1.10 Matrix Representation of Graphs

Definitions:

In this section, we introduce two kinds of matrix representations of a graph, that is, the adjacency matrix and incidence matrix of the graph.

A graph $G$ with the vertex-set $V(G) = \{x_1, x_2, \ldots, v_v\}$ can be described by means of matrices. The adjacency matrix of $G$ is a $v \times v$ matrix

$$A(G) = (a_{ij}) \text{, where } a_{ij} = \mu(x_i, x_j) = |E_G(x_i, x_j)|.$$  

For example, for the digraph $D$ and the undirected graph $G$ shown in Figure 1.26, their adjacency matrices $A(D)$ and $A(G)$ are as follows.

$$A(D) = \begin{pmatrix} 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \quad A(G) = \begin{pmatrix} 0 & 2 & 1 & 1 \\ 2 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}.$$  

The incidence matrix of a loopless graph $G$ is a $v \times \varepsilon$ matrix

$$M(G) = (m_x(e)), \quad x \in V(G) \text{ and } e \in E(G),$$

where, if $G$ is directed, then

$$m_x(e) = \begin{cases} 1, & \text{if } x \text{ is the tail of } e; \\ -1, & \text{if } x \text{ is the head of } e; \\ 0, & \text{otherwise}, \end{cases}$$

and if $G$ is undirected, then

$$m_x(e) = \begin{cases} 1, & \text{if } e \text{ is incident with } x; \\ 0, & \text{otherwise}. \end{cases}$$

For example, for the digraph $D$ and the undirected graph $G$ shown in Figure 1.26, the incidence matrix $M(D - a_7)$ and $M(G)$ are as follows.

$$M(D - a_7) = \begin{pmatrix} 1 & 1 & 0 & 0 & -1 & -1 \\ -1 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & -1 & 1 & 0 \end{pmatrix},$$

$$M(G) = \begin{pmatrix} 1 & 1 & 0 & 0 & -1 & -1 \\ -1 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & -1 & 1 & 0 \end{pmatrix}.$$
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\[
M(G) = \begin{pmatrix}
1 & 1 & 0 & 0 & 1 & 1 & 0 \\
1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 2
\end{pmatrix}.
\]

The adjacency matrix or the incidence matrix of a graph is another representation of the graph, and it is this form that a graph can be commonly stored in computers. The matrix representation of a graph is often convenient if one intends to use a computer to obtain some information or solve a problem concerning the graph. This kind of representation of a graph is conducive to study properties of the graph by means of algebraic methods.

Let
\[
\sigma = \begin{pmatrix}
1 & 2 & \cdots & n \\
i_1 & i_2 & \cdots & i_n
\end{pmatrix}
\]
be a permutation of the set \{1, 2, \ldots, n\}. Then we obtain an \( n \times n \) permutation matrix \( P = (p_{ij}) \) defined by
\[
p_{ij} = \begin{cases}
1, & \text{if } j = \sigma(i); \\
0, & \text{otherwise}.
\end{cases}
\]

It is not difficult to see that the adjacency matrices of two isomorphic graphs are permutedly similar. In other words, assume that \( A \) and \( B \) are the adjacency matrices of two isomorphic graphs \( G \) and \( H \), respectively, then there exists a \( v \times v \) permutation matrix \( P \) such that \( A = P^{-1}BP \).

Similarly, the incidence matrices of two isomorphic graphs are permutedly equivalent. In other words, assume that \( M \) and \( N \) are the incidence matrices of two isomorphic graphs \( G \) and \( H \), respectively, then there exist a \( v \times v \) permutation matrix \( P \) and an \( \varepsilon \times \varepsilon \) permutation matrix \( Q \) such that \( M = PNQ \).

**Relationship between Matrix and Graphical Representations:**

It is these properties that makes us convenient to study structures of graphs by using their matrix representations. We now present a very useful result on the adjacency matrix of a graph as follows.

**Theorem 1.11** Let \( A \) be the adjacency matrix of a digraph \( G \) with the vertex set \( \{x_1, x_2, \ldots, x_V\} \). Then the entry in position \((i, j)\) of \( A^k \) is the number of different \((x_i, x_j)\)-walks of length \( k \) in \( G \).

**Proof:** The proof is by induction on \( k \). The result is obvious for \( k = 1 \) since there exist \( a_{ij} \) \((x_i, x_j)\)-walks of length one if and only if there exist \( a_{ij} \) edges from
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Let \( A^{k-1} = \left( a^{(k-1)}_{ij} \right) \) and assume that \( a^{(k-1)}_{ij} \) is the number of different \((x_i, x_j)\)-walks of length \( k - 1 \) in \( G \); furthermore, let \( A^k = \left( a^{(k)}_{ij} \right) \). Since \( A^k = A^{k-1} \cdot A \), we have

\[
a^{(k)}_{ij} = \sum_{l=1}^{v} a^{(k-1)}_{il} \cdot a_{lj}.
\]

(1.11)

Every \((x_i, x_j)\)-walk of length \( k \) in \( G \) consists of an \((x_i, x_l)\)-walk of length \( k - 1 \), where \( x_l \) \((1 \leq l \leq v)\) is adjacent to \( x_j \), followed by an edge from \( x_l \) to \( x_j \). Thus by the induction hypothesis and the equation (1.20), we have the desired result.

It should be noted that walks could not be replaced by paths in Theorem 1.11 in general.

It is easy to see that there is the unique \((x, y)\)-walk of length \( n \) for any pair \((x, y)\) of vertices in \( B(d, n) \). We obtain from Theorem 1.11 immediately that if \( A \) is the adjacency matrix of \( B(d, n) \), then \( A^n = \mathbf{J} \), where \( \mathbf{J} \) is an \( n \)-square matrix all of whose entries are 1. Similarly, if \( A \) is the adjacency matrix of \( K(d, n) \), then \( A^n + A^{n-1} = \mathbf{J} \).

**Some Examples:**

We will, in Section 1.11 this book, introduce an important application of the adjacency matrix of a graph, specially Theorem 1.11, in matrix theory. We here give three examples, which are important results in graph theory, to show that adjacency and incidence matrices are very useful for studying graphs.

In Example 1.6.3, we show that if \( G \) is a strongly connected digraph of order \( v \) and the maximum degree \( \Delta \), then

\[
v \leq 1 + \Delta + \Delta^2 + \cdots + \Delta^{k-1} + \Delta^k = \begin{cases} k + 1, & \text{for } \Delta = 1; \\ \frac{\Delta^{k+1} - 1}{\Delta - 1}, & \text{for } \Delta > 1. \end{cases}
\]

Digraphs attaining this upper bound are called \((\Delta, k)\)-Moore digraphs.

The following example is due to Plesnik and Znom (1974), and rediscovered by Bridges and Toueg (1980).

**Example 1.10.1** There is no \((\Delta, k)\)-Moore digraph for \( \Delta \geq 2 \) and \( k \geq 2 \).

**Proof:** Assume that \( G \) is a \((\Delta, k)\)-Moore digraph whose order \( n \) reaches the Moore bound defined in (1.6), and let \( A \) be the adjacency matrix of \( G \). By the exercise 1.6.2, \( G \) is a \( \Delta \)-regular and simple digraph. Furthermore, by Theorem 1.11,
we have
\[ \mathbf{I} + \mathbf{A} + \mathbf{A}^2 + \cdots + \mathbf{A}^k = \mathbf{J}, \tag{1.12} \]
where \( \mathbf{I} \) is an identity square matrix. The expression (1.12) implies that \( \mathbf{J} \) is a polynomial in \( \mathbf{A} \), and so the matrices \( \mathbf{A} \) and \( \mathbf{J} \) have a common set of eigenvectors.

It is not difficult to show that \( \Delta \) is an eigenvalue of \( \mathbf{A} \) (see the exercise 1.10.6). Let \( r \) be any eigenvalue other than \( \Delta \), and let \( \mathbf{X} \) be an eigenvector corresponding to \( r \). Noting that the zero, as an eigenvalue of \( \mathbf{J} \), has the multiplicity \( n - 1 \), we have
\[ \mathbf{AX} = r\mathbf{X}, \quad \mathbf{JX} = 0. \]

By (1.12), we obtain the relation
\[ 1 + r + r^2 + \cdots + r^k = 0. \tag{1.13} \]
The expression (1.13) shows that \( r \) has the multiplicity \( (k + 1) \) as the unite root, i.e., \( r^{k+1} = 1 \). Let \( r_1, r_2, \cdots, r_{n-1} \) be \( n - 1 \) eigenvalues of \( \mathbf{A} \) other than \( \Delta \). By Theorem 1.11, all the main diagonal entries of \( \mathbf{A}^i (1 \leq i \leq k) \) are 0, that is,
\[ \text{Tr}\, \mathbf{A}^i = 0, \quad i = 1, 2, \cdots, k. \]
Thus the sum of the eigenvalues of \( \mathbf{A}^i \)
\[ \Delta^i + \sum_{j=1}^{n-1} r_j^i = 0, \quad i = 1, 2, \cdots, k. \tag{1.14} \]
Since \( r_j r_j = |r_j|^2 = 1 = r_j^{k+1} \), it follows that \( r_j^{-1} = \overline{r_j} = r_j^k \), where \( \overline{r_j} \) is the conjugate complex number of \( r_j \). Setting \( i = 1 \) and \( i = k \) in (1.23), respectively, we have
\[ -\Delta = \sum_{j=1}^{n-1} r_j, \quad -\Delta^k = \sum_{j=1}^{n-1} r_j^k. \]
Taking the conjugates of the above expressions and noting (1.14), we have that
\[ -\Delta = \sum_{j=1}^{n-1} r_j^{-1} = \sum_{j=1}^{n-1} r_j^k = -\Delta^k, \]
which holds if and only if either \( k = 1 \) or \( \Delta = 1 \). This contradicts to our assumption and, thus, the conclusion follows.

By Example 1.10.1, a digraph with the maximum degree \( \Delta \) and diameter 2 has order at most \( \Delta^2 + \Delta \). We have known that the Kautz digraph \( K(\Delta, 2) \) had order \( \Delta^2 + \Delta \). Therefore, \( K(\Delta, 2) \) is a maximum \( (\Delta, 2) \)-digraph, which is the unique known maximum \( (\Delta, 2) \)-digraph up to now.
Similarly, if \( G \) is a connected graph of order \( v \) and the maximum degree \( \Delta \), then
\[
v \leq 1 + \Delta + \Delta(\Delta - 1) + \cdots + \Delta(\Delta - 1)^2 + \Delta(\Delta - 1)^{k-1}
\]
\[
= \begin{cases} 
2k + 1, & \text{for } \Delta = 2; \\
\frac{\Delta(\Delta - 1)^k - 2}{\Delta - 2}, & \text{for } \Delta > 2.
\end{cases}
\]
Graphs attaining this upper bound are called \((\Delta, k)\)-Moore graphs.

**Example 1.10.2 (Hoffman and Singleton, 1960)** There is no undirected \((\Delta, 2)\)-Moore graph for \( \Delta \neq 2, 3, 7, 57 \).

**Proof** Assume that \( G \) is an undirected \((\Delta, 2)\)-Moore graph of order \( n \). Then \( G \) is \( \Delta \)-regular. The adjacency matrix \( A = A(G) \) is a real symmetric \( n \)-square matrix with all main diagonal entries 0. Since \( G \) is \( \Delta \)-regular, \( \Delta \) is an eigenvalue of \( A \). Let \( I \) be the identity \( n \)-square matrix, and \( J \) be an \( n \)-square matrix all of whose entries are 1. Then \( n \) is an eigenvalue of \( J \), otherwise are 0. Note \( d(G) = 2 \). By Theorem 1.11, all main diagonal entries of \( A^2 \) are \( \Delta \), otherwise are 0 or 1, and the \((i, j)\)-th entry of \( A^2 \) is 0 if and only if the corresponding two vertices are adjacent in \( G \), that is the \((i, j)\)-th entry of \( A \) is 1. It follows that
\[
A^2 + A - (\Delta - 1)I = J. \tag{1.15}
\]
This implies that \( J \) is a polynomial in \( A \). So \( A \) and \( J \) have a common set of eigenvectors. Suppose that one of these is \( X \) corresponding to the eigenvalue \( \Delta \). Then
\[
AX = \Delta X, \quad JX = nX.
\]
For this eigenvector, the expression (1.15) supplies the relation \( \Delta^2 + 1 = n \).

Let \( Y \) be any other eigenvector of \( A \) corresponding to an eigenvalue \( r \). Then
\[
AY = rY, \quad JY = 0.
\]
Using (1.15), we obtain the relation
\[
r^2 + r - (\Delta - 1) = 0.
\]
Hence \( A \) has two other distinct eigenvalues:
\[
r_1 = \frac{1}{2}(-1 + \sqrt{4\Delta - 3}), \quad r_2 = \frac{1}{2}(-1 - \sqrt{4\Delta - 3}).
\]
Since \( A \) is a real symmetric matrix, it has only real eigenvalues. Thus both \( r_1 \) and \( r_2 \) are real numbers.
If $\Delta$ is such that $r_1$ and $r_2$ are not rational, then each has multiplicity \( \frac{1}{2}(n - 1) \) as an eigenvalue of $A$ since $A$ is rational. Since all main diagonal entries of $A$ are 0, by a result on the trace of a matrix, the sum of the eigenvalues of $A$ is 0. Namely

\[
\Delta + \frac{1}{2}(n - 1)(r_1 + r_2) = \Delta - \frac{1}{2}\Delta^2 = 0. \tag{1.16}
\]

The value of $\Delta$ satisfying (1.16) is only $\Delta = 2$, for which $n = 5$ and the corresponding undirected $(2,2)$-Moore graph is an undirected cycle $C_5$.

The values of $\Delta$ for which $r_1$ and $r_2$ are rational are those for which there is an integer $s$ such that $s^2 = 4\Delta - 3$. Thus

\[
r_1 = \frac{1}{2}(s - 1), \quad r_2 = -\frac{1}{2}(s + 1).
\]

Let $t$ be the multiplicity of $r_1$. Then the sum of the eigenvalues of $A$ is

\[
\Delta + ts - \frac{1}{2} + (n - 1 - t)s - \frac{1}{2} = 0.
\]

Using the relations $n = 1 + \Delta^2$ and $s^2 = 4\Delta - 3$, we have that

\[
s^5 + s^4 + 6s^3 - 2s^2 + (9 - 32t)s = 15. \tag{1.17}
\]

Since the equation (1.17) requires solutions in integers, the only candidates for $s$ are the factors of 15. These possible solutions are:

- $s = \pm 1, \quad t = 0, \quad \Delta = 1, \quad n = 2;
- s = \pm 3, \quad t = 5, \quad \Delta = 3, \quad n = 10;
- s = \pm 5, \quad t = 28, \quad \Delta = 7, \quad n = 50;
- s = \pm 15, \quad t = 1729, \quad \Delta = 57, \quad n = 3250.$

There is no undirected graph of degree 1 and diameter 2. The theorem follows. \(\blacksquare\)

The undirected $(7,2)$-Moore bound is $m(7,2) = 50$, the corresponding undirected $(7,2)$-Moore graph is determined by Hoffman-Singleton. The uniqueness of the undirected $(3,2)$- and $(7,2)$-Moore graphs have been shown by Hoffman and Singleton.

The undirected $(57,2)$-Moore has order 3250, the corresponding undirected $(57,2)$-Moore graph might exist, but no one has been able to construct (or prove the nonexistence of) such a graph so far.

**Example 1.10.3** Let $M$ be the incidence matrix of a digraph $G$ without loops, and let $M_i$ be the matrix obtained from $M$ by deleting the $i$th row. Then the algebraic cofactor of any entry in $MM^T$ is equal to the determinant $\det(M_iM_i^T)$, where $M^T$ denotes the transpose of $M$. 

Proof: Suppose that the vertex-set of $G$ is $\{x_1, x_2, \cdots, x_v\}$, and let $N = MM^T$.

Suppose that the entry in position $(i,j)$ of $N$ is $n_{ij}$. Then $N$ is symmetric and

$$n_{ij} = \begin{cases} d_G(x_i) = d_G^+(x_i) + d_G^-(x_i), & \text{for } j = i; \\ -\mu(x_i, x_j) - \mu(x_j, x_i), & \text{for } j \neq i. \end{cases}$$

Thus the sum of any row and the sum of any column of $N$ all are 0. It is a routine algebraic exercise to show that the algebraic cofactors of all entries in $MM^T$ have the same value (the exercise 1.10.5). Let $N_{ij}$ be the algebraic cofactors of $n_{ij}$ in $MM^T$, and, without loss of generality, suppose

$$N_{ij} = N_{11}, \quad \forall \ 1 \leq i, j \leq v.$$ 

Let $\alpha_1$ be the first row vector of $M$. Then

$$N = MM^T = \begin{pmatrix} \alpha_1 \\ M_1 \end{pmatrix} \cdot \begin{pmatrix} \alpha_1^T \\ M_1^T \end{pmatrix} = \begin{pmatrix} \alpha_1 \alpha_1^T \\ M_1 \alpha_1 \\ M_1 M_1^T \end{pmatrix}.$$ 

Thus, we have

$$N_{ij} = N_{11} = \det (M_1 M_1^T), \quad \forall \ 1 \leq i, j \leq v$$

as desired.

We conclude this section with some remarks. Let $A$ be the adjacency matrix of an undirected graph $G$ with the vertex-set $\{x_1, x_2, \cdots, x_v\}$, $M$ the incidence matrix of any oriented graph $D$ of $G$, and let $B$ be the $v \times v$ diagonal matrix with the main diagonal entries $b_{ii} = d_G(x_i)$. It is easily shown that (the exercise 1.10.5) $MM^T = B - A$, which is called **Laplace matrix** in the literature and textbook on graph theory.

We have known from Example 1.10.3 that all the algebraic cofactors of entries in $MM^T$ have the same value, the determinant $\det (M_1 M_1^T)$. This value is a very important invariant of isomorphic graphs. We will, in Section 2.3, know what this invariant is.

Exercises: 1.10.4, 1.10.5, 1.10.6
Exercises

1.10.6 Let \( A \) be the adjacency matrix of a graph \( G \) (undirected or directed). The eigenvalues of \( A \) is referred to as the eigenvalues of \( G \); the characteristic polynomial \( \det(\lambda I - A) \) is referred to as the characteristic polynomial of \( G \). Suppose that characteristic polynomial of \( G \) is

\[
P_G(\lambda) = \det(\lambda I - A) = \lambda^v + c_1\lambda^{v-1} + \cdots + c_{v-1}\lambda + c_v.\]

(a) Count the characteristic polynomials of the following two graphs.

(b) Prove

\[
c_k = \sum_{H \in \mathcal{M}_k} (-1)^{\omega(H)}, \quad k = 1, 2, \ldots, v,
\]

where \( \mathcal{M}_k \) is the set of (1-) 2-regular subgraphs with order \( k \) of (di)graphs of \( G \). (M.Milic (1964), H. Sachs (1964), L.Spialter (1964))

(c) Prove that \( c_1 = 0; \ -c_2 = \varepsilon; \) and \(-c_3\) is equal to twice the number of triangles in \( G \).

(d) Prove that if \( \lambda_1, \lambda_2, \ldots, \lambda_v \) are all eigenvalues of \( G \), then

(i) \( \lambda_1 + \lambda_2 + \cdots + \lambda_v = -c_1; \)

(ii) the number of different directed closed walks of length \( k \) in \( G \)

is \( (\lambda_1^k + \lambda_2^k + \cdots + \lambda_v^k). \)

(e) Let \( \lambda \) be the maximum eigenvalue of \( G \). Prove that

(i) \( \delta^+ \leq \lambda \leq \Delta^+ \), and \( \delta^- \leq \lambda \leq \Delta^- \) (or \( \delta \leq \lambda \leq \Delta \)),

and the equalities hold if and only if \( G \) is regular;

(ii) if \( G \) is strongly connected and regular, then \( \lambda \) has the

multiplicity 1.

(f) Prove that a strongly connected digraph of diameter \( d \) has at least \( d + 1 \)

distinct eigenvalues.