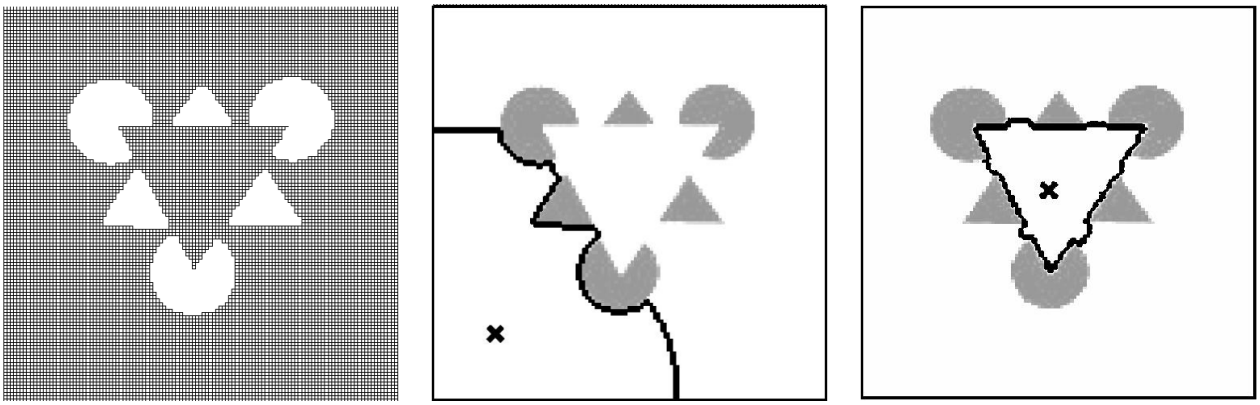
(a) (b)

Fig. 6. (a) Image used to benchmark the effects of a changing `scale` and `stop` parameter. (b) This tiled figure demonstrates the results of varying the `scale` (vertical) and `stop` (horizontal) parameters when processing the image in (a), showing a large range of stable solutions. `scale` range: 300–30, `stop` range: $1 \times 10^{-5.5}$–$1 \times 10^{-4.5}$.

B. Methods of image segmentation

As in the case of point clustering, it is not clear, *a priori*, how to impose a graph structure on an image. Since pixels define the discrete input, a simple choice for nodes is the pixels and their values. Traditional neighborhood connectivity employs a 4-connected or 8-connected topology [67]. Another approach, taken by Shi and Malik [3] is to use a fully connected neighborhood within a parameterized radius of each node. We chose to use a minimal 4-connected topology since the matrix L becomes less sparse as more edges are added to the graph, and a graph with more edges requires more time to solve equation (16). Edge weights were generated from intensity values in the case of a grayscale image or from RGB color values in the case of a color image using equation (22).

The isoperimetric algorithm is controlled by only two parameters: the `scale` parameter β of equation (22) and the `stop` parameter used to end the recursion. The `scale` affects how sensitive the algorithm is to changes in feature space (e.g., RGB, intensity), while the `stop` parameter determines the maximum acceptable isoperimetric ratio a partition must generate in order to accept it and continue the recursion. In order to illustrate the dependence of the results on parameterization, a sweep of the two-dimensional parameter space was performed on individual natural images. An example of this parameter-sweep is shown using a natural image, with the `scale` parameter on the vertical and the `stop` parameter on the horizontal (Figure 6). It can be seen that the solution is similar over a broad range with respect to changes in `scale` and that the effect of raising the `stop` parameter (i.e., making more partitions admissible) is to generate a greater number of small partitions.



(a) (b) (c)

Fig. 7. The Kaniza triangle illusion with the single bipartition outlined in black and the ground node marked with an 'x'. (a) The graph being segmented. (b) Isoperimetric partition using a ground point in the corner. (c) Isoperimetric partition using a ground point inside the triangle. Uniform weights ($\beta = 0$) were employed in both cases.

C. Completion

Study of the classic Kaniza illusion [68] suggests that humans segment objects based on something beyond perfectly connected edge elements. The isoperimetric algorithm was used to segment the image in Figure 7, using only one level of recursion with all nodes corresponding to the black "inducers" removed. In this case, choice of the ground node is important for determining the single bipartition. If the ground node is chosen inside the illusory triangle, the resulting partition is the illusory triangle. However, if the ground is chosen outside, the triangle partition is not produced, but instead a partition that hugs the corner in which the ground is located. In this way, the ground node may be considered as representing something like an "attentional" point, since it induces a partition that favors the region of the ground node. However, note that these partitions are compatible with each other, suggesting that the choice of ground may affect only the order in which partitions are found. We believe that the ability to "complete" an object boundary is an important quality for a segmentation algorithm, since natural images frequently contain weak object boundaries.

D. Segmentation of natural images

Having addressed issues regarding stability and completion, we proceed to examples of the segmentation found by the isoperimetric algorithm when applied to natural images. Examples of the segmentation found by the isoperimetric algorithm for some natural images are displayed in Figure 8. All results in the example segmentations were obtained using the same two parameters. It should be emphasized in comparisons of segmentations produced by the Ncuts algorithm that the authors of Ncuts make use of a more fully connected neighborhood as well as fairly sophisticated spatial filtering (e.g., oriented Gabor filters at multiple scales) in order to aid in textural segmentation. The demonstrations with the

isoperimetric algorithm used a basic 4-connected topology and no spatial filtering at all. Consequently, the segmentations produced by the isoperimetric algorithm should be expected to perform less well on textural cues. However, for general grayscale images, it appears to perform well, with increased numerical stability and a speed advantage of more than an order of magnitude over Ncuts (based on our TMMATLAB implementation of both algorithms). Furthermore, because of the implementation (e.g., 4-connected lattice, no spatial filtering), the isoperimetric algorithm makes use of only two parameters, compared to the four basic parameters (i.e., radius, two weighting parameters and the recursion stop criterion) required in the Ncuts paper [3].

The asymptotic (formal) time complexity of Ncuts is roughly the same as the isoperimetric algorithm. Both algorithms have an initial stage in which nodal values are computed that requires approximately $\mathcal{O}(n)$ operations (i.e., via Lanczos or conjugate gradient). Generation of the nodal values is followed in both algorithms by an identical cutting operation. Using the TMMATLAB sparse matrix solver for the linear system required by the isoperimetric algorithm and the Lanczos method (TMMATLAB employs ARPACK [69] for this calculation) to solve the eigenvalue problem required by Ncuts, the time was compared for a 10000×10000 L matrix (i.e., a 100×100 pixel image) representing a 4-connected graph (for both algorithms). Since other aspects of the algorithms are the same (e.g., generating weights from the image, cutting the indicator vector, etc.), and because solving for the indicator vector is the main computational hurdle, we only compare the time required to solve for the indicator vector. On a 1.4GHz AMD Athlon with 512K RAM, the time required to approximate the Fiedler vector in equation (25) was 7.1922 seconds while application of the direct solver to the isoperimetric partitioning equation (16) required 0.5863 seconds. In terms of actual computation time (using TMMATLAB), this result means that solving the central computation for the isoperimetric algorithm is more than an order of magnitude faster than solving the central computation required by the Ncuts algorithm.

E. Stability

Stability of the solution for both the isoperimetric algorithm and the spectral algorithms differs considerably, as does the perturbation analysis for the solution to a system of equations versus the solution to the eigenvector problem [52]. Differentiating equations (16) and (25) with respect to an edge weight reveals that the derivative of the solution to the spectral (23) and Ncuts (25) equations is highly dependent on the current Fiedler value, even taking degenerate solutions for some values (see Appendix II). By contrast, the derivative of the isoperimetric solution has no poles. Instability in spectral methods due to algebraic multiplicity of the Fiedler value is a common problem in implementation of these algorithms (see [70]). This analysis suggests that the Ncuts algorithm may be more unstable to minor changes in an image than the isoperimetric algorithm.

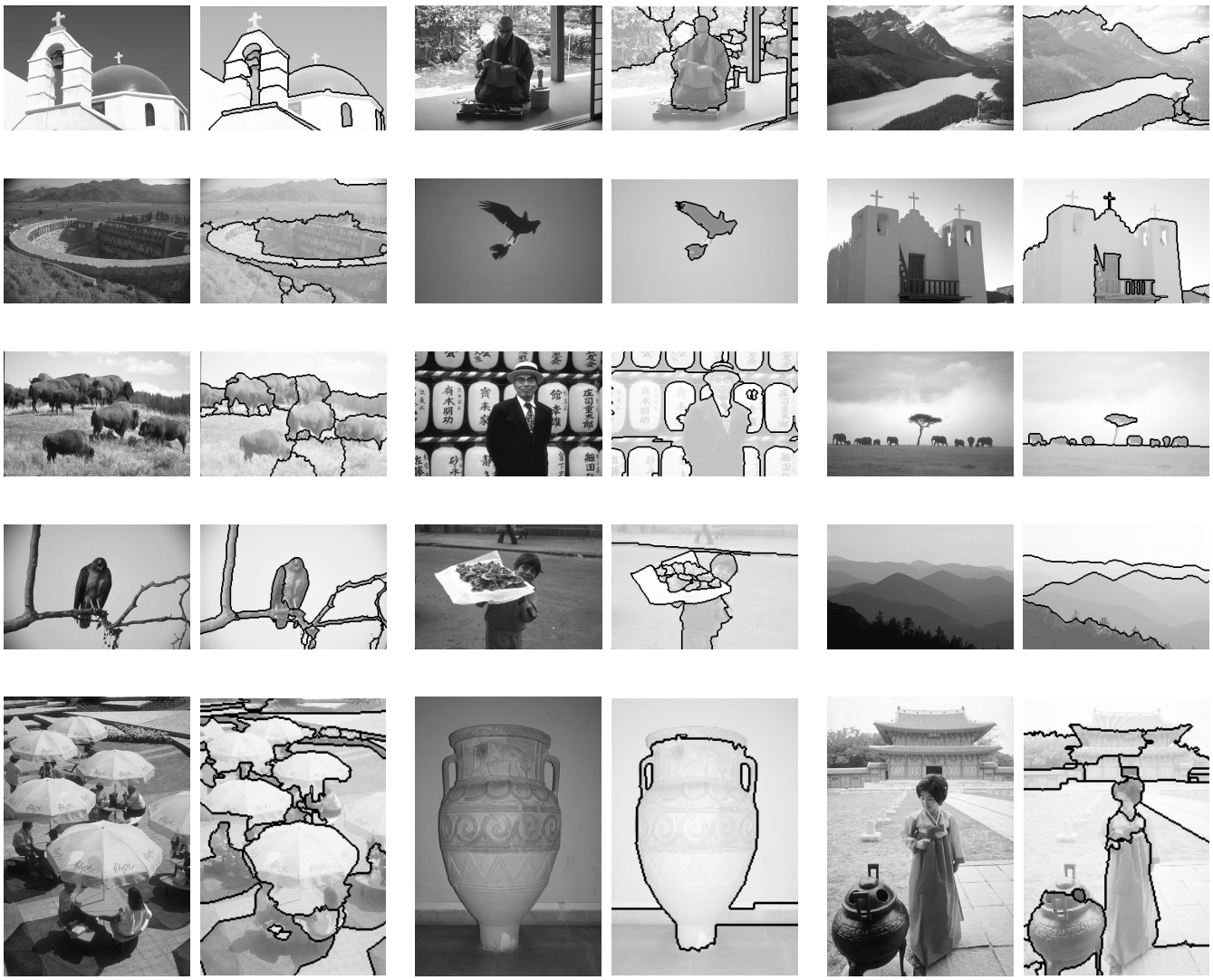
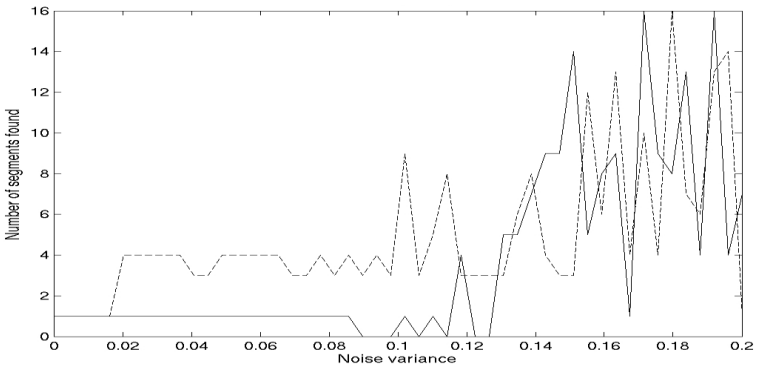


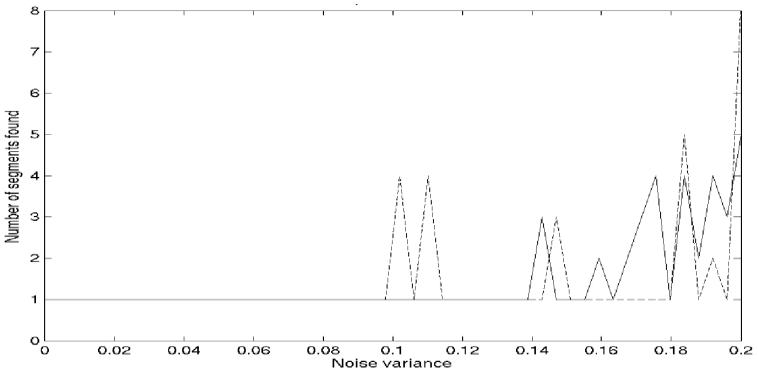
Fig. 8. Examples of segmentations produced by the isoperimetric algorithm using the same parameters ($\beta = 95$, `stop` = 10^{-5}). Our ™MATLAB implementation required approximately 10–15 seconds to segment each image. Additional segmentation results from our publicly available image database may by found at `http://eslab.bu.edu/publications/grady2003isoperimetric/`

The sensitivity of Ncuts (our implementation) and the isoperimetric algorithm to noise is compared using a quantitative and qualitative measure. First, each algorithm was applied to an artificial image of a white circle on a black background, using a 4-connected lattice topology. Increasing amounts of additive, multiplicative and shot noise were applied, and the number of segments output by each algorithm was recorded. Results of this comparison are recorded in Figure 9.

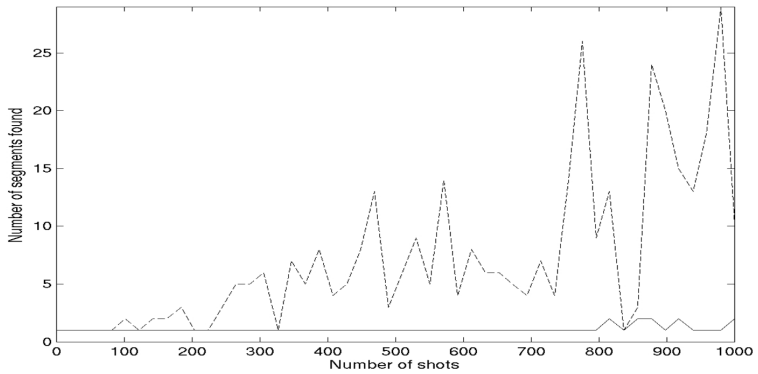
In order to visually compare the result of the segmentation algorithms applied to progressively noisier images, the isoperimetric and Ncuts algorithms were applied to a relatively simple natural image of red blood cells. The isoperimetric algorithm operated on a 4-connected lattice, while Ncuts was applied to an 8-connected lattice, since we had difficulty finding parameters that would cause Ncuts to give a good segmentation of the original image if a 4-connected lattice was used.



(a) Additive noise



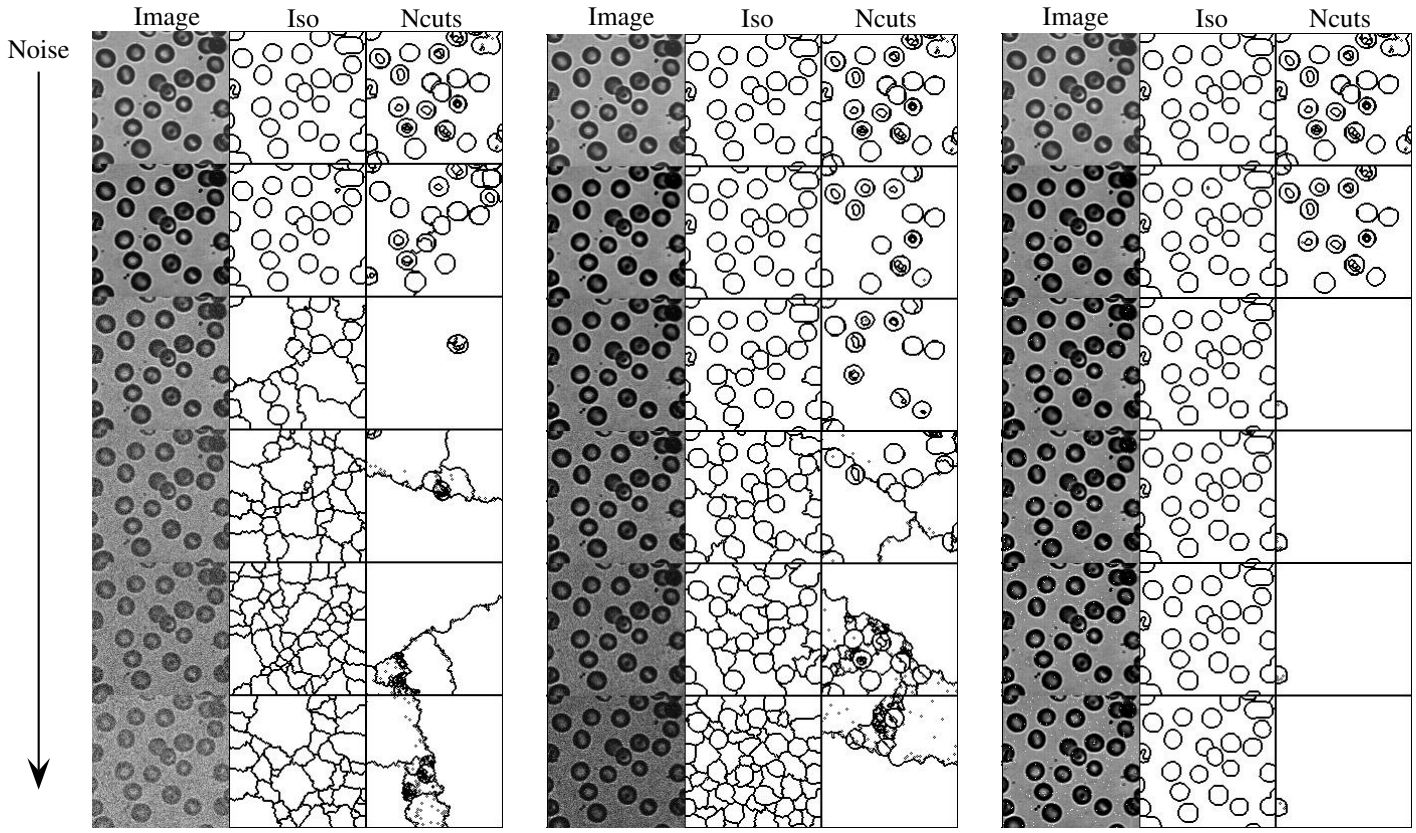
(b) Multiplicative noise



(c) Shot noise

Fig. 9. Stability analysis relative to additive, multiplicative and shot noise for an artificial image of a white circle on a black background, for which the correct number of segments should be one. The x-axis represents an increasing noise variance for the additive and multiplicative noise, and an increasing number of "shots" for the shot noise. The y-axis indicated the number of segments found by each algorithm. The solid line represents the results of the isoperimetric algorithm and the dashed line represents the results of the Ncuts algorithm. The underlying graph topology was the 4-connected lattice with $\beta = 95$ for the isoperimetric algorithm and $\beta = 35$ for the Ncuts algorithm. Ncuts `stop` criterion = 10^{-2} (relative to the Ncuts criterion) and isoperimetric `stop` criterion = 10^{-5}. In all cases, the isoperimetric algorithm outperforms Ncuts, most dramatically in response to shot noise. The β and `stop` values for each algorithm were chosen empirically to produce the best results for that algorithm in response to noise.

In both comparisons, additive, multiplicative, and shot noise were used to test the sensitivity of the two algorithms to noise. The additive noise was zero mean Gaussian noise with variance ranging from 1–20% of the brightest luminance. Multiplicative noise was introduced by multiplying each pixel by a unit mean Gaussian variable with the same variance range as above. Shot noise was added to the image by randomly selecting pixels that were fixed to white. The number of "shots" ranged from 10 to 1,000. The above discussion of stability is illustrated by the comparison in Figure 10. Although additive and multiplicative noise heavily degrades the solution found the Ncuts algorithms, the isoperimetric algorithm degrades more gracefully. Even the presence of a significant amount of shot noise does not seriously disrupt the isoperimetric algorithm, but it significantly impacts the convergence of Ncuts to any solution.



(a) Additive noise (b) Multiplicative noise (c) Shot noise

Fig. 10. Stability analysis relative to additive, multiplicative and shot noise. Each row represents an increasing amount of noise of the appropriate type. The top row in each subfigure is the segmentation found for the `blood1.tif` image packaged with ™MATLAB (i.e., zero noise). Each figure is divided into three columns representing the image with noise, isoperimetric segmentation and Ncuts segmentation from left to right respectively. The underlying graph topology was the 4-connected lattice for isoperimetric segmentation and an 8-connected lattice for Ncuts segmentation (due to failure to obtain quality results with a 4-connected lattice) with $\beta = 95$ for the isoperimetric algorithm and $\beta = 35$ for the Ncuts algorithm. Ncuts `stop` criterion = 5×10^{-2} (relative to the Ncuts criterion) and isoperimetric `stop` criterion = 10^{-5}. Results were slightly better for additive noise, and markedly better for multiplicative and shot noise. Note that the β and `stop` values for each algorithm were chosen empirically to produce the best results for that algorithm in response to noise. (a) Additive noise. (b) Multiplicative noise. (c) Shot noise.

IV. Conclusion

We have presented a new algorithm for graph partitioning that attempts to find sets with a low isoperimetric ratio. Our algorithm was then applied to the problems of data point clustering and image segmentation. The algorithm was compared with Ncuts to demonstrate that it is faster and more stable, while providing visually comparable results with less pre-processing. The isoperimetric algorithm additionally admits interpretation in terms of circuit theory, random walks and combinatorial PDEs, lending the depth of these well-researched literatures to analysis of the algorithm's behavior. The (MATLAB) code used to generate all the figures in this paper will be available upon publication at `http://eslab.bu.edu/publications/grady2005isoperimetric/` using the Graph Analysis Toolbox [71] available at `http://eslab.bu.edu/software/graphanalysis/`.

Developing algorithms to process a distribution of data on graphs is an exciting area. Many biological sensory units are non-uniformly distributed in space (e.g., vision, somatic sense) with spatial distribution often differing radically between species [72]. The ability to develop algorithms that allow the designer a free hand in choosing the distribution of sensors (or data of any sort) represents a large step over existing algorithms that require a regular, shift-invariant lattice.

These initial findings are encouraging. Since the graph representation is not tied to any notion of dimension, the algorithm applies equally to graph-based problems in N-dimensions as it does to problems in two dimensions. Suggestions for future work are applications to segmentation in space-variant architectures, supervised or unsupervised learning, 3-dimensional segmentation, and the segmentation/clustering of other areas that can be naturally modeled with graphs.

Appendix I
Connectivity

The purpose of this section is to prove that regardless of how a ground is chosen, the partition containing the grounded node (i.e., the set S) must be connected, independent of how a threshold (i.e., cut) is chosen. The strategy for proving this will be to show that every node has a path to ground such that each node in that path has a monotonically decreasing potential.

Proposition 1: If the set of vertices, V, is connected then, for any α, the subgraph with vertex set $N \subseteq V$ defined by $N = \{v_i \in V | x_i < \alpha\}$ is connected when x_0 satisfies $L_0 x_0 = f_0$ for any $f_0 \geq 0$.

This proposition follows directly from proof of the following

Lemma 1: For every node, v_i, there exists a path to the ground node, v_g, defined by $P_i = \{v_i, v^1, v^2, \ldots, v_g\}$ such that $x_i \geq x^1 \geq x^2 \geq \ldots \geq 0$, when $L_0 x_0 = f_0$ for any $f_0 \geq 0$.

Proof: By equation (16) each non-grounded node assumes a potential

$$x_i = \frac{1}{d_i} \sum_{e_{ij} \in E} x_j + \frac{f_i}{d_i}, \tag{26}$$

i.e., the potential of each non-grounded node is equal to a nonnegative constant added to the (weighted) average potential of its neighbors. Note that (26) is a combinatorial formulation of the Mean Value Theorem [73] in the presence of sources.

For any connected subset, $S \subseteq V, v_g \notin S$, denote the set of nodes on the boundary of S as $S_b \subset V$, such that $S_b = \{v_i |\, e_{ij} \in E,\, \exists\, v_j \in S,\, v_i \notin S\}$.

Now, either

1) $v_g \in S_b$, or
2) $\exists\, v_i \in S_b$, such that $x_i \leq \min x_j,\, \forall\, v_j \in S$ by (26), since the graph is connected.

Therefore, every node has a path to ground with a monotonically decreasing potential, by induction (i.e., start with $S = \{v_i\}$ and add nodes with a nonincreasing potential until ground is reached). ■

APPENDIX II
SENSITIVITY ANALYSIS

Previous work in circuit theory allows for a straightforward analysis of the sensitivity of the isoperimetric, spectral, and normalized cuts algorithms. Here we specifically examine the sensitivity to the edge weights for these three algorithms.

Sensitivity to a single, general parameter, s, is developed in this section. Sensitivity computation for many parameters (e.g., all the weights in a graph) may be obtained efficiently using the adjoint method [74].

A. Isoperimetric

Given the vector of degrees, d, the Laplacian matrix, L, and the reduced Laplacian matrix L_0, the isoperimetric algorithm requires the solution to

$$L_0 x_0 = d_0. \tag{27}$$

The sensitivity of the solution to equation (27) with respect to a parameter s may be determined from

$$L_0 \frac{\partial x_0}{\partial s} = -\frac{\partial L_0}{\partial s} x_0 + \frac{\partial d_0}{\partial s}. \tag{28}$$

Since L_0, x_0 are known (for a given solution to equation (27) and $\frac{\partial L_0}{\partial s}$ may be determined analytically, $\frac{\partial x_0}{\partial s}$ may be solved for as a system of linear equations (since L_0 is nonsingular) in order to yield the derivative at a point x_0.

B. Spectral

The spectral method solves the equation

$$Lx = \lambda_2 x, \tag{29}$$

where λ_2 is the Fiedler value. The sensitivity of the solution to equation (29) to a parameter s is more complicated, but proceeds in a similar fashion from the equation

$$\frac{\partial L}{\partial s}x + L\frac{\partial x}{\partial s} = \frac{\partial \lambda_2}{\partial s}x + \lambda_2\frac{\partial x}{\partial s}. \tag{30}$$

The term $\frac{\partial \lambda_2}{\partial s}$ may be calculated from the Rayleigh quotient for λ_2 and the chain rule. The Rayleigh quotient is

$$\lambda = \frac{x^T L x}{x^T x}. \tag{31}$$

The chain rule determines $\frac{\partial \lambda_2}{\partial s}$ by $\frac{\partial \lambda_2}{\partial s} = \frac{\partial \lambda_2}{\partial x}\frac{\partial x}{\partial s}$. This may be solved by finding $\frac{\partial \lambda_2}{\partial x}$ from the Rayleigh quotient via

$$\frac{\partial \lambda_2}{\partial x} = 2Lx(x^T x)^{-1} - 2x^T L x (x^T x)^{-2} x. \tag{32}$$

Equation (32) allows us to solve for $\frac{\partial \lambda_2}{\partial s}$ via equations (30) and (32)

$$\left(L - \left(\frac{\partial \lambda_2}{\partial x}^T x + \lambda_2\right) I\right)\frac{\partial x}{\partial s} = \frac{\partial L}{\partial s}x. \tag{33}$$

Equation (33) also gives a system of linear equations which may be solved for $\frac{\partial x}{\partial s}$ since all the other terms are known or may be determined analytically.

C. Normalized Cuts

The normalized cuts algorithm [3] requires the solution to

$$D^{-\frac{1}{2}} L D^{-\frac{1}{2}} x = \lambda_2 x, \tag{34}$$

where D is a diagonal vector with $D_{ii} = d_i$. In a similar fashion to the above treatment on the spectral algorithm, the sensitivity of x with respect to a parameter s may be determined using the Rayleigh quotient and the chain rule.

Employing the chain rule, taking the derivative of equation (34) with respect to s and rearranging yields

$$\left(D^{-\frac{1}{2}} L D^{-\frac{1}{2}} - \left(\frac{\partial \lambda_2}{\partial x}^T x + \lambda_2\right) I\right)\frac{\partial x}{\partial s} = \left(2\frac{\partial D^{-\frac{1}{2}}}{\partial s} L D^{-\frac{1}{2}} + D^{-\frac{1}{2}}\frac{\partial L}{\partial s} D^{-\frac{1}{2}}\right) x. \tag{35}$$

Again, this is a system of linear equations for $\frac{\partial x}{\partial s}$. For Ncuts, the eigenvalue corresponds to $D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$

instead of L, so $\frac{\partial \lambda_2}{\partial x}$ must be recomputed from the Rayleigh quotient. The result of this calculation is

$$\frac{\partial \lambda_2}{\partial x} = 2D^{-\frac{1}{2}}LD^{-\frac{1}{2}}x(x^Tx)^{-1} - 2x^TD^{-\frac{1}{2}}LD^{-\frac{1}{2}}x(x^Tx)^{-2}x. \tag{36}$$

D. Sensitivity to a weight

Using the results above, it is possible to analyze the effect of a specific parameter by finding $\frac{\partial L}{\partial s}$, $\frac{\partial d}{\partial s}$ and $\frac{\partial D^{-\frac{1}{2}}}{\partial s}$ for the specific parameter in question. The value for $\frac{\partial L_0}{\partial s}$ is determined from $\frac{\partial L}{\partial s}$ simply by deleting the row and column corresponding to the grounded node. For a specific weight, w_{ij}, these quantities become

$$\left(\frac{\partial d}{\partial w_{ij}}\right)_{v_i} = \begin{cases} 1 & \text{if } e_{ij} \text{ is incident on } v_i, \\ 0 & \text{otherwise,} \end{cases} \tag{37}$$

and

$$\left(\frac{\partial D^{-\frac{1}{2}}}{\partial w_{ij}}\right)_{v_p v_q} = \begin{cases} -\frac{1}{2}d_p^{-\frac{3}{2}} & \text{if } p = q,\ p = i \text{ or } p = j, \\ 0 & \text{otherwise.} \end{cases} \tag{38}$$

The matrix $\frac{\partial L}{\partial w_{ij}}$ equals the L matrix of a graph with an edge set reduced to just $E = \{e_{ij}\}$. The degree of node v_i is specified by d_i.

Equations (28), (30) and (35) demonstrate that the derivative of the isoperimetric solution is never degenerate (i.e., the left hand side is always nonsingular for a connected graph), whereas the derivative of the spectral and normalized cuts solutions may be degenerate depending on the current state of the Fiedler vector and value.

APPENDIX III
FULLY CONNECTED GRAPHS

The isoperimetric algorithm will produce an unbiased solution to equation (16) when applied to fully connected graphs with uniform weights. Any set with cardinality equal to half the cardinality of the vertex set and its complement is an isoperimetric set for a fully connected graph with uniform weights. For a uniform edge weight, $w(e_{ij}) = \kappa$ for all $e_{ij} \in E$, the solution, x_0, to equation (16) will be $x_i = 1/\kappa$ for all $v_i \in V$. The use of the median or ratio cut method will choose half of the nodes arbitrarily. Although it should be pointed out that using a median or ratio cut to partition a vector of randomly assigned potentials will also produce equal sized (in this case optimal) partitions, the solution to equation (16) is unique for a specified ground (in contrast to spectral partitioning or Ncuts, which has $n-1$ solutions) and explicitly gives no node a preference since all the potentials are equal.

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