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Applied Mathematics Letters 18 (2005) 917–922

Applied Mathematics Letters

www.elsevier.com/locate/aml

On the pseudo-inverse of the Laplacian of a bipartite graph☆

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Received 6 July 2004; accepted 15 July 2004

Abstract

We provide an efficient method to calculate the pseudo-inverse of the *Laplacian* of a bipartite graph, which is based on the pseudo-inverse of the *normalized Laplacian*.

Keywords: Laplacian; Pseudo-inverse; Bipartite graph

1. Introduction

In [1], an elegant connection is made between random walks on graphs and electrical network theory. Quantities like *probability of absorption* and *average commute time* in graphs have their counterpart in electrical networks. Recently, these quantities have been applied in *collaborative filtering* [2] and they involve the *Laplacian* of large bipartite graphs. It is shown in [3] that the above quantities can be derived from the pseudo-inverse of this Laplacian.

In this short note, we give an efficient way to compute the pseudo-inverse of the Laplacian of an undirected bipartite graph. Such a graph $G = (V, E)$ is defined by a set of vertices V and a set of edges E between these vertices. Let n be the number of vertices then the *adjacency* matrix of the graph G is a matrix $A \in \mathbb{R}^{n\times n}$ with $A_{ij} = 1$ if $(i, j) \in E$ and $A_{ij} = 0$ otherwise. In the case of a weighted graph $A_{ij} > 0$ if $(i, j) \in E$ and $A_{ij} = 0$ otherwise.

☆ Supported by the Belgian Programme on Inter-university Poles of Attraction, initiated by the Belgian State, Prime Minister's Office for Science, Technology and Culture and by a concerted research project on Algorithmic Challenges in Large Networks, funded by the Université catholique de Louvain.
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0893-9659/$ - see front matter
doi:10.1016/j.aml.2004.07.034

We assume in this document that the vertices of the bipartite graph are labelled such that the edges are between the first m vertices and the $k := n - m$ remaining ones. If the graph is also undirected then the adjacency matrix A is symmetric and has the following block form:

$$A = \left[\begin{array}{c|c} 0_{m\times m} & B \\ \hline B^T & 0_{k\times k} \end{array}\right],$$

where B is a $m \times k$ non-negative matrix. Without loss of generality we can assume that $m \geq k$ since otherwise one only needs to relabel the vertices. Define then the diagonal matrix D with diagonal entries $D_{ii} := \sum_{j=1}^{n} A_{ij}$. This is the so-called *degree matrix* of G and the Laplacian matrix L of G is then defined as:

$$L = D - A = \left[\begin{array}{c|c} D_1 & -B \\ \hline -B^T & D_2 \end{array}\right],$$

where D_1 and D_2 are the diagonal blocks of D. Notice that D is invertible when G is connected.

It easily follows from the definition of D that the symmetric matrix L is singular since e_n (the column vector of n 1's) is in the null space of L. We derive in this paper an efficient method to compute the pseudo-inverse L^+ of this Laplacian matrix. Let us recall that the pseudo-inverse (or generalized inverse) M^+ of a matrix M is uniquely defined by the four equations: $MM^+M = M$, $M^+MM^+ = M^+$, $M^+M = (M^+M)^T$ and $MM^+ = (MM^+)^T$ [4].

2. The normalized Laplacian

Assuming that D is invertible, one can scale L to obtain a *normalized Laplacian* $\tilde{L}$, defined as:

$$\tilde{L} := D^{-1/2} L D^{-1/2} = I_n - D^{-1/2} A D^{-1/2}$$

which then has the following form:

$$\tilde{L} = \left[\begin{array}{c|c} I_m & -D_1^{-1/2} B D_2^{-1/2} \\ \hline -D_2^{-1/2} B^T D_1^{-1/2} & I_k \end{array}\right] = \left[\begin{array}{c|c} I_m & -\tilde{B} \\ \hline -\tilde{B}^T & I_k \end{array}\right]. \tag{1}$$

While computing the pseudo-inverse of the Laplacian requires the eigen-decomposition of L, this is much simpler for the normalized Laplacian since one can make use of the singular value decomposition (SVD) of $\tilde{B}$. The following result shows the relation between the SVD of $\tilde{B}$ and the generalized inverse of $\tilde{L}$.

Theorem 1. *Let the SVD of the $m \times k$ matrix $\tilde{B}$ be given by*

$$\tilde{B} = U \begin{bmatrix} I_{m_1} & 0 \\ 0 & \Sigma \\ 0 & 0 \end{bmatrix} V^T = \begin{bmatrix} U_1 & U_2 & U_3 \end{bmatrix} \begin{bmatrix} I_{m_1} & 0 \\ 0 & \Sigma \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1 & V_2 \end{bmatrix}^T$$

where $k = m_1 + m_2$, $m = m_1 + m_2 + m_3$, $U_i \in \mathbb{R}^{m\times m_i}$, $V_i \in \mathbb{R}^{k\times m_i}$ and where $\Sigma \in \mathbb{R}^{m_2\times m_2}$ has no singular values equal to 1. Then the matrix $\tilde{L}$ has a decomposition

$$\tilde{L} = \left[\begin{array}{c|c} U & 0 \\ \hline 0 & V \end{array}\right] \left[\begin{array}{ccc|cc} I_{m_1} & & & -I_{m_1} & \\ & I_{m_2} & & & -\Sigma \\ & & I_{m_3} & & \\ \hline -I_{m_1} & & & I_{m_1} & \\ & -\Sigma & & & I_{m_2} \end{array}\right] \left[\begin{array}{c|c} U^T & 0 \\ \hline 0 & V^T \end{array}\right] \tag{2}$$

and a generalized inverse

$$\tilde{L}^+ = \left[\begin{array}{c|c} U & 0 \\ \hline 0 & V \end{array}\right] \left[\begin{array}{ccc|cc} \frac{1}{4} I_{m_1} & & & -\frac{1}{4} I_{m_1} & \\ & \Sigma_1 & & & \Sigma_2 \\ & & I_{m_3} & & \\ \hline -\frac{1}{4} I_{m_1} & & & \frac{1}{4} I_{m_1} & \\ & \Sigma_2 & & & \Sigma_1 \end{array}\right] \left[\begin{array}{c|c} U^T & 0 \\ \hline 0 & V^T \end{array}\right] \tag{3}$$

where $\Sigma_1 := (I_{m_2} - \Sigma^2)^{-1}$ *and* $\Sigma_2 := \Sigma \Sigma_1$.

Proof. It follows by inspection that $\tilde{L}^+$ satisfies the four equations for the pseudo-inverse. □

Corollary 1. *The pseudo-inverse* $\tilde{L}^+$ *can be written using* $U_{12} := [\ U_1\ U_2\ ]$ *only as follows:*

$$\tilde{L}^+ = \left[\begin{array}{c|c} I_m & 0 \\ \hline 0 & 0 \end{array}\right] + \left[\begin{array}{c|c} U_{12} & 0 \\ \hline 0 & V \end{array}\right] \left[\begin{array}{cc|cc} -\frac{3}{4} I_{m_1} & & -\frac{1}{4} I_{m_1} & \\ & \Sigma_1 - I_{m_2} & & \Sigma_2 \\ \hline -\frac{1}{4} I_{m_1} & & \frac{1}{4} I_{m_1} & \\ & \Sigma_2 & & \Sigma_1 \end{array}\right] \left[\begin{array}{c|c} U_{12}^T & 0 \\ \hline 0 & V^T \end{array}\right]. \tag{4}$$

Proof. This follows from (3) and the identity $U_3 U_3^T = I_m - U_{12} U_{12}^T$. □

Corollary 2. *The semidefinite matrices* $\tilde{L}$ *and* $\tilde{L}^+$ *have the following explicit eigen-decomposition:*

$$\tilde{L} = U_{\tilde{L}} \Sigma_{\tilde{L}} U_{\tilde{L}}^T, \quad \tilde{L}^+ = U_{\tilde{L}} \Sigma_{\tilde{L}}^+ U_{\tilde{L}}^T$$

where

$$U_{\tilde{L}} = \frac{1}{\sqrt{2}} \left[\begin{array}{ccc|cc} -U_1 & -U_2 & -\sqrt{2} U_3 & U_1 & U_2 \\ \hline V_1 & V_2 & 0 & V_1 & V_2 \end{array}\right], \qquad \Sigma_{\tilde{L}} = \left[\begin{array}{ccc|cc} 2 I_{m_1} & & & & \\ & I_{m_2} + \Sigma & & & \\ & & I_{m_3} & & \\ \hline & & & 0_{m_1} & \\ & & & & I_{m_2} - \Sigma \end{array}\right]$$

and

$$\Sigma_{\tilde{L}}^+ = \left[\begin{array}{ccc|cc} \frac{1}{2} I_{m_1} & & & & \\ & (I_{m_2} + \Sigma)^{-1} & & & \\ & & I_{m_3} & & \\ \hline & & & 0_{m_1} & \\ & & & & (I_{m_2} - \Sigma)^{-1} \end{array}\right]. \tag{5}$$

Proof. Due to the scaling (1), it follows that $\|\tilde{B}\|_2 \le 1$ and hence that $\tilde{L} \ge 0$. The decomposition then follows from (2) and $U_{\tilde{L}} U_{\tilde{L}}^T = I$. □

It is important to note that when $m \gg k$ computing a pseudo-inverse via (4) is more economical than via the eigenvalue decomposition of an $(m+k) \times (m+k)$ matrix, since this would require $O(m+k)^3$ floating point operations (flops) instead of the $O(mk^2)$ needed for the SVD approach (see [4] for an operation count of the so-called economical SVD approach).

3. Projectors and pseudo-inverses

For an $n \times \ell$ matrix M one can define the projectors Π_M on the image of M and Π_{M^T} on the image of M^T, using the pseudo inverse of M (see [4]):

$$\Pi_M = MM^+, \qquad \Pi_{M^T} = M^+M.$$

It is often simpler to write it in terms of orthogonal bases V_M and U_M of the respective kernels of M and M^T:

$$\Pi_M = I_n - V_M V_M^T, \qquad \Pi_{M^T} = I_\ell - U_M U_M^T$$

and these can e.g. be obtained from an orthogonal decomposition of M. This is especially useful when the dimension of the kernels is small compared to the dimensions n and ℓ of the matrix M. For an irreducible undirected bipartite graph, the Laplacian L is symmetric and its kernel is known to be of dimension 1 and spanned by e_n and hence $\Pi_L = \Pi_{L^T} = I_n - \frac{1}{n}e_n e_n^T$.

In order to compute the pseudo-inverse of the Laplacian matrix L from the normalized Laplacian matrix, we make use of the following result:

Theorem 2. *Given $M \in \mathbb{R}^{n\times\ell}$, then for any invertible matrices D_1 and D_2 we have:*

$$M^+ = \Pi_{M^T} D_2 (D_1 M D_2)^+ D_1 \Pi_M. \tag{6}$$

Proof. It follows from $\Pi_M = MM^+$, $\Pi_{M^T} = M^+M$ that

$$\begin{aligned}\Pi_{M^T} D_2 (D_1 M D_2)^+ D_1 \Pi_M &= M^+ M D_2 (D_1 M D_2)^+ D_1 M M^+ \\ &= M^+ D_1^{-1} (D_1 M D_2)(D_1 M D_2)^+ (D_1 M D_2) D_2^{-1} M^+ \\ &= M^+ D_1^{-1} (D_1 M D_2) D_2^{-1} M^+ = M^+ M M^+ = M^+. \quad \square\end{aligned}$$

If we apply this result to compute the pseudo-inverse of the Laplacian matrix L then the pseudo-inverse of L is:

$$L^+ = \Pi_L D^{-1/2} (D^{-1/2} L D^{-1/2})^+ D^{-1/2} \Pi_L = \Pi_L D^{-1/2} \tilde{L}^+ D^{-1/2} \Pi_L. \tag{7}$$

Suppose that G is connected, then the kernel of L is spanned by e_n and

$$L^+ = \left(I_n - \frac{1}{n} e_n e_n^T\right) D^{-1/2} \tilde{L}^+ D^{-1/2} \left(I_n - \frac{1}{n} e_n e_n^T\right). \tag{8}$$

If the graph G is not connected, then one can relabel the first m vertices and the last k vertices such that the permuted matrix B has the form

$$P_m B P_k = \begin{bmatrix} B_1 & & & \\ & \ddots & & \\ & & B_t & \\ & & & 0 \end{bmatrix}, \tag{9}$$

and where each subgraph

$$A_i = \left[\begin{array}{c|c} 0_{m_i \times m_i} & B_i \\ \hline B_i^T & 0_{k_i \times k_i} \end{array}\right]$$

is now connected. The complexity of the relabelling is proportional to the number of edges in the graph (see [5]). Moreover the pseudo-inverse of the Laplacian then amounts to a block arrangement of the pseudo-inverses of the smaller Laplacians. Notice also that for each connected subgraph, the condition that the corresponding degree matrix D_i is invertible is automatically satisfied.

Remark 1. If a graph consists of two (or more) chained bipartite graphs, then the adjacency matrix A has the form

$$A = \begin{bmatrix} & B_1 & & & \\ B_1^T & & B_2 & & \\ & B_2^T & & \ddots & \\ & & \ddots & & B_\ell \\ & & & B_\ell^T & \end{bmatrix}.$$

This can also be relabelled in an adjacency matrix of the type found in bipartite graphs. For $\ell = 2$ and $\ell = 3$ this would e.g. yield

$$P^T A P = \left[\begin{array}{cc|c} & & B_1 \\ & & B_2^T \\ \hline B_1^T & B_2 & \end{array}\right], \qquad P^T A P = \left[\begin{array}{cc|cc} & & B_1 & \\ & & B_2^T & B_3 \\ \hline B_1^T & B_2 & & \\ & B_3^T & & \end{array}\right].$$

The same techniques can therefore also be applied for computing the pseudo-inverse of the Laplacian of such graphs.

Remark 2. If only the r dominant eigenvectors of L^+ are needed, they can be approximated by the r dominant eigenvectors of $\tilde{L}^+$. In fact, (5) yields the exact eigen-decomposition of $\tilde{L}^+$. One can use the orthogonal basis $\tilde{U}_r$ corresponding to the r largest eigenvalues of $\tilde{L}^+$ to approximate the r corresponding dominant eigenvectors of L^+ as follows:

$$U_r := \Pi_L D^{-1/2} \tilde{U}_r. \tag{10}$$

This initial approximation can be used in an iterated procedure to compute the r dominant eigenvectors of L^+.

4. Concluding remarks

We have presented a method for calculating the pseudo-inverse of the Laplacian of a bipartite graph. The method will have a good performance when the two subsets are very different in size and/or when the graph is decomposed into smaller connected bipartite subgraphs.

Acknowledgements

We thank professor Marco Saerens from the Information Systems Research Unit, IAG, University of Louvain for drawing our attention to this topic. The first author was supported by a Belgian FRIA fellowship.

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