Lecture #11 Notes Summary

Graph Theory for Block Designs

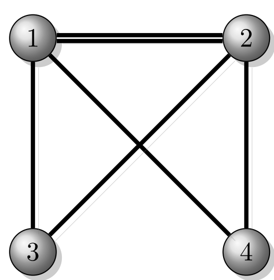
Concurrence and Levy Graphs

Definition 1 (Concurrence Graph)**.** Let ξ be a block design (t treatments, b blocks of size k). The Concurrence Graph (CG) of ξ is the graph with t vertices that contains $\lambda_{i,j}$ edges between i and j (that is, one edge of weight $\lambda_{i,j}$).

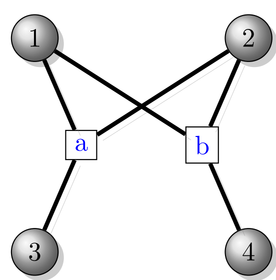
Definition 2 (Levi Graph)**.** Let ξ be a block design (t treatments, b blocks of size k). The Levi Graph (LG) of ξ is a bipartite graph with $t+b$ vertices, one for each treatment and one for each block; the node corresponding to treatment i is connected to the node of block j iff i appears in block j.

Consider the following design:

$$\xi = \begin{array}{|c|c|} \hline 1 & 1 \\ 2 & 2 \\ 3 & 4 \\ \hline \end{array}.$$



Concurrence Graph



Levi Graph

#1

Definition 3 (Laplacian of a graph)**.** Let $G=(V,E)$ be a graph with n nodes, and edges of weights w_e ($\forall e \in E$). The degree of i in G is $\deg(i) = \sum_{(i,j)\in E} w_{ij}$. The Laplacian matrix of G is the $n \times n$ symmetric matrix such that:

$$L_{i,j} = \begin{cases} \deg(i) & \text{if } i = j \\ -w_{ij} & \text{if } (i,j) \in E \\ 0 & \text{otherwise.} \end{cases}$$

Observe that the Laplacian matrix of a design, $L = kR - \Lambda$, coincide with the Laplacian matrix of its CG. For example, the Laplacian matrix of the design ξ above is

$$\begin{pmatrix} 4 & -2 & -1 & -1 \\ -2 & 4 & -1 & -1 \\ -1 & -1 & 2 & 0 \\ -1 & -1 & 0 & 2 \end{pmatrix}.$$

The next proposition shows that L can be written as a sum of rank-one positive semidefinite matrices, hence the same holds for C and $C \in \mathbb{S}_+^t$.

Proposition 1. *Let $\boldsymbol{e}_{ij}$ be the vector with a* 1 *on coordinate i,* -1 *on coordinate j, and* 0 *everywhere else. Then,*

$$L = \sum_{(i,j)\in E} w_{i,j} \boldsymbol{e}_{ij} \boldsymbol{e}_{ij}^T \succeq 0.$$

Proof. Just check with the definition of L. □

Note that the previous expression looks like the standard form of the information $M(\xi) = \sum_i w_i \boldsymbol{a}(x_i)\boldsymbol{a}(x_i)^T$ in the linear model. In particular, for a block design with blocks of size $k = 2$, we can write $C = \frac{1}{k} L = \frac{1}{k} \sum_{i\neq j} w_{i,j} \boldsymbol{e}_{ij} \boldsymbol{e}_{ij}^T$, where $w_{i,j}$ denotes the number of times that i and j are tested together in a block. For blocks of larger size, we can also write $C = \frac{1}{k} \sum_{B\in\mathcal{B}} w_B M_B$, where $\mathcal{B}$ denotes the set of all blocks of size k, and $M_B = \sum_{i\neq j \in B} \boldsymbol{e}_{ij} \boldsymbol{e}_{ij}^T \in S_+^t$ is a matrix of rank $k-1$ (this is the Laplacian of the small clique on the vertices of B) and w_B indicates the number of times that block B is chosen in the design.

We have seen in last Lecture that the information matrix of a design is $C = \frac{1}{k} L$. Recall that it is not possible to estimate the vector of treatment effects $\boldsymbol{\tau}$. So it is not surprising that L is singular:

Proposition 2. *The Laplacian matrix of a graph is singular, and $\mathbf{1} := [1, 1, \ldots, 1]^T$ is an eigenvector associated to the eigenvalue* 0*. Moreover, the multiplicity of the eigenvalue* 0 *corresponds to the number of connected components in G.*

Proof. By definition of L, it is clear that the rows of L sum to 0, so $L\,\mathbf{1} = \mathbf{0}$. From Proposition 1 L can be written as EE^T, where E is a matrix with one column of the form $\boldsymbol{e}_{ij}$ for each (simple) edge of G. We have $\ker L = \ker EE^T = \ker E^T$, so $\boldsymbol{u}$ is in the nullspace of L iff $E^T \boldsymbol{u} = \mathbf{0}$, which implies that $\boldsymbol{u}$ is constant on each connected component of G. Hence, the multiplicity of 0 as eigenvalue of L, that is, the dimension of $\ker L$, is the number of connected components of G. □

The information matrix is singular for all designs, so the $A-$, $E-$, and $D-$ criterion are always equal to zero. But if we are interested in estimating all treatment differences $\tau_i - \tau_j$, we obtain a well-posed problem. Geometrically, the confidence ellipsoids are unbounded in the direction of the vector $\mathbf{1}$, but we can *minimize* the projection of the confidence ellipsoids in the subspace that is orthogonal to $\mathbf{1}$.

Definition 4. A block design (with t treatments, and b blocks of size k) is called $E-$, $A-$, or $D-$optimal if its information matrix C has $t-1$ nonzero eigenvalues (that is, the CG of the design is connected), and is such that

- **E-optimality** the smallest nonzero eigenvalue is maximum
- **A-optimality** the harmonic average of the nonzero eigenvalues is maximum
- **D-optimality** the geometric average of the nonzero eigenvalues is maximum,

over all block designs of b blocks of size k with t treatments.

Laplacian eigenvalues of graphs

We will now see that these functions of the Laplacian eigenvalues have nice graph-theoretical interpretations.

Recall that the optimal variance for the estimation of $\tau_i - \tau_j$ is $\sigma^2(\boldsymbol{e}_{ij}^T C^- \boldsymbol{e}_{ij}) = k\sigma^2(\boldsymbol{e}_{ij}^T L^- \boldsymbol{e}_{ij})$. The next proposition gives an interesting sense to this quantity:

Proposition 3. *Let $G = (V, E)$ be a connected graph with n nodes, and edges of weights w_e ($\forall e \in E$). Consider an electrical network with n nodes, with a resistor of $w_{i,j}\Omega$ connecting edges i and j. Assume that a current of 1 Ampere flow from node i to node j. The voltage between i and j is called the* effective resistance *between i and j, and is equal to*

$$R_{ij} = \boldsymbol{e}_{ij}^T L^- \boldsymbol{e}_{ij} = L_{ii}^\dagger + L_{jj}^\dagger - 2L_{ij}^\dagger.$$

Proof. From the relation $L = \sum_{(i,j)\in E} w_{i,j} \boldsymbol{e}_{ij} \boldsymbol{e}_{ij}^T$, we see that L can be written as EE^T, where E is a matrix with one column of the form $\boldsymbol{e}_{ij}$ for each (simple) edge of G. Let $\boldsymbol{p}$ be a vector of potentials at the nodes of G and $\boldsymbol{x}$ be a vector of currents on the edges of G (counted and oriented in the same order as in the matrix E). Ohm's Law and Kirchhoff's voltage law can be written as $E^T\boldsymbol{p} = \boldsymbol{x}$ (because the resistors are of one Ω, so the drop of potentials between 2 connected nodes is equal to the current on the corresponding edge), and Kirchhoff's current law is $E\boldsymbol{x} = \boldsymbol{e}_{ij}$. Thus, we obtain $EE^T\boldsymbol{p} = L\boldsymbol{p} = \boldsymbol{e}_{ij}$, and since $\boldsymbol{e}_{ij}$ is orthogonal to the nullspace of L (it is a contrast vector), we have $\boldsymbol{p} = L^\dagger \boldsymbol{e}_{ij}$ (up to some constant). So $R_{ij} = \boldsymbol{e}_{ij}^T \boldsymbol{p} = \boldsymbol{e}_{ij}^T L^- \boldsymbol{e}_{ij}$. □

Theorem 4. *The average of all pairwise effective resistances is equal to 2 divided by the harmonic average of the nonzero eigenvalues of the Laplacian.*

Proof. $\sum_{i=1}^t \sum_{j\neq i} R_{ij} = \sum_{i=1}^t \sum_{j\neq i} L_{ii}^\dagger + L_{jj}^\dagger - 2L_{ij}^\dagger = 2(t-1)\operatorname{trace} L^\dagger - 2\sum_{i=1}^t \sum_{j\neq i} L_{ij}^\dagger$. Now, note that $\mathbf{1}$ is an eigenvector of $L^\dagger$ associated to the eigenvalue 0. So for all i, $L_{ii}^\dagger = -\sum_{j\neq i} L_{ij}^\dagger$. Thus,

$$\sum_{i=1}^t \sum_{j\neq i} R_{ij} = 2(t-1)\operatorname{trace} L^\dagger + 2\sum_{i=1}^t L_{ii}^\dagger = 2t \operatorname{trace} L^\dagger,$$

and the eigenvalues of $L^\dagger$ are 0 and the inverses of the nonzero eigenvalues of L. □

We now give a result that gives an interpretation of the $D-$criterion for block designs.

Theorem 5. *Kirchhoff's matrix-tree theorem Let G be a connected graph on n vertices, with $w_{ij} \in \mathbb{Z}_+$ representing the "number of simple edges between i and j". Then the following three quantities are equal:*

1. *the number of spanning trees of G;*
2. *$\frac{1}{n}\times$ the product of the nonzero eigenvalues of L;*
3. *any cofactor of L, that is, $(-1)^{i+j}\times$ the determinant obtained by deleting row i and column j.*

Proof. in Exercises □

Remark 6. The results seen today also work with the Levi Graph (LG) of the design. More precisely,

- The effective resistance between i and j in the LG is equal to $k\,\times$ the effective resistance in the CG.
- The number of spanning trees in the LG is $k^{b-v+1}\,\times$ the number of spanning trees in the CG.
- So $A-$optimal designs maximize the average effective resistance of the LG, and $D-$optimal designs maximize the number of spanning trees in the LG.

Exercises

1. Consider the designs

$$\xi_1 = \begin{array}{|c|c|c|} \hline 1 & 2 & 1 \\ 2 & 3 & 2 \\ 3 & 5 & 4 \\ \hline \end{array} \qquad \text{and} \qquad \xi_2 = \begin{array}{|c|c|c|} \hline 2 & 1 & 1 \\ 3 & 2 & 3 \\ 4 & 5 & 5 \\ \hline \end{array}.$$

   - Construct the CG and the LG of the design.
   - Which of these 2 designs is better according to the $D-$criterion?
   - Which of these 2 designs is better for the estimation of $\tau_4 - \tau_5$?

2. Proof of the matrix-tree theorem. In this proof we only show that the number of spanning trees of G is equal to the $(1,1)-$minor of the Laplacian. The result for the other minors can be obtained by adding rows and column to others. The result with the product of the nonzero eigenvalues uses the coefficients of the characteristic polynomial of L to show that the product of the nonzero eigenvalues must be equal to the sum of the n principal minors of L.

   We admit the Binet-Cauchy formula: let A and B be two matrices of size $n \times m$, with $m \geq n$. Then, we have

$$\det AB = \sum_S \det A[S] \det B[S],$$

   where the sum goes over all subsets $S \subseteq \{1, \ldots, m\}$ of cardinality n, and $A[S]$ denotes the $n \times n-$submatrix of A formed by its columns indexed in S.

   - Recall that $L = EE^T$ for a matrix E with n rows and $\sum_{i<j} w_{ij}$ columns.
   - Let F be the matrix obtained by removing the first row of E. Write the first principal minor of L as a function of F. What does the Binet-Cauchy fomula tell ?
   - To conclude, show that $\det F[S] = \pm 1$ iff the edges indexed by S form a tree, and $\det F[S] = 0$ otherwise (by induction).