Chapter 4

Average Mixing

Theorem: Let X be a graph on n vertices with simple eigenvalues. If X is regular or has a non-trivial automorphism, then

$$\mathrm{rk}(\widehat{M}) < n.$$

Proof. Let $\{x_1, x_2, \ldots, x_n\}$ be a set of orthonormal eigenvectors of X for eigenvalues $\theta_1, \theta_2, \ldots, \theta_n$. Let N be the matrix whose j-th column is

$$x_j \circ x_j.$$

Since X has simple eigenvalues,

$$\widehat{M} = NN^T.$$

It suffices to show that

$$\mathrm{rk}(N) < n.$$

Suppose X is regular. Without loss of generality assume

$$x_1 = \frac{1}{\sqrt{n}}\mathbf{1}.$$

Then

$$N\mathbf{1} = nNe_1 = \mathbf{1}.$$

So the columns of N are linearly dependent. Now suppose X has a non-trivial automorphism P. We have

$$APx_j = \theta_j Px_j.$$

Since θ_j is simple,

$$Px_j = \pm x_j.$$

It follows that

$$P(x_j \circ x_j) = (Px_j) \circ (Px_j) = x_j \circ x_j.$$

Thus $PN = N$. Choose any vector y such that $P^T y \neq y$. Then we have

$$N^T y = N^T (P^T y).$$

This implies that $\operatorname{rk}(N) < n$. $\square$

4.0.8 Lemma. *Let $A, B \succcurlyeq 0$ and let $C = A + B$. Then*

$$\mathrm{rk}(C) \geq \max\{\mathrm{rk}(A), \mathrm{rk}(B)\}.$$

Proof. We have
$$\ker(C) = \ker(A) \cap \ker(B),$$
so
$$\mathrm{col}(A) + \mathrm{col}(B) \subseteq \mathrm{col}(C).6$$
□

4.0.9 Lemma. *Consider two rank-one orthogonal projections $E_1 = xx^T$ and $E_2 = yy^T$. Then the following statements are equivalent.*

(i) $E_1^{\circ 2}$ *is parallel to* $E_2^{\circ 2}$.

(ii) $E_1^{\circ 2} = E_2^{\circ 2}$.

(iii) $x^{\circ 2} = y^{\circ 2}$

(iv) $x = Dy$ *for some diagonal matrix* D *with entries* ± 1. □

4.0.10 Lemma. *Let E be an orthogonal projection.*

(i) If $\mathrm{rk}(E) = 1$, *then* $\mathrm{rk}(E^{\circ 2}) = 1$.

(ii) If $\mathrm{rk}(E) \geq 2$, *then* $\mathrm{rk}(E^{\circ 2}) \geq 2$.

Proof. To see the second statement, suppose $\mathrm{rk}(E) = 2$ and write

$$E = E_1 + E_2 + \cdots$$

where each E_i has rank one. Then

$$E^{\circ 2} \succcurlyeq E_1^{\circ 2} + E_2^{\circ 2} + E_1 \circ E_2.$$

If $E_1^{\circ 2} \neq E_2^{\circ 2}$, then $E_1^{\circ 2}$ and $E_2^{\circ 2}$ are not parallel and thus have different column spaces. Therefore $\mathrm{rk}(E^{\circ 2}) \geq 2$. If $E_1^{\circ 2} = E_2^{\circ 2}$, then we can write $E_1 = xx^T$ and $E_2 = yy^T$, where $y = Dx$ for some diagonal matrix D whose entries are ± 1. Now

$$E_1 \circ E_2 = (xx^T) \circ (Dxx^T D) = DE_1^{\circ 2} D.$$

Note $E_1^{\circ 2} + DE_1^{\circ 2} D$ is block diagonal and hence has rank at least two. □

4.0.11 Lemma. *If the average mixing matrix*

$$\widehat{M} = E_1^{\circ 2} + E_2^{\circ 2} + \cdots .$$

has rank one, then $E_i^{\circ^2}$ is a multiple of J, for each i. □

4.0.12 Lemma. *For any orthogonal projection E, we have*

$$\operatorname{rk}(E^{\circ 2}) \geq \operatorname{rk}(E).$$

Proof. We can write E as the Gram matrix of

$$\{u_1, u_2, \dots, u_n\},$$

where each $u_i \in \mathbb{R}^\ell$. Then

$$E_{ij}^2 = \langle u_i \otimes u_i, u_j \otimes u_j \rangle.$$

That is, $E^{\circ 2}$ is the Gram matrix of

$$\{u_1 \otimes u_1, \cdots, u_n \otimes u_n\}.$$

Suppose $\operatorname{rk}(E) = k$. Let $\{u_1, u_2, \dots, u_k\}$ be k linearly independent columns of E. We show that

$$\{u_1 \otimes u_1, \cdots, u_k \otimes u_k\}$$

are linearly independent. Assume

$$\sum_{i=1}^{k} a_i u_i \otimes u_i = 0.$$

By the isomorphism

$$u_i \otimes u_i \mapsto u_i \otimes u_i^T,$$

we have

$$\sum_{i=1}^{k} a_i u_i u_i^T.$$

Equivalently,

$$UDU^T = 0$$

where U is the $\ell \times k$ matrix whose columns are $u_1, u_2, \ldots, u_k$, and D is the diagonal matrix whose entries are $a_1, a_2, \ldots, a_k$. Since U has full column rank, there is an invertible matrix P such that

$$PU = \begin{pmatrix} I \\ 0 \end{pmatrix}.$$

Hence

$$0 = PUDU^T P^T = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix}.$$

Therefore $D = 0$. □

4.0.13 Lemma. *Let E be a spectral idempotent of X with*

$$\mathrm{rk}(E^{\circ 2}) = 2.$$

Then E has two disjoint eigenvectors.

Proof. Let x and y be any two orthonormal eigenvectors of E. If they are disjoint, then we are done. Otherwise, write $E = E_1 + E_2$, where $E_1 = xx^T$ and $E_2 = yy^T$. Then

$$E^\circ = FF^T$$

where

$$F = \begin{pmatrix} x \circ x & y \circ y & \sqrt{2} x \circ y \end{pmatrix}.$$

Since $\mathrm{rk}(F) = 2$, either $x \circ x = y \circ y$, which shows $x + y$ and $x - y$ are two disjoint eigenvectors, or

$$x \circ y = a x \circ x + b y \circ y$$

for some a and b. Take the inner product of both sides with $\mathbf{1}$. Since the left hand side is 0, while the right hand side is $a + b$, we must have $a + b = 0$ and $a \neq 0$. Thus

$$x_i y_i = a(x_i^2 - y_i^2).$$

It follows that $x_i = 0$ if and only if $y_i = 0$. For all i where x and y are non-zero, the above equation tells us that

$$\frac{x_i}{y_i} = \frac{1 \pm \sqrt{1 + 4a^2}}{2a}.$$

Moreover, both ratio should appear since $x \neq y$. Now let

$$t = \frac{1 + \sqrt{1 + 4a^2}}{2a}, \quad s = \frac{1 - \sqrt{1 + 4a^2}}{2a}.$$

The vectors $x - ty$ and $x - sy$ are disjoint eigenvectors of E. □

4.0.14 Lemma. *Suppose*

$$\widehat{M} = E_1^{\circ 2} + E_2^{\circ 2} + \cdots$$

with

$$\operatorname{rk}(E_1^{\circ 2}) = \operatorname{rk}(E_2^{\circ 2}) = \operatorname{rk}(\widehat{M}) = 2.$$

Then

$$E_1^{\circ 2} = E_2^{\circ 2} = \begin{pmatrix} (xx^T)^{\circ 2} & 0 \\ 0 & (yy^T)^{\circ 2} \end{pmatrix}$$

for some unit vectors x and y.

Proof. From previous lemma we see

$$E_i = \begin{pmatrix} x_i x_i^T & 0 \\ 0 & y_i y_i^T \end{pmatrix}.$$

Since $\widehat{M}$ has the same rank as $E_i^{\circ 2}$,

$$\operatorname{col}(\widehat{M}) = \operatorname{col}(E_i^{\circ}) = \operatorname{col}\begin{pmatrix} x_i^{\circ 2} & 0 \\ 0 & y_i^{\circ 2} \end{pmatrix}.$$

Therefor $x_1^{\circ 2} = x_2^{\circ 2}$ and $y_1^{\circ 2} = y_2^{\circ 2}$. $\square$

4.0.15 Lemma. *Suppose*

$$\widehat{M} = E^{\circ 2} + F^{\circ 2} + \cdots$$

with

$$\operatorname{rk}(\widehat{M}) = \operatorname{rk}(E^{\circ 2}) = 2, \quad \operatorname{rk}(F^{\circ 2}) = 1.$$

Then

$$F = \begin{pmatrix} \frac{1}{\sqrt{\alpha}} D & 0 \\ 0 & \frac{1}{\sqrt{\beta}} S \end{pmatrix} \begin{pmatrix} xx^T & xy^T \\ yx^T & yy^T \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{\alpha}} D & 0 \\ 0 & \frac{1}{\sqrt{\beta}} S \end{pmatrix}$$

where

$$\begin{pmatrix} x \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ y \end{pmatrix}$$

are orthonormal eigenvectors of E,

$$\frac{1}{\alpha} + \frac{1}{\beta} = 1,$$

and D and S are some diagonal matrices with ± 1 entries.

Proof. We have
$$E^{\circ 2} = \begin{pmatrix} (xx^T)^{\circ 2} & 0 \\ 0 & (yy^T)^{\circ 2} \end{pmatrix}$$
and
$$F^{\circ 2} = \begin{pmatrix} (zz^T)^{\circ 2} & (zw^T)^{\circ 2} \\ (wz^T)^{\circ 2} & (ww^T)^{\circ 2} \end{pmatrix}.$$
Since
$$\operatorname{rk}(E^{\circ 2} + F^{\circ 2}) = \operatorname{rk}(E^{\circ 2}) = 2,$$
it follows that $(xx^T)^{\circ 2} + (zz^T)^{\circ 2}$ is parallel to $(wz^T)^{\circ 2}$. Take the inner product of both vectors with $\mathbf{1}^T$ and we get

$$x^{\circ 2} = \alpha z^{\circ 2}$$

for some α, that is
$$z = \frac{1}{\sqrt{\alpha}} Dx$$
for some diagonal matrix D with ± 1 entries. Similarly,

$$w = \frac{1}{\sqrt{\beta}} Sy$$

for some diagonal matrix S with ± 1 entries. Finally,

$$\frac{1}{\alpha} + \frac{1}{\beta} = \langle \mathbf{1}, z^{\circ 2} + w^{\circ 2} \rangle = 1.$$ □

4.0.16 Lemma. *Let X be a graph whose eigenvalues are not all simple, and suppose $\operatorname{rk}(\widehat{M}) = 2$. Then X has two strongly cospectral classes.*

Proof. Write
$$\widehat{M} = E_1^{\circ 2} + \cdots + E_k^{\circ 2} + F_1^{\circ} + \cdots,$$
with
$$\operatorname{rk}(\widehat{M}) = \operatorname{rk}(E_i^{\circ 2}) = 2, \quad \operatorname{rk}(F_j^{\circ 2}) = 1.$$
By previous lemma, if E_1 has orthonormal eigenvectors

$$\begin{pmatrix} x \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ y \end{pmatrix}$$

then each F_j has eigenvector

$$\begin{pmatrix} \frac{1}{\sqrt{\alpha_j}} Dx \\ \frac{1}{\sqrt{\beta_j}} Dy \end{pmatrix}.$$

Thus

$$1 = I_{uu} = \sum_i (E_i)_{uu} + \sum_j (F_j)_{uu}$$

is either

$$\left(k + \sum_j \frac{1}{\alpha_j} \right) x_u^2$$

or

$$\left(k + \sum_j \frac{1}{\beta_j} \right) y_u^2.$$

Hence $x^{\circ 2}$ and $y^{\circ 2}$ are both constant. It follows that $(E_i)_{uu}$ takes two values, and $(F_j)_{uu}$ takes two values. Moreover, all columns of F_j are parallel, and the structure of E_i shows it has two parallel classes. Therefore X has exactly two strongly cospectral classes. □

4.0.17 Lemma. *Let X be a regular graph on $n \geq 4$ vertices. If X has simple eigenvalues, then* $\operatorname{rk}(\widehat{M}) \leq n-3$.

Proof. Let $\{x_1, x_2, \ldots, x_n\}$ be a set of orthonormal eigenvectors of X for eigenvalues $\theta_1, \theta_2, \ldots, \theta_n$. Let N be the matrix whose r-th column is

$$x_r \circ x_r.$$

Since X has simple eigenvalues,

$$\widehat{M} = NN^T.$$

Suppose X is k-regular and

$$x_1 = \frac{1}{\sqrt{n}}\mathbf{1}.$$

We show that $\operatorname{null}(N) \geq 3$. First note that

$$\begin{aligned} N \begin{pmatrix} \theta_1^j \\ \cdots \\ \theta_n^j \end{pmatrix} &= \sum_r \theta_r^j x_j \circ x_j \\ &= \sum_r \theta_r^j \left((x_j x_j^T) \circ I\right) \mathbf{1} \\ &= \left(A^j \circ I\right) \mathbf{1}. \end{aligned}$$

Plug in $j = 0, 1, 2$ and we get three vectors in $\ker(N)$:

$$N(\mathbf{1} - ne_1) = 0$$

$$N \begin{pmatrix} \theta_1 \\ \cdots \\ \theta_n \end{pmatrix} = 0$$

$$N \begin{pmatrix} \theta_1^2 - k \\ \cdots \\ \theta_n^2 - k \end{pmatrix} = 0$$

If the three vectors are linearly dependent, then there are α, β and γ such that for all $r \geq 2$,

$$\alpha(\theta_r^2 - k) + \beta\theta_r + \gamma = 0.$$

Thus there are at most two values for $\theta_2, \theta_3, \ldots, \theta_n$ to take. Since X has simple eigenvalues, it must have fewer than 4 vertices. □