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

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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.

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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 $\tilde{L}$, 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

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

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.

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