TECHNISCHE UNIVERSITÄT
CHEMNITZ

A note on Fiedler vectors interpreted as graph realizations

C. Helmberg S. Reiss

Preprint 2010-1

Fakultät für Mathematik

Impressum:
Herausgeber:
Der Dekan der
Fakultät für Mathematik
an der Technischen Universität Chemnitz
Sitz:
Reichenhainer Straße 39
09126 Chemnitz
Postanschrift:
09107 Chemnitz
Telefon: (0371) 531-22000
Telefax: (0371) 531-22009
E-Mail: dekanat@mathematik.tu-chemnitz.de
Internet:
http://www.tu-chemnitz.de/mathematik/
ISSN 1614-8835 (Print)

A note on Fiedler vectors interpreted as graph realizations

Christoph Helmberg and Susanna Reiss*

August 13, 2009

Abstract

The second smallest eigenvalue of the Laplace matrix of a graph and its eigenvectors, also known as Fiedler vectors in spectral graph partitioning, carry significant structural information regarding the connectivity of the graph. Using semidefinite programming duality we offer a geometric interpretation of this eigenspace as optimal solution to a graph realization problem. A corresponding interpretation is also given for the eigenspace of the maximum eigenvalue of the Laplacian.

Keywords: spectral graph theory, semidefinite programming, eigenvalue optimization, embedding, graph partitioning

MSC 2000: 05C50; 90C22, 90C35, 05C10, 05C78

Consider an undirected simple graph $G := (N, E)$ with node set $N := \{1, \ldots, n\}$, edge set $E \subseteq \{\{i, j\} : i, j \in N, i \neq j\}$ and edge weights $c \in \mathbb{R}^E_+$. For brevity we write ij instead of $\{i, j\}$. Defining symmetric $N \times N$ matrices $E_{ij} := (e_i - e_j)(e_i - e_j)^\top$, where e_i denotes the i-th column of the identity matrix I, the weighted Laplacian of G is the matrix $L_c(G) := \sum_{ij \in E} c_{ij} E_{ij}$. If G is clear from the context we simply write L_c and we also drop the subscript c if $c = \mathbf{1}$. Here and in the following $\mathbf{1}$ denotes the vector of all ones of appropriate dimension. Spectral properties of L are a central topic in spectral graph theory [2, 10, 1], we recall the basic facts needed in the sequel. Because the matrices E_e are positive semidefinite and $\mathbf{1}$ is an eigenvector of E_e to the eigenvalue zero, this also holds for L_c. For $c > 0$ the second smallest eigenvalue $\lambda_2(L_c)$ is nonzero if and only if G is connected. Fiedler [3, 4, 5] proved several further relationships between $\lambda_2(L_c)$, its eigenvectors, and the connectivity of the graph and coined the name *algebraic connectivity* for $\lambda_2(L)$. In his honor, eigenvectors to λ_2 are also called Fiedler vectors. They form the basis of spectral graph partitioning heuristics, see, *e.g.*, [12] and the references therein. In [5, 6] Fiedler introduced the *absolute algebraic connectivity*,

$$\hat{a}(G) := \max\{\lambda_2(L_c) : c \in \mathbb{R}^E_+, \sum_{e \in E} c_e = |E|\}. \tag{1}$$

Göring et al. [8] give a scaled dual semidefinite programming formulation (for symmetric matrices $A, B \in \mathbb{R}^{k \times k}$ we use the inner product $\langle A, B\rangle := \operatorname{trace}(AB)$ and $A \succeq 0$ if A is positive semidefinite),

$$\begin{array}{rll} \frac{|E|}{\hat{a}(G)} = \text{maximize} & \langle I, X\rangle & \\ \text{subject to} & \langle E_{ij}, X\rangle \leq 1 & \text{for } ij \in E, \\ & \langle \mathbf{1}\mathbf{1}^\top, X\rangle = 0, & \\ & X \succeq 0. & \end{array} \tag{2}$$

Via a gram representation $X = V^\top V$ with $V = [v_1, \ldots, v_n] \in \mathbb{R}^{n \times N}$ this provides a dual interpretation of $\hat{a}(G)$ in form of the following graph realization problem ($\|\cdot\|$ denotes the Euclidean

*Fakultät für Mathematik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany. {helmberg, susanna.reiss}@mathematik.tu-chemnitz.de

norm),

$$\frac{|E|}{\hat{a}(G)} = \begin{array}{ll} \text{maximize} & \sum_{i\in N}\|v_i\|^2 \\ \text{subject to} & \|v_i - v_j\| \le 1 \qquad \text{for } ij \in E, \\ & \sum_{i\in N} v_i = 0, \\ & v_i \in \mathbb{R}^n \text{ for } i \in N. \end{array} \tag{3}$$

An optimal solution of (3) spreads out the nodes as far as possible while keeping adjacent nodes at distance at most one and the barycenter in the origin. The emphasis of [8] was to exhibit connections between the eigenspace of $\hat{a}(G)$ and structural properties of the graph, but at the same time this problem also showed up in several other contexts, see [11] for relations to fastest mixing Markov chains, maximum variance unfolding and conductivity maximization. In [9] the graph realization problem (3) was generalized to include node weights and edge lengths for the purpose of introducing a minor monotone graph parameter, the *rotational dimension* of the graph. In this note we introduce edge length variables $l \in \mathbb{R}^E$ in (2) (in squared form) and study the problem of optimizing the spread by varying edge lengths within a limited total norm $\|l\|^2 \le |E|$,

$$\begin{array}{ll} \text{maximize} & \langle I, X\rangle \\ \text{subject to} & \langle E_{ij}, X\rangle \le l_{ij}^2 \quad \text{for } ij \in E, \\ & \langle \mathbf{1}\mathbf{1}^\top, X\rangle = 0, \\ & \sum_{ij\in E} l_{ij}^2 \le |E|, \\ & l^2 \in \mathbb{R}^E, X \succeq 0. \end{array} \tag{4}$$

Putting $X = V^\top V$ as before, the corresponding graph realization problem reads

$$\begin{array}{ll} \text{maximize} & \sum_{i\in N}\|v_i\|^2 \\ \text{subject to} & \|v_i - v_j\| \le l_{ij} \qquad \text{for } ij \in E, \\ & \sum_{i\in N} v_i = 0, \\ & \sum_{ij\in E} l_{ij}^2 \le |E|, \\ & l \in \mathbb{R}^E,\ v_i \in \mathbb{R}^n \text{ for } i \in N. \end{array} \tag{5}$$

Our main result is the following.

Theorem 1 *Given a connected graph $G = (N, E)$, let $V = [v_1, \ldots, v_n]$ be an optimal solution of (5). Then $\sum_{i\in N}\|v_i\|^2 = \frac{|E|}{\lambda_2(L(G))}$ and for $u \in \mathbb{R}^n$ the vector $V^\top u$ is an eigenvector of $\lambda_2(L(G))$.*

Proof. The semidefinite dual to (4) reads

$$\begin{array}{ll} \text{minimize} & |E|\rho \\ \text{subject to} & \sum_{ij\in E} w_{ij}E_{ij} + \mu\mathbf{1}\mathbf{1}^\top \succeq I, \\ & \rho - w_{ij} = 0 \quad \text{for } ij \in E, \\ & w \in \mathbb{R}_+^E, \rho \ge 0, \mu \in \mathbb{R}. \end{array} \tag{6}$$

Because G is connected, the second smallest eigenvalue $\lambda_2(L_w)$ can be increased arbitrarily by choosing $w > 0$ large enough. This proves that (6) is strictly feasible, therefore semidefinite duality theory ensures that the optimal values of (6) and (4) coincide. By connectedness of G this value is strictly positive. Given an optimal primal-dual pair of solutions $\rho > 0$, $w = \rho\mathbf{1}$, μ and $X = V^\top V$, semidefinite complementarity yields $V^\top V(\rho L + \mu\mathbf{1}\mathbf{1}^\top - I) = 0$, so $LV^\top = \frac{1}{\rho}V^\top$, hence the columns of $V^\top$ are contained in the eigenspace of $\lambda_2(L) = \frac{1}{\rho}$. ■

The theorem also implies that the optimal solution of (5) is rank one (*i.e.*, the optimal graph realization is one dimensional) whenever $\lambda_2(L) = \frac{1}{\rho}$ has multiplicity one. Conversely, each eigenvector to $\lambda_2(L)$ gives rise to an optimal solution of (5), as we show next.

Theorem 2 *Given a connected graph $G = (N, E)$, let $u \in \mathbb{R}^n$, $\|u\| = 1$, be an eigenvector to $\lambda_2(L(G))$. An optimal solution of (4) is $X = \frac{|E|}{\lambda_2(L(G))}uu^\top$ and $l_{ij}^2 = \frac{|E|}{\lambda_2(L(G))}(u_i - u_j)^2$, $ij \in E$.*

Proof. To check feasibility, observe that u is orthogonal to the eigenvector $\mathbf{1}$ of $\lambda_1(L)$, so $\langle \mathbf{1}\mathbf{1}^\top, X\rangle = 0$. For $ij \in E$, $\langle E_{ij}, X\rangle = \frac{|E|}{\lambda_2(L)} u^\top E_{ij} u = \frac{|E|}{\lambda_2(L)}(u_i - u_j)^2 = l_{ij}^2$, thus $\sum_{ij\in E} l_{ij}^2 = \frac{|E|}{\lambda_2(L)} u^\top L u = |E|$. As $\langle I, X\rangle = \frac{|E|}{\lambda_2(L)}$, optimality follows from Theorem 1. ■

The two theorems together assert that an optimal solution of maximum rank to (4) (as delivered, *e.g.*, by interior point methods) gives a geometric view of the entire eigenspace of $\lambda_2(L)$. Indeed, suppose the columns of $U \in \mathbb{R}^{N\times k}$ with $U^\top U = I_k$ span the eigenspace to $\lambda_2(L)$, then the convex combination $X = \frac{|E|}{k\lambda_2(L)} UU^\top$ with $l_{ij}^2 = \langle E_{ij}, X\rangle$ for $ij \in E$ is a corresponding maximum rank solution of (4) and its k-dimensional realization (5) is given by the columns of $V = \sqrt{\frac{|E|}{k\lambda_2(L)}} U^\top$.

It was shown in [7] that $\lambda_{\max}(L_c)$ allows to derive structural results and graph realizations complementing those obtained for $\lambda_2(L_c)$ in [8]. Likewise, analogous results to two theorems above can be formulated for $\lambda_{\max}(L)$ via the program

$$\begin{array}{rll} \text{minimize} & \langle I, X\rangle & \\ \text{subject to} & \langle E_{ij}, X\rangle \geq l_{ij}^2 & \text{for } ij \in E, \\ & \sum_{ij\in E} l_{ij}^2 \geq |E|, & \\ & l^2 \in \mathbb{R}_+^E, X \succeq 0, & \end{array} \tag{7}$$

and the corresponding graph realization problem

$$\begin{array}{rll} \text{minimize} & \sum_{i\in N} \|v_i\|^2 & \\ \text{subject to} & \|v_i - v_j\| \geq l_{ij} & \text{for } ij \in E, \\ & \sum_{ij\in E} l_{ij}^2 \geq |E|, & \\ & l \in \mathbb{R}_+^E,\ v_i \in \mathbb{R}^n \text{ for } i \in N. & \end{array} \tag{8}$$

We state the corresponding theorems without proof as the arguments are almost identical.

Theorem 3 *Given a connected graph $G = (N, E)$, let $V = [v_1, \ldots, v_n]$ be an optimal solution of (8). Then $\sum_{i\in N} \|v_i\|^2 = \frac{|E|}{\lambda_{\max}(L(G))}$ and for $u \in \mathbb{R}^n$ the vector $V^\top u$ is an eigenvector of $\lambda_{\max}(L(G))$.*

Theorem 4 *Given a connected graph $G = (N, E)$, let $u \in \mathbb{R}^n$, $\|u\| = 1$, be an eigenvector to $\lambda_{\max}(L(G))$. An optimal solution of (7) is $X = \frac{|E|}{\lambda_{\max}(L(G))} uu^\top$ and $l_{ij}^2 = \frac{|E|}{\lambda_{\max}(L(G))}(u_i - u_j)^2$, $ij \in E$.*

References

[1] T. Biyikoglu, J. Leydold, and P. F. Stadler. *Laplacian Eigenvectors of Graphs*, volume 1915 of *Lecture Notes in Mathematics*. Springer, Berlin Heidelberg, 2007.

[2] D. Cvetković, M. Doob, and H. Sachs. *Spectra of Graphs. Theory and application.* J. A. Barth Verlag, Leipzig, 3rd edition, 1995.

[3] M. Fiedler. Algebraic connectivity of graphs. *Czechoslovak Mathematical Journal*, 23:298–305, 1973.

[4] M. Fiedler. A property of eigenvectors of nonnegative symmetric matrices and its application to graph theory. *Czechoslovak Mathematical Journal*, 25:619–633, 1975.

[5] M. Fiedler. Laplacian of graphs and algebraic connectivity. *Combinatorics and Graph Theory*, 25:57–70, 1989.

[6] M. Fiedler. Absolute algebraic connectivity of trees. *Linear and Multilinear Algebra*, 26:85–106, 1990.

[7] F. Göring, C. Helmberg, and S. Reiss. Graph realizations associated with minimizing the maximum eigenvalue of the Laplacian. Preprint 2009-10, Fakultät für Mathematik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany, May 2009. Submitted.

[8] F. Göring, C. Helmberg, and M. Wappler. Embedded in the shadow of the separator. *SIAM J. Optim.*, 19(1):472–501, 2008.

[9] F. Göring, C. Helmberg, and M. Wappler. The rotational dimension of a graph. Preprint 2008-16, Fakultät für Mathematik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany, Oct. 2008. To appear in J. Graph Theory.

[10] B. Mohar. Graph Laplacians. In L. W. Beineke and R. J. Wilson, editors, *Topics in algebraic graph theory*, volume 102 of *Encyclopedia of Mathematics and Its Applications*, pages 113–136. Cambridge University Press, 2004.

[11] J. Sun, S. Boyd, L. Xiao, and P. Diaconis. The fastest mixing Markov process on a graph and a connection to a maximum variance unfolding problem. *SIAM Review*, 48(4):681–699, 2006.

[12] U. von Luxburg, M. Belkin, and O. Bousquet. Consistency of spectral clustering. *The Annals of Statistics*, 36(2):555–586, 2008.