# Chapter 8

# 초콜릿 시럽 Linear Algebra

*I cannot pour chocolate sauce over asparagus.*

George Szell

*Yes we can. Yes we did.*

Barack Obama

## 8.1 Basic linear algebra

선형대수에서 배운 내용을 상기해봅시다.

### 8.1.1 Coordinatization

1. abstract vector space $V$ over $k$, basis and dimension
2. linear transformation and isomorphism
3. the coordinate vector $[v]_B$ of $v \in V$ with relative to a basis $B$, $V \cong k^n$.
4. the representation $[T]_{BC}$ of $T : V \to W$
5. similar matrices: $[T]_B$, $[T]_C$, and basis change matrix $P_{C \leftarrow B}$

동일한 선형변환을 다른 기저를 이용하여 표현한 두 행렬은 서로 닮았고 similar, 따라서 많은 성질을 서로 공유합니다.

**Proposition 8.1.** *If $A$ and $B$ are similar, then*

$$\det(A) = \det(B) \qquad \textit{and} \qquad tr(A) = tr(B).$$

*Proof.* First prove/recall that $tr(XY) = tr(YX)$ and $\det(XY) = \det(X)\det(Y)$. ☐

### 8.1.2 Eigenvector and eigenvalues

1. the determinant of a square matrix $A$
2. the invertibility of $A$
3. the characteristic equation, eigenvalues and eigenvectors of $A$
4. diagonalization of $A$: algebraic and geometric multiplicity of $\lambda$.

### 8.1.3 Jordan canonical form

A Jordan matrix is a block diagonal matrix whose diagonal block is a Jordan block.

**Theorem 8.2.** *Every matrix $A \in M_n(\mathbb{C})$ is similar to a Jordan matrix.*

### 8.1.4 Cayley-Hamilton theorem

Let $A \in M_n(\mathbb{C})$. For a polynomial $f(x) = c_k x^k + \cdots + c_1 x + c_0$, we define the matrix

$$f(A) = c_k A^k + \cdots + c_1 A + c_0 I_n.$$

Note that if $A$ and $B$ are similar then $f(A)$ and $f(B)$ are similar.

**Theorem 8.3.** *Let $ch_A(x) = \det(xI - A)$ be the characterisitc polynomial of $A \in M_n(\mathbb{C})$. Then, $ch_A(A)$ is the zero matrix.*

With a fixed $A \in M_n(\mathbb{C})$, define an action of $k[x]$ on $k^n$:

$$k[x] \times k^n \to k^n, \quad (f(x), v) \mapsto f(A)v.$$

Note that $f(A)v = 0$ for all $v \in k^n$ if and only if $f(A)$ is the zero matrix. We let $I$ be the set of all $f(x) \in k[x]$ such that $f(A)$ is the zero matrix. Then, it is an ideal and from the fact that $k[x]$ is a principal ideal domain, there is $m(x) \in I$ such that

$$I = \{g(x)m(x) : g(x) \in k[x]\}.$$

Then, the Cayley-Hamilton theorem says that the characteristic polynomial of $A$ is in the ideal and thus the ideal is non-trivial. A monomic generator of the ideal $I$ is called the minimal polynomial of $A$. We remark that the Cayley-Hamilton theorem can be helpful to compute $A^{-1}$ and $A^m$ for a large $m$.

To prove the theorem, we let $J$ be the Jordan canonical form of $A$, thus $Q^{-1}AQ = J$ for some $Q \in M_n(\mathbb{C})$. Then, from

$$ch_A(A) = ch_A(QJQ^{-1}) = Q\, ch_A(J)Q^{-1}$$

it is enough to prove that $ch_A(J)$ is the zero matrix.

## 8.2 Diagonalization of symmetric matrices

### 8.2.1 Eigenvalues of symmetric matrices

For $A \in M_n(\mathbb{C})$, write $A^*$ for the conjugate of the transpose $A^T$. A complex square matrix $A$ is <u>Hermitian</u>, if

$$A^* = A.$$

Note that a real symmetric matrix is Hermitian.

**Theorem 8.4.** *If $A \in M_n(\mathbb{C})$ is Hermitian, then the eigenvalues of $A$ are real.*

*Proof.* Let $Av = \lambda v$ for some $\lambda \in \mathbb{C}$ and nonzero $v \in \mathbb{C}^n$. Then, $v^*(Av) = v^*(\lambda v) = \lambda v^* v$ and

$$\lambda(v^*v) = v^*Av = v^*A^*(v^*)^* = (v^*Av)^* = (\lambda v^*v)^* = \overline{\lambda}(v^*v).$$

When $v^T = \begin{bmatrix} c_1 & c_2 & \cdots & c_n \end{bmatrix}$, since

$$v^*v = \sum_{i=1}^{n} c_i\overline{c_i} = \sum_{i=1}^{n} |c_i|^2 > 0$$

we have $\overline{\lambda} = \lambda$ and thus $\lambda$ is real. $\square$

### 8.2.2 Orthogonal diagonalization

Recall that a $n \times n$ matrix $A$ is called diagonalizable, if it is similar to a diagonal matrix.

**Theorem 8.5.** *A matrix $A \in M_n(\mathbb{C})$ is diagonalizable if and only if there is a basis of $\mathbb{C}^n$ consisting of eigenvectors $v_1, ..., v_n$ of $A$. In this case, if $\lambda_i$ are eigenvalues of $A$ corresponding to $v_i$ then*

$$Q^{-1}AQ = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \quad \textit{where} \quad Q = \begin{bmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{bmatrix}.$$

Recall that $U \in M_n(\mathbb{C})$ is a unitary matrix if and only if the set of column vectors of $U$ is an orthonormal basis of $\mathbb{C}^n$ with respect to the standard Hermitian inner product of $\mathbb{C}^n$; $P \in M_n(\mathbb{R})$ is orthogonal if and only if the set of columns vectors of $P$ is an orthonormal basis of $\mathbb{R}^n$ with repect to the standard inner product.

**Theorem 8.6.** *$A \in M_n(\mathbb{C})$ is Hermitian if and only if $A$ is unitarily diagonalizable. $A \in M_n(\mathbb{R})$ is symmetric if and only if $A$ is orthogonally diagonalizable.*

## 8.3 Positive definite matrix

벡터공간 $\mathbb{R}^n$에 정의된 dot product를 일반화하는 한가지 방법은 다음 관찰로부터

$$v \cdot w = v^T w = v^T I_n w$$

항등행렬 $I_n$을 일반화하는 것이겠습니다.

$$\langle v, w \rangle = v^T A w.$$

교환법칙 $\langle v, w \rangle = \langle w, v \rangle$이 성립하려면 $A$는 대칭행렬이어야 합니다. 또한 미적분 등에서 보았듯이 dot product를 이용하여 벡터의 길이를 $|v| = \sqrt{v \cdot v}$로 정의하려면 모든 벡터에 대해 $v \cdot v \geq 0$이고 등호는 오직 영벡터에 대해서만 성립하는 성질이 중요합니다. 이로부터 다음과 같은 성질의 행렬들을 공부해보고자 합니다.

**Definition 8.7.**
1. *A symmetric matrix $A \in M_n(\mathbb{R})$ is positive semidefinite (PSD), if $v^T A v \geq 0$ for all $v \in \mathbb{R}^n$.*
2. *A symmetric matrix $A \in M_n(\mathbb{R})$ is positive definite (PD), if $A$ is PSD and $v^T A v = 0$ holds only when $v = \mathbf{0}$.*

A positive definite symmetric bilinear form on $\mathbb{R}^n$ is called an inner product. The following map is an inner product, if $A$ is symmetric and positive definite.

$$\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}, \quad (v, w) \mapsto v^T A w.$$

**Lemma 8.8.** *If $A \in M_n(\mathbb{R})$ is PSD then the eigenvalues of $A$ is greater than or equal to $0$.*

*Proof.* Suppose that $Av = \lambda v$ for nonzero $v \in \mathbb{R}^n$. Then,

$$v^T A v = v^T \lambda v = \lambda v^T v.$$

Since $v^T v \geq 0$ and $v^T A v \geq 0$, $\lambda \geq 0$. If $A$ is PD, $v \neq 0$ implies $\lambda > 0$. $\square$

**Lemma 8.9.** *If $B$ is $n \times m$ real matrix, then $BB^T$ is symmetric and PSD.*

*Proof.* The matrix $A = BB^T$. is symmetric, because $A^T = (BB^T)^T = (B^T)^T B^T = BB^T = A$. We want to show that $u^T A u \geq 0$ for all $u \in \mathbb{R}^n$:

$$u^T A u = u^T (BB^T) u = (u^T B)(B^T u) = (u^T B)(u^T B)^T \geq 0.$$

□

**Theorem 8.10.** *If $A \in M_n(\mathbb{R})$ is symmetric, then the following statements are equivalent.*

1. *A is PSD.*
2. *All eigenvalues of A are greater than or equal to 0.*
3. *$A = BB^T$ for some $B \in M_{n\times m}(\mathbb{R})$.*

*Proof.* Let us prove (1) → (2) → (3) → (1). Since (1) → (2) (Lemma 8.8) and (3) → (1) (Lemma 8.9) are already proved, we are left to show (2) → (3).

Suppose that (2) is true. Since $A$ is symmetric, $A$ is orthogonally diagaonalizable (Theorem 8.6). Thus, for some orthogonal matrix $P$,

$$P^T AP = D = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} = \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_n} \end{pmatrix}^2 .$$

Let's write

$$\begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_n} \end{pmatrix} = \sqrt{D}.$$

Then,

$$A = PDP^T = P(\sqrt{D}\sqrt{D})P^T = (P\sqrt{D})(\sqrt{D}^T P^T) = (P\sqrt{D})(P\sqrt{D})^T.$$

□

## 8.4 Eigenvalues of principal submatrices

For a square matrix $A$, its square submatrix $B$ is a principal submatrix, if the diagonal entries of $B$ lie on the diagonal of $A$. More explicitly, $B$ is a $k \times k$ principal submatrix of $A$ such that

$$(B)_{ab} = (A)_{i_a i_b}$$

for all $a, b$ with $i_1 < i_2 < \cdots < i_k$. Note that the adjacency matrix $A_H$ of an induced subgraph $H$ of $G$ is a principal submatrix of $A_G$

### 8.4.1 Positivity

**Lemma 8.11.** *Let $A \in M_n(\mathbb{R})$ be symmetric and PSD. Then, every principal submatrix of $A$ is also symmetric and PSD.*

*Proof.* Let $A' \in M_k(\mathbb{R})$ be a principal submatrix of $A$ by choosing $i_1, ..., i_k$ rows and columns of $A$. Then, since $A$ is symmetric

$$(A')_{ab} = (A)_{i_a i_b} = (A)_{i_b i_a} = (A')_{ba}$$

and thus $A'$ is symmetric.

Net, to prove that $A'$ is PSD, we need to show $x^T A' x \geq 0$ for all $x \in \mathbb{R}^k$. For each

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} \in \mathbb{R}^k,$$

let us define

$$\tilde{x} = \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \vdots \\ \tilde{x}_n \end{bmatrix} \text{ where } \tilde{x}_l = \begin{cases} x_m & \text{if } l = i_m \text{ for some } 1 \leq m \leq k \\ 0 & \text{otherwise.} \end{cases}$$

Then, we claim that $x^T A' x = \tilde{x}^T A \tilde{x}$. This is because

$$\tilde{x}^T A \tilde{x} = \sum_{s=1}^{n} \sum_{t=1}^{n} \tilde{x}_s A_{st} \tilde{x}_t = \sum_{s'=1}^{k} \sum_{t'=1}^{k} x_{s'} (A')_{s't'} x_{t'} = x^T A' x.$$

Since $A$ is PSD, $\tilde{x}^T A \tilde{x} \geq 0$ and therefore, $x^T A' x \geq 0$. $\square$

뒤에서 대칭행렬의 고윳값과 그 principal sumbtrix의 고윳값과의 관계에 대한 일반적인 내용을 증명할 예정인데, 먼저 positivity 성질을 활용하여 쉽게 증명할 수 있는 간단한 내용부터 보겠습니다.

**Theorem 8.12.** *Let $B$ be a $k \times k$ principal submatrix of a $n \times n$ symmetric matrix $A$. Let $\lambda^A$ and $\lambda^B$ be the set of all eigenvalues of $A$ and $B$ respectively. Then,*

$$\max \lambda^A \geq \max \lambda^B \geq \min \lambda^B \geq \min \lambda^A.$$

*Proof.* The second inequality $\max \lambda^B \geq \min \lambda^B$ is trivial. Let us prove the first inequality.

1. Let $\sigma$ be any eigenvalue of $(\max \lambda^A I_n - A)$ and $v$ be an eigenvector corresponding to $\sigma$. Since $\max \lambda^A I_n - A$ is symmetric, we know that $\sigma$ is a real number.

2. Then, we have
$$\begin{aligned}(\max \lambda^A I_n - A)v &= \sigma v \\ Av &= (\max \lambda^A - \sigma)v,\end{aligned}$$
which shows that $(\max \lambda^A - \sigma)$ is an eigenvalue of $A$.

3. Since $\max \lambda^A$ is the largest eigenvalue of $A$, we have
$$\max \lambda^A \geq (\max \lambda^A - \sigma),$$
from which we conclude that $\sigma \geq 0$ and then $(\max \lambda^A I_n - A)$ is PSD by Theorem 8.10.

4. Being a principal submatrix of $(\max \lambda^A I_n - A)$, the matrix $(\max \lambda^A I_k - B)$ is symmetric and PSD. by Theorem 8.11. Thus, all the eigenvalues of $(\max \lambda^A I_k - B)$ are nonnegative.

5. Now let $\mu$ be any eigenvalue of $B$ and $w$ be a corresponding eigenvector. Then, from $Bw = \mu w$, we have
$$(\max \lambda^A I_k - B)w = (\max \lambda^A - \mu)w$$
which shows that $(\max \lambda^A - \mu)$ is an eigenvalue of $(\max \lambda^A I_k - B)$ and thus
$$\max \lambda^A - \mu \geq 0.$$

6. This shows that for all eigenvalues $\mu$ of $B$, we have $\max \lambda^A \geq \mu$ and can conclude that $\max \lambda^A \geq \max \lambda^B$.

The proof of the last inequality is similar and left as an exercise to the reader □

### 8.4.2 Courant-Fischer theorem

**Lemma 8.13.** *Let $S$ be a $k$-dimensional subspace of $\mathbb{C}^n$. The map from the set of all unit vectors in $S$ to $\mathbb{R}$ defined by*
$$f(x) = x^* Ax$$
*has absolute maximum and minimum values.*

**Theorem 8.14** (Courant-Fischer Theorem). *Let $A \in M_n(\mathbb{C})$ is a Hermitian matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then, for $1 \leq k \leq n$*

$$\begin{aligned}\lambda_k &= \max_{S \subset \mathbb{C}^n} \left\{ \min_{x \in S} \{x^* A x : \|x\| = 1\} \mid \dim S = k \right\} \\ &= \min_{S \subset \mathbb{C}^n} \left\{ \max_{x \in S} \{x^* A x : \|x\| = 1\} \mid \dim S = n - k + 1 \right\}.\end{aligned}$$

*It is also called the min-max theorem.*

*Proof.*

1. Let us prove the first equality. Since $A$ is Hermitian, $A$ is unitarily diagonalizable. Let $u_i \in \mathbb{C}^n$ be orthonormal eigenvectors corresponding to eigenvalues $\lambda_i$. Then, $\{u_1, u_2, \ldots, u_n\}$ is an orthonormal basis of $\mathbb{C}^n$.

$$u_i^* u_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

2. Let $T$ be a subspace of $\mathbb{C}^n$ spanned by $\{u_k, u_{k+1}, ..., u_n\}$ and choose any $k$-dimensional subspace $S$ of $\mathbb{C}^n$. Since $\dim T + \dim S > n$, their intersection $S \cap T$ is a nontrivial subspace of $\mathbb{C}^n$ and we can choose a unit vector $x_0 \in S \cap T$.

3. Being an element in $T$, the vector $x_0$ can be written as

$$x_0 = \sum_{i=k}^{n} c_i u_i$$

for some $c_i \in \mathbb{C}$ and $\|x_0\|^2 = 1$, or $x_0^* x_0 = 1$, implies that

$$\left( \sum_{i=k}^{n} c_i u_i \right)^* \left( \sum_{i=k}^{n} c_i u_i \right) = \sum_{i,j=k}^{n} \overline{c_i} c_j \, u_i^* u_j = \sum_{i=k}^{n} |c_i|^2 = 1. \tag{8.1}$$

4. Next let us show that $x_0^* A x_0 \le \lambda_k$.

$$\begin{aligned} x_0^* A x_0 &= \left(\sum_{i=k}^{n} c_i u_i\right)^* A \left(\sum_{j=k}^{n} c_j u_j\right) = \left(\sum_{i=k}^{n} c_i u_i\right)^* \left(\sum_{j=k}^{n} c_j A u_j\right) \\ &= \left(\sum_{i=k}^{n} c_i u_i\right)^* \left(\sum_{j=k}^{n} c_j \lambda_j u_j\right) = \sum_{i,j=k}^{n} \overline{c_i} c_j \lambda_j u_i^* u_j = \sum_{j=k}^{n} |c_j|^2 \lambda_j \\ &\le \sum_{j=k}^{n} |c_i|^2 \lambda_k = \lambda_k. \end{aligned}$$

In the last line, we applied the equality (8.1).

5. Since $x_0$ is a unit vector in $S$

$$\min_{x \in S} \{x^* A x : \|x\| = 1\} \le \lambda_k.$$

Moreover, since we chose a $k$-dimensional subspace $S$ of $\mathbb{C}^n$ arbitrarily,

$$\max_{S \subset \mathbb{C}^n} \left\{ \min_{x \in S} \{x^* A x : \|x\| = 1\} \mid \dim S = k \right\} \le \lambda_k. \tag{8.2}$$

6. Next, let $S'$ be the subspace of $\mathbb{C}^n$ spanned by $u_1, u_2, ..., u_k$ and choose a unit vector $x_1 \in S'$. Then,

$$x_1 = \sum_{i=1}^{k} c_i' u_i$$

for some $c_i' \in \mathbb{C}$ and using a computation similar to (8.1), we have

$$\sum_{i=1}^{k} |c_i'|^2 = 1. \tag{8.3}$$

7. Now we want to show that $x_1^* A x_1 \ge \lambda_k$.

$$\begin{aligned} {x_1}^* A x_1 &= \left(\sum_{i=1}^{k} {c'}_i u_i\right)^* A \left(\sum_{j=1}^{k} {c'}_j u_j\right) = \left(\sum_{i=1}^{k} {c'}_i u_i\right)^* \left(\sum_{j=1}^{k} {c'}_j A u_j\right) \\ &= \left(\sum_{i=1}^{k} {c'}_i u_i\right)^* \left(\sum_{j=1}^{k} {c'}_j \lambda_j u_j\right) = \sum_{i=1}^{k} |c_i'|^2 \lambda_i \\ &\ge \sum_{i=1}^{k} |c_i'|^2 \lambda_k = \lambda_k \end{aligned}$$

In the last line, we applied the equality (8.3).

8. Since $x_1$ is an arbitrary unit vector in $S'$,

$$\min_{x\in S'}\{x^*Ax : x \in S',\ \|x\| = 1\} \geq \lambda_k.$$

Therefore,

$$\max_{S'\subset\mathbb{C}^n}\left\{\min_{x\in S'}\{x^*Ax : \|x\| = 1\} \mid \dim S' = k\right\} \geq \lambda_k. \tag{8.4}$$

9. Finally, we obtain the first equality from (8.2) and (8.4). The proof of the second equality is similar and left as an exercise to the reader.

□

### 8.4.3 Cauchy's interlacing theorem

**Theorem 8.15** (Cauchy's Interlacing Theorem). *Let $A \in M_n(\mathbb{C})$ is Hermitian with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. For a principal submatrix $B \in M_k(\mathbb{C})$ of $A$ with eigenvalues $\mu_1 \geq \mu_2 \geq \dots \mu_k$,*

$$\lambda_j \geq \mu_j \geq \lambda_{n-k+j}$$

*for $j = 1, 2, \dots, k$.*

*Proof.* 1. It is enough to prove the theorem for the matrix $B$ obtained by erasing the last $n-k$ rows and columns of $A$ (why?).

2. Consider the subspace $T$ of $\mathbb{C}^n$ spanned by vectors of the form

$$y = \begin{bmatrix} z_1 \\ \vdots \\ z_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Then, $T \cong \mathbb{C}^k$.

3. By Theorem 8.14, for $1 \leq j \leq k$,

$$\begin{aligned}\lambda_j &= \max_{S \subset \mathbb{C}^n} \left\{ \min_{x \in S} \{x^* A x : \|x\| = 1\} \mid \dim S = j \right\} \\ &\geq \max_{S \subset T} \left\{ \min_{y \in S} \{y^* A y : \|x\| = 1\} \mid \dim S = j \right\}\end{aligned}$$

4. Every element $y$ in $T$ can be written as, using an element $z \in \mathbb{C}^k$,

$$y = \begin{bmatrix} z \\ 0 \end{bmatrix}$$

   and then $y^* A y = z^* B z$.

5. Thus,

$$\begin{aligned}\lambda_j &\geq \max_{S \subset T} \left\{ \min_{y \in S} \{y^* A y : \|y\| = 1\} \mid \dim S = j \right\} \\ &= \max_{S \subset \mathbb{C}^k} \left\{ \min_{z \in S} \{z^* B z : \|z\| = 1\} \mid \dim S = j \right\} = \mu_j.\end{aligned}$$

6. For the other inequality, note that the eigenvalues of $-A$ are $-\lambda_n \geq \cdots \geq -\lambda_1$. Then, using the same argument, we obtain

$$-\lambda_{n-\alpha+1} \geq -\mu_{k-\alpha+1}$$

   for $1 \leq \alpha \leq k$. Thus,

$$\mu_j \geq \lambda_{n-k+j} \tag{8.5}$$

   by substituting $k - \alpha + 1 = j$.

□

See ‘Cauchy’s interlace theorem for Hermitian matrices’ by Suk-Geun Hwang, the American Mathematical Monthly, Feb 2004 and ‘A very short proof of Cauchy’s interlace theorem for eigenvalues of Hermitian matrices’ by Steve Fisk, the American Mathematical Monthly, Feb 2005.

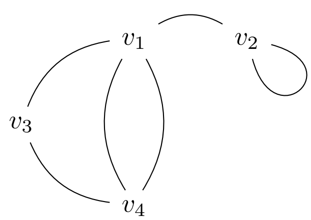
# Chapter 9

# 인접 행렬과 근접 행렬

## 9.1 Adjacency Matrix

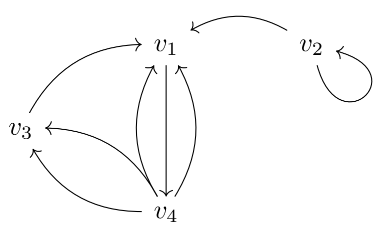
**Definition 9.1.** *Let $G = (V, E)$ be a undirected graph with $|V| = n$, the adjacency matrix $A_G$ of $G$ is the $n \times n$ matrix whose $(i, j)$ entry is the number of edges incident with both $v_i$ and $v_j$.*

**Example 9.2.**

$G =$ 


$$A_G = \begin{bmatrix} 0 & 1 & 1 & 2 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 2 & 0 & 1 & 0 \end{bmatrix}$$

**Example 9.3.** *When $G$ is a directed graph, we let $(A_G)_{ij}$ be the number of edges from $v_i$ to $v_j$.*

$G =$ 


$$A_G = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 \end{bmatrix}.$$

**Lemma 9.4.** *If $G$ is undirected then $A_G$ is symmetric $A_G^T = A_G$.*

**Proposition 9.5.** *The eigenvalues of $A_G$ of a undirected graph $G$ are real.*

*Proof.* Since $A_G$ is symmetric, the statement follows from Theorem 8.4. $\square$

When we study an adjacency matrix of a graph $G$, the vertex labeling is not important. It is because the adjacency matrices of isomorphic graphs $G$ and $G'$ are similar and two similar matrices have the same eigenvalues.

**Theorem 9.6.** *If $G$ and $G'$ are isomorphic to each other then $P^{-1}A_GP = A_{G'}$ for some permutation matrix $P$.*

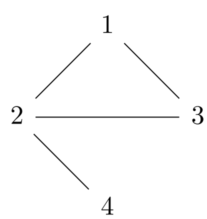
*Proof.* Let $G = (V, E)$ with $|V| = n$. Consider the permutation matrix $P$ defined by $(P)_{ij} = 1$ if and only if $\phi(v_i) = {v_j}'$ and $P_{ij} = 0$ otherwise. Then, for every $(i, j)$,

$$\begin{aligned}(A_GP)_{ij} &= \sum_{k=1}^{n}(A_G)_{ik}(P)_{kj} = (A_G)_{is} \quad \text{for } \phi(v_s) = v_j \\ &= (A_{G'})_{tj} = \sum_{k=1}^{n}(P)_{ik}(A_{G'})_{kj} = (PA_{G'})_{ij} \quad \text{for } \phi(v_i) = v_t.\end{aligned}$$

Thus, $A_GP = PA_{G'}$. Since every permutation matrix invertible, we obtain the statement. $\square$

**Example 9.7.** *Verify the above theorem with the following example.*

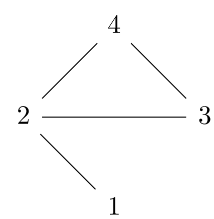
$G$




$A_G$

$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$G'$




$A_{G'}$

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

**Lemma 9.8.** *The trace $\mathrm{tr}(A_G)$ of $A_G$ counts the number of loops in $G$.*

**Theorem 9.9.** *The $(i, j)$ entry of the $k$th power of $A_G$ is equal to the number of walks of length $k$ from $v_i$ to $v_j$.*

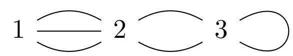
*Proof.* Use mathematical induction on $k$. By the definition of adjacency matrix, $(A_G)_{ij}$ is the number of walks from $v_i$ to $v_j$ of length 1. Suppose that $(A_G^{k-1})_{ij}$ is the number of walks from $v_i$

to $v_j$ of length $k-1$. Then,

$$(A_G^k)_{ij} = ((A_G^{k-1})\,A_G)_{ij} = \sum_{l=1}^{n}(A_G^{k-1})_{il}(A_G)_{lj}$$

implies that $({A_G}^k)_{ij}$ is the summation of walks of length $k$ from $v_i$ to $v_j$ via $v_l$ for all $v_l \in V$. $\square$

**Example 9.10.** *Verify the above theorem for the following graph.*

$G =$ 


$$A_G = \begin{bmatrix} 0 & 3 & 0 \\ 3 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix} \qquad A_G^2 = \begin{bmatrix} 9 & 0 & 6 \\ 0 & 13 & 2 \\ 6 & 2 & 5 \end{bmatrix} \qquad A_G^3 = \begin{bmatrix} 0 & 39 & 6 \\ 39 & 4 & 28 \\ 6 & 28 & 9 \end{bmatrix}$$

For the rest of this section, we will focus on undirected simple graphs. Recall that if $G$ is simple, then $(A_G)_{ij} = 1$ if and only if $i \neq j$ and $v_i$ adjacent to $v_j$. Otherwise, $(A_G)_{ij} = 0$.

**Theorem 9.11.** *Let $G = (V, E)$ be a simple graph.*

1. $\mathrm{tr}(A_G) = 0$.
2. $\mathrm{tr}(A_G^2) = 2|E|$.
3. $\mathrm{tr}(A_G^3) = 6 \times ($*the number of triangles in* $G)$.

*Proof.* $\square$

**Proposition 9.12.** *Let $G = (V, E)$ be a simple graph with $n$ vertices and $\lambda_1 \geq \cdots \geq \lambda_n$ be the eigenvalues of its adjacency matrix $A_G$. Then,*

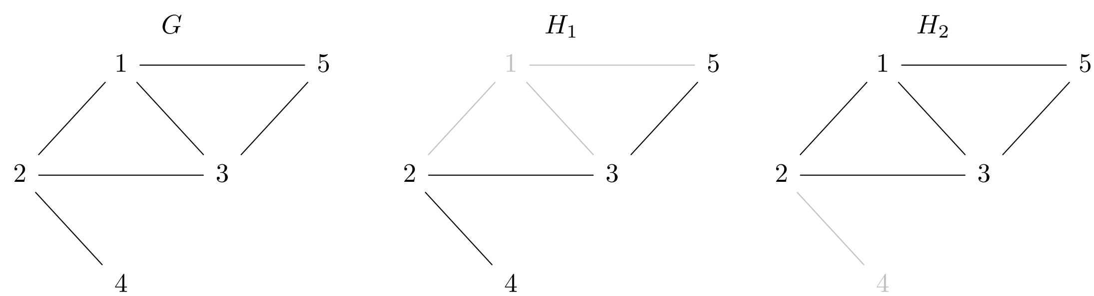
1. $\prod_{i=1}^{n} \lambda_i = \det A_G$.
2. $\sum_{i=1}^{n} \lambda_i = 0$.
3. $\sum_{i=1}^{n} \lambda_i^2 = 2|E|$.
4. $\sum_{i<j} \lambda_i \lambda_j = -|E|$.

*Proof.* For (1) and (2), note that the product and sum of eigenvalues are equal to the determinant and the trace of $A_G$. For (3), use the first statement in the above theorem. Statement (4) follows from (2) and (3). $\square$

## 9.2 Induced subgraphs and their adjacency matrices

Let $G = (V_G, E_G)$ be a simple graph. Recall the following definitions: $H = (V_H, E_H)$ is a subgraph of $G$, if $V_H \subseteq V_G$ and $v$ and $w$ are adjacent in $H$ implies $v$ and $w$ are adjacent in $G$. $H = (V_H, E_H)$ is an induced subgraph of $G$, if $H$ is a subgraph of $G$ and $v$ and $w$ are adjacent in $G$ implies $v$ and $w$ are adjacent in $H$ for $v, w \in V_H$.

**Example 9.13.** *Note that $H_1$ and $H_2$ are induced subgraphs of $G$. We can obtain $A_{H_1}$ and $A_{H_2}$ by erasing the rows and columns of $A_G$ corresponding to missing vertices.*




$A_G$

$$\begin{array}{c|c} & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{bmatrix} \end{array}$$

$A_{H_1}$

$$\begin{array}{c|c} & \begin{matrix} 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \end{array}$$

$A_{H_2}$

$$\begin{array}{c|c} & \begin{matrix} 1 & 2 & 3 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 5 \end{matrix} & \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

**Lemma 9.14.** *Let $H$ be an induced subgraph of a graph $G$. Then, $A_H$ is a principal submatrix of $A_G$*

**Theorem 9.15.** *Let $H$ be an induced subgraph of $G$. If $\lambda_1 \geq \cdots \geq \lambda_n$ are the eigenvalues of $A_G$ and $\mu_1 \geq \cdots \geq \mu_k$ are the eigenvalues of $A_H$ then we have*

$$\lambda_j \geq \mu_j \geq \lambda_{n-k+j}$$

*for $j = 1, 2, ..., k$.*

*Proof.* Since $A_H$ is a principal submatrix of $A_G$, the statement follows from Cauchy's interlace theorem. □

## 9.3 Graph energy

분자 molecule 구조를, 원자 atoms는 꼭짓점으로 결합 bonds은 선분으로 나타내어, 그래프로 표현할 수 있겠습니다. 화학 그래프 이론 chemical graph theory는 이러한 분자의 그래프 표현을 통해 분자의 화학적 특성을 그래프 이론을 이용하여 연구하는 분야입니다. 여기서는 그래프 인접행렬의 고윳값에 절댓값을 씌워 더한 값을 주어진 그래프의 에너지로 정의하는데, 유명한 (미해결) 문제 중 하나로, 꼭짓점의 갯수가 같은 그래프들 중 에너지가 가장 큰 그래프는 무엇인지를 결정하라는 문제가 있습니다.

**Definition 9.16.** *Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of the adjacency matrix of a graph $G$. Then, the energy of $G$ is*

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

이 값은 HMO 등 여러 이론적 가정을 기반으로 한 화학 모델에서 실제 에너지로서 의미를 갖고 있으나, 몇몇 가정들이 더 이상 널리 받아들여지지 않으면서 자연스럽게 그래프 에너지도 실제 화학적인 불변량이라기 보다는 그래프의 불변량으로 한정하여 이해되고 있습니다. 정리하면, 그래프 에너지는 실제 화학 분야 응용으로는 제약이 있으나 수학적 대상으로 여전히 활발히 연구되고 있습니다.

**Theorem 9.17** (the Coulson integral formula (1940))**.** *Let $G$ be a graph with $n$ vertices and $\phi(G,x)$ be the characteristic polynomial of the adjacency matrix of $G$.*

$$\phi(G,x) = \det(xI_n - A_G).$$

*Then, the energy of $G$ is*

$$E(G) = \frac{1}{\pi}\,\mathrm{pv}\int_{-\infty}^{+\infty}\left[n - x\frac{d}{dx}\ln\phi(G,ix)\right]dx$$

Here, the integration means the principal value of the integral, i.e.,

$$\mathrm{pv}\int_{-\infty}^{+\infty} = \lim_{a\to\infty}\int_{-a}^{a}$$

*Proof.* See Graph Energy by Xueliang Li, Yongtang Shi and Ivan Gutman, Chapter 3. □

**Theorem 9.18.** *Let $G$ be a simple graph. For any vertx $v$ of $G$,*

$$E(G-v) \leq E(G).$$

*Thus, if $H$ is an induced subgraph of $G$ then $E(H) \leq E(G)$.*

*Proof.* Use Theorem 9.15. ☐

The edge version of the above theorem is not known.

**Theorem 9.19** (McClelland's bounds (1971))**.** *Let $G$ be a simple graph with $n$ vertices and $m$ edges. Then,*

$$\sqrt{2m + n(n-1)|\det A_G|^{2/n}} \ \leq \ E(G) \ \leq \sqrt{2mn}.$$

*Proof.* To the vectors $x = (1, ..., 1)$ and $y = (|\lambda_1|, ..., |\lambda_n|)$, apply the Cauchy-Schwartz inquality to obtain

$$E(G) = |E(G)| = |x \cdot y| \leq \|x\| \, \|y\| = \sqrt{n}\sqrt{\sum_{i=1}^{n} \lambda_i^2} = \sqrt{n}\sqrt{2m},$$

which gives the upper bound. In the last step we used Proposition 9.12.

To obtain the lower bound, let us observe that

$$E(G)^2 = \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 = \sum_{i=1}^{n} |\lambda_i|^2 + 2\sum_{i<j} |\lambda_i \lambda_j|$$

The second term is, using the AM-GM inequality of $|\lambda_i \lambda_j|$,

$$2\sum_{i<j} |\lambda_i \lambda_j| = n(n-1)\, AM \geq n(n-1)\, GM$$

Then, the GM is

$$GM = \left(\prod_{i<j} |\lambda_i \lambda_j|\right)^{2/(n^2-n)} = \left(\prod_{i=1}^{n} |\lambda_i|^{n-1}\right)^{2/(n^2-n)} = \left(\prod_{i=1}^{n} |\lambda_i|\right)^{2/n}.$$

Therefore,

$$\begin{aligned} E(G)^2 &\geq \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 + n(n-1)\left(\prod_{i=1}^{n} |\lambda_i|\right)^{2/n} \\ &= 2m + n(n-1)|\det A_G|^{2/n}. \end{aligned}$$

where in the last line we applied Proposition 9.12. □

**Theorem 9.20** (Koolen and Moulton (2001, 2003))**.** *Let $G$ be a simple graph with $n$ vertices. Then*

$$E(G) \leq \frac{n}{2}(\sqrt{n}+1).$$

*Moreover, if $G$ is bipartite then*

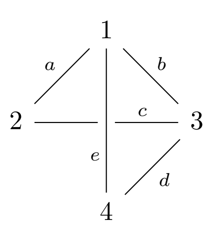
$$E(G) \leq \frac{n}{\sqrt{8}}(\sqrt{n}+\sqrt{2}).$$

## 9.4 Incidence matrix and line graph

**Definition 9.21.** *Let $G = (V, E)$ be a simple graph with $|V| = n$ and $|E| = m$. The* <u>*incidence matrix*</u> *$B_G$ of $G$ is an $m \times n$ matrix such that*

$$(B_G)_{ij} = \begin{cases} 1 & \text{if } e_i \text{ is incident with } v_j \\ 0 & \text{otherwise.} \end{cases}$$

**Example 9.22.** *Note that only two entries in each row are 1 and the others 0.*

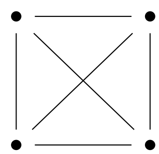
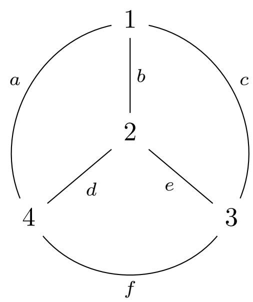



$$\begin{array}{cc} & V \\ & \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ E \; \begin{array}{c} a \\ b \\ c \\ d \\ e \end{array} & \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

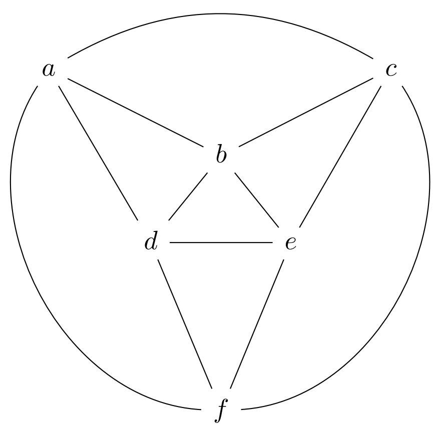
**Definition 9.23** (Line graph of $G$)**.** *Let $G$ be a simple graph. The <u>line graph</u> $L(G)$ of $G$ is a graph such that*

1. *there is a bijection between the vertex set of $L(G)$ and the edge set of $G$,*
2. *two vertices $v$ and $w$ in $L(G)$ are adjacent if and only if two edges in $G$ corresponding to $v$ and $w$ are incident with the same vertex.*

**Example 9.24.** *Let us label the edges of $K_4$.*

$K_4 =$  $\cong$ 


*Then, the line graph of $K_4$ is*

$L(K_4) =$ 


**Lemma 9.25.** *Let $G$ be a simple graph with $n$ vertices and $m$ edges. Then,*

$$B_G\,(B_G)^T = A_{L(G)} + 2I_m.$$

*Proof.* The identity easily follows from the following two observations.

1. Let $B = B_G$ be the incidence matrix of $G$. Then,

$$(BB^T)_{ij} = \begin{cases} 2 & \text{if } i = j \\ 1 & \text{if two different edges } e_i \text{ and } e_j \text{ in } G \text{ are incident with the same vertex} \\ 0 & \text{otherwise.} \end{cases}$$

2. On the other hand, we have

$$A_{L(G)} = \begin{cases} 1 & \text{if } e_i \text{ and } e_j \text{ in } G \text{ are incident with the same vertex} \\ 0 & \text{otherwise.} \end{cases}$$

□

**Theorem 9.26.** *Let $G$ be a simple graph with $n$ vertices and $m$ edges. Then, all the eigenvalues of $A_{L(G)}$ are greater than or equal to $-2$.*

*Proof.* Let $B = B_G$ and $\lambda$ be an eigenvalue of $A_{L(G)}$. Then,

$$A_{L(G)}v = \lambda v.$$

for some nonzero vector $v$. By replacing $A_{L(G)}$ by $BB^T - 2I_m$ (Theorem 9.25), we obtain

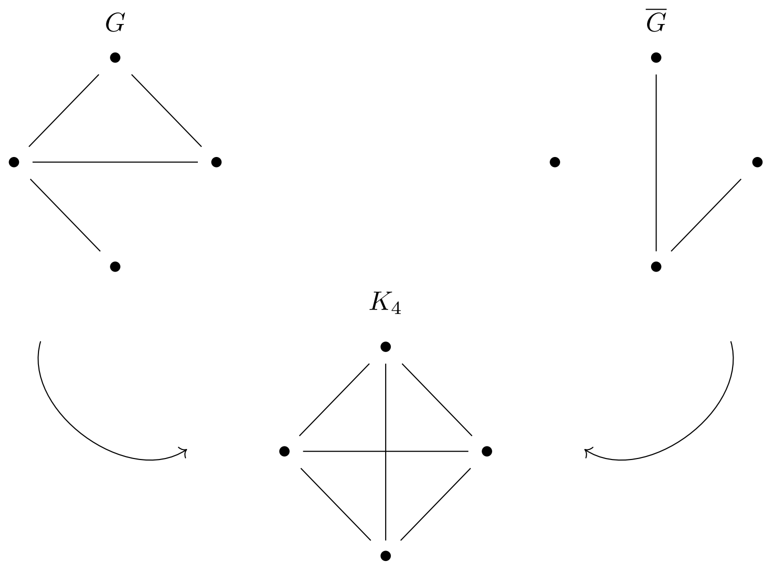
$$BB^T v = (\lambda + 2)v$$

and thus $(\lambda+2)$ is an eigenvalue of $BB^T$. Since all the eigenvalues of $BB^T$ are nonnegative (Theorem 8.10), we conclude that $\lambda \geq -2$. □

## 9.5 Complement Graphs

**Definition 9.27.** *The complement of a simple graph $G$ a graph $\overline{G}$ on the same vertex set $G$ such that two vertices in $\overline{G}$ are adjacent if and only if they are not adjacent in $G$.*

**Example 9.28.**




**Lemma 9.29.** *For a simple graph $G$,*

$$(A_G + A_{\overline{G}})_{ij} = \begin{cases} 1 & \text{if } i \neq j, \\ 0 & \text{if } i = j. \end{cases}$$

Let us write $J_n$ for the $n \times n$ matrix all whose entries are 1.

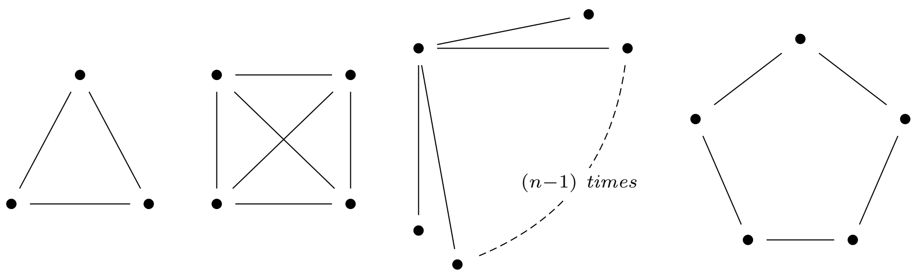
**Proposition 9.30.** *For a simple graph $G$ with $n$ vertices,*

$$A_G + A_{\overline{G}} + I_n = J_n.$$

Recall that a graph is $k$-regular, if the degree of every vertex is $k$.

**Lemma 9.31.** *Let $G$ be a simple graph with $n$ vertices which is not $K_n$. If $G$ is $k$-regular, then $\overline{G}$ is $(n-1-k)$-regular.*

**Example 9.32.**




| $K_3$ | $K_4$ | $K_n$ | $C_5$ |
| --- | --- | --- | --- |
| 2-*regular* | 3-*regular* | $(n-1)$-*regular* | 2-*regular* |

**Proposition 9.33.** *Let $G$ be a $k$-regular simple graph. Then, $k$ is an eigenvalue of $A_G$.*

*Proof.* Assume that $G$ has $n$ vertices. Let us write $\mathbf{1}_n$ for the vector in $\mathbb{R}^n$ all whose entries are 1. Then, from the observation that the sum of entries in $i$th row of $A_G$ is equal to the degree of the $i$th vertex, we have

$$A_G\mathbf{1}_n = k\mathbf{1}_n.$$

□

**Theorem 9.34.** *Let $G$ be a $k$-regular simple graph with $n$ vertices. Then, the following statements are true.*

1. *If $k, \theta_2, \theta_3, \ldots, \theta_n$ are the eigenvalues of $A_G$ then the following are the eigenvalues of $A_{\overline{G}}$.*

$$n-k-1, -1-\theta_2, -1-\theta_3, ..., -1-\theta_n.$$

2. *The eigenvectors of $A_G$ and $A_{\overline{G}}$ are the same.*

*Proof.* By Lemma 9.31 and Proposition 9.33, we know that $(n-k-1)$ is an eigenvalue of $A_{\overline{G}}$ with the eigenvector $\mathbf{1}_n$. For $2 \leq i \leq n$, let $v_i$ be an eigenvector of $A_G$ corresponding to $\theta_i$:

$$A_G v_i = \theta_i v_i.$$

By Corollary 9.30, we have $A_{\overline{G}} = J_n - I_n - A_G$ and thus

$$\begin{aligned} A_{\overline{G}} v_i &= (J_n - I_n - A_G) v_i \\ &= J_n v_i - v_i - A_G v_i \\ &= J_n v_i + (-1-\theta_i) v_i. \end{aligned}$$

Since $A_G$ is symmetric and thus orthogonally diagonalizable, we can further assume that the eigenvectors $\mathbf{1}_n, v_2, ..., v_n$ form an orthogonal basis of $\mathbb{R}^n$. In particular, $\mathbf{1}_n \cdot v_i = 0$ for all $i = 2, 3, ..., n$. This shows that $J_n v_i = \mathbf{0}$ for all $i$. Therefore.

$$A_{\overline{G}} v_i = (-1 - \theta_i) v_i.$$

□

**Example 9.35.** *Verify the above theorem for the following examples.*