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降维理论中特征值的估计*
Eigenvalue Estimation in Dimensionality Reduction Theory

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摘要:利用谱降维方法可以归结为求解带权图 Laplacican 矩阵 $L(G)$ 的特征值 λ_{n-t} 对应的特征向量这一理论,通过代数方法估计 λ_{n-t} 的下界,并讨论非带权图的情况下 λ_{n-t} 的下界.

关键词:带权图 Laplacian 矩阵 特征值 降维理论
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Abstract: The application of spectral dimension reduction method can be attributed to solve the eigenvectors corresponding to the eigenvalues of weighted graph Laplacican matrix $L(G)$. The lower bound of λ_{n-t} is given by using algebra method, and discussed the case of non-weighted graph.

Key words: weighted graph, Laplacian matrix eigenvalue, dimensionality reduction theory

降维问题的一般化描述为:设 $x_1, x_2, \cdots, x_n$ 是 R^l 上的 n 个点,找出 R^m 上的 n 个点 $y_1, y_2, \cdots, y_n$,用 y_i 表示 x_i, $1 \leqslant i \leqslant n$,这里 $m < l$.

设 $G=(V,E,w)$ 是带权无向简单连通图,其中顶点集 $V=\{v_1, v_2, \cdots, v_n\}$, $E=E(G)$ 是 G 的边集合.若 d_i 表示顶点 v_i 在 G 中的度, $N(i)$ 表示顶点 v_i 在 G 中的邻域,从而有 $|N(i)|=d_i$.对于 G 中每条边赋予一个正权值,即 $w_{i,j}\begin{cases} >0, 若\ v_iv_j \in E(G) \\ =0, 否则 \end{cases}$,令 $w_i = \sum_{j=1}^{n} w_{i,j}$.带权图 G 的 Laplacian 矩阵定义为 $L(G)=D-W$,其中 W 是 G 的权值矩阵, D 是对角阵,其对角线上第 i 个元素为 w_i.易知:(1) $L(G)$ 是对角占优的对称矩阵,从而 $L(G)$ 是半正定矩阵;(2) $L(G)$ 的最小特征值为 0,对应的特征向量为 1,且当 G 是连通图时,特征值 0 的重数为 1.不妨设 $\lambda_1, \lambda_2, \cdots, \lambda_{n-1}, \lambda_n=0$ 为 $L(G)$ 的所有特征值(按值的大小以降序排列).将 G 中每个顶点所表示的 l 维向量降维成为 m 维向量,并保存顶点大部分有用的信息,相当于求解[1]:

$$\underset{Y^TDY=I}{\arg\min}\ \mathrm{tr}(Y^TLY),$$

即计算拉普拉斯矩阵 L 除最小特征值 0 外前 m 个最小特征值对应的特征向量,分别记为 $y_1, y_2, \cdots, y_m$,则矩阵 $Y=[y_1y_2\cdots y_m]$ 即为所求. $x_i \to (f_1(i), f_2(i), \cdots, f_m(i))$,特别地,利用上述降维理论取 $m=1$ 的特殊情况可以将每个顶点映射成实数,此时 y 可以通过求解 L 的次小特征值对应的特征向量得到.因此在理论上估计带权图 Laplacian 矩阵除最小特征值 0 外,前 m 个最小特征值的范围对实际应用有着重要的指导作用.为方便表述,记 λ_{n-t} 表示除最小特征值 0 外第 t 小特征根, $1 \leqslant t \leqslant m$.

文献[2]给出关于最大特征值的一个上界,因此对于 λ_{n-t} 有

$$\frac{1}{2}\max_{v_iv_j \in E(G)}\{w_i + w_j + \sum_{\substack{v_kv_i \in E(G)\\ v_kv_j \notin E(G)}} w_{i,k} + \sum_{\substack{v_kv_j \in E(G)\\ v_kv_i \notin E(G)}} w_{j,k} + \sum_{\substack{v_kv_j \in E(G)\\ v_kv_i \in E(G)}} |w_{i,k} - w_{j,k}|\} \geqslant \lambda_{n-t} > 0.$$

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文献[3]给出 λ_{n-1} 的一个下界,并讨论非带权图的情况.本文运用文献[3]的证明方法,扩展该文的结果,给出 $\lambda_{n-t}(1\leqslant t\leqslant n)$ 的一个下界,并讨论非带权图的情况.文中涉及的符号和标记若没有特别说明,则与文献[4,5]一致.

定理1 设 G 是 n 阶简单连通带权图,则

$$\lambda_{n-t}\geqslant \frac{1}{2}\min_{v_iv_j\in E(G)}\Big\{w_i+w_j-\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}-\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}-\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}|w_{i,k}-w_{j,k}|\Big\}.$$

证明 设 $x=[x_1,x_2,\cdots,x_n]^{\mathrm{T}}$ 是对应特征值 λ_{n-t} 的特征向量,即

$$Lx=\lambda_{n-t}x, \tag{1}$$

则有 $x\neq 0$ 且 $\sum_{k=1}^{n}x_k=0$. 设 $x_i=\max\{x_1,x_2,\cdots,x_n\}$,则 $x_i>0$. 令 $x_j=\min\{x_k:v_kv_i\in E(G)\}$,则 $\forall k$: $v_kv_i\in E(G)$,有 $x_j\leqslant x_k$. 由(1)式可得

$$\lambda_{n-t}x_i=w_ix_i-\sum_{v_kv_i\in E(G)}w_{i,k}x_k;\lambda_{n-t}x_j=w_jx_j-\sum_{v_kv_j\in E(G)}w_{j,k}x_k. \tag{2}$$

将(2)式中的两式相减,再由 $x_j\leqslant x_k\leqslant x_i$ 得

$$\begin{aligned}\lambda_{n-t}(x_i-x_j)&=w_ix_i-w_jx_j+\sum_{v_kv_j\in E(G)}w_{j,k}x_k-\sum_{v_kv_i\in E(G)}w_{i,k}x_k=w_ix_i-w_jx_j+\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}x_k+\\&\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}w_{j,k}x_k-\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}x_k-\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\in E(G)}}w_{i,k}x_k\geqslant\\&w_ix_i-w_jx_j+x_j\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}+x_k\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}w_{j,k}-\\&x_i\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}-x_k\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}w_{i,k}=w_ix_i-w_jx_j+\\&x_j\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}-x_i\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}+\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}(w_{j,k}-w_{i,k})x_k.\end{aligned}$$

令

$$S_{i,j}=w_ix_i-w_jx_j+x_i\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}-x_j\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}+\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}(w_{j,k}-w_{i,k})x_k,$$

则有

$$\begin{aligned}S_{i,j}&=w_i(x_i-x_j)+w_j(x_i-x_j)+w_ix_j-w_jx_i+x_i\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}-x_j\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}+\\&\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}(w_{j,k}-w_{i,k})x_k=\frac{1}{2}w_i(x_i-x_j)+\frac{1}{2}w_j(x_i-x_j)+\frac{1}{2}(x_i-x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}+\\&\frac{1}{2}(x_i-x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}+\frac{1}{2}(x_i+x_j)\Big(w_i-\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}\Big)-\frac{1}{2}(x_i+x_j)\Big(w_j-\\&\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}\Big)+\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}(w_{j,k}-w_{i,k})x_k=\\&\frac{1}{2}w_i(x_i-x_j)+\frac{1}{2}w_j(x_i-x_j)+\frac{1}{2}(x_i-x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}+\frac{1}{2}(x_i-x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}+\\&\frac{1}{2}(x_i+x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\in E(G)}}w_{i,k}-\frac{1}{2}(x_i+x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}w_{j,k}+\\&\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}(w_{j,k}-w_{i,k})x_k=\frac{1}{2}w_i(x_i-x_j)+\frac{1}{2}w_j(x_i-x_j)+\\&\frac{1}{2}(x_i-x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}+\frac{1}{2}(x_i-x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}+\frac{1}{2}(x_i+x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}(w_{i,k}-w_{j,k})+\\&\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}(w_{j,k}-w_{i,k})x_k=\frac{1}{2}w_i(x_i-x_j)+\frac{1}{2}w_j(x_i-x_j)+\\&\frac{1}{2}(x_i-x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}}w_{i,k}+\frac{1}{2}(x_i-x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}+\frac{1}{2}\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}}(w_{i,k}-w_{j,k})(x_i-x_k+\\&x_j-x_k).\end{aligned}$$

因此有

$$\lambda_{n-t}(x_i-x_j)\geqslant w_ix_i-w_jx_j+x_j\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}}w_{j,k}-$$

$$x_i \sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}} w_{i,k} + \sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} (w_{j,k}-w_{i,k})x_k = S_{i,j} - (x_i - x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}} w_{j,k} - (x_i - x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}} w_{i,k} = \frac{1}{2}w_i(x_i - x_j) + \frac{1}{2}w_j(x_i - x_j) + \frac{1}{2}(x_i - x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}} w_{i,k} + \frac{1}{2}(x_i - x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}} w_{j,k} + \frac{1}{2}\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} (w_{i,k}-w_{j,k})\cdot (x_i - x_k + x_j - x_k) - (x_i - x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}} w_{j,k} - (x_i - x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}} w_{i,k} = \frac{1}{2}w_i(x_i - x_j) + \frac{1}{2}w_j(x_i - x_j) - \frac{1}{2}(x_i - x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}} w_{i,k} - \frac{1}{2}(x_i - x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}} w_{j,k} + \frac{1}{2}\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} (w_{i,k}-w_{j,k})(x_i - x_k + x_j - x_k).$$

而

$$\frac{1}{2}\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} (w_{i,k}-w_{j,k})(x_i - x_k + x_j - x_k) \geqslant \frac{1}{2}\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} |w_{i,k}-w_{j,k}|(x_j - x_k) + \frac{1}{2}\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} |w_{i,k}-w_{j,k}|(x_k - x_i) = \frac{1}{2}(x_j - x_i)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} |w_{i,k}-w_{j,k}|,$$

从而

$$\lambda_{n-1}(x_i - x_j) \geqslant \frac{1}{2}w_i(x_i - x_j) + \frac{1}{2}w_j(x_i - x_j) - \frac{1}{2}(x_i - x_j)\sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}} w_{i,k} - \frac{1}{2}(x_i - x_j)\cdot \sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}} w_{j,k} - \frac{1}{2}(x_i - x_j)\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} |w_{i,k}-w_{j,k}|. \quad (3)$$

若 $x_i = x_j$，则 $\forall k: v_kv_i \in E(G)$，有 $x_j = x_k$. 从而由(2)式可知 $\lambda_{n-1}x_i = w_ix_i - \sum_{v_kv_i\in E(G)} w_{i,k}x_k = w_ix_i - w_ix_i = 0$. 从而必有 $\lambda_{n-1} = 0$，与假设矛盾. 因此 $x_i - x_j > 0$. 在(3)式左右两边同时除 $x_i - x_j$，即得

$$\lambda_{n-1} \geqslant \frac{1}{2}\min_{v_iv_j\in E(G)}\{w_i + w_j - \sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}} w_{i,k} - \sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}} w_{j,k} - \sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} |w_{i,k}-w_{j,k}|\}.$$

易知下界大于等于0.

推论1 当 G 是非带权图时，$\lambda_{n-1} \geqslant \min_{v_iv_j\in E(G)} |N(i) \cap N(j)|$.

证明 此时对 $\forall\, v_iv_j \in E(G)$，有 $w_{i,j} = 1$. 从而 $w_i = d_i, w_j = d_j$，$w_i - \sum_{\substack{v_kv_i\in E(G)\\ v_kv_j\notin E(G)}} w_{i,k} = w_j - \sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\notin E(G)}} w_{j,k} = |N(i) \cap N(j)|$，$\sum_{\substack{v_kv_j\in E(G)\\ v_kv_i\in E(G)}} |w_{i,k} - w_{j,k}| = 0$. 代入定理1，结论成立.

注1 本文得到带权连通图次小特征根的下界. 由于 G 是连通图，因此 $\lambda_{n-1} > 0$ 恒成立. 但是由分析可知我们得到的下界并非严格大于0，如何得到 λ_{n-1} 严格大于0的下界还有待进一步研究.

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