

Möbius Inversion of Random Acyclic Directed Graphs

By Joel E. Cohen

Suppose a random acyclic digraph has adjacency matrix A with independent columns or independent rows. Then the mean Möbius inverse of the zeta matrix $I+A$ is the Möbius inverse of the mean zeta matrix, i.e., $E[(I+A)^{-1}] = [I + E(A)]^{-1}$.

The purpose of this note is to show that, under natural conditions, the mean Möbius inverse of a random acyclic directed graph (digraph) equals the Möbius inverse of the mean acyclic digraph.

Let the vertex set V be $\{1, \dots, n\}$ for a fixed integer n , $1 < n < \infty$, and let R be a subset of $V \times V$. An element $(i, j) \in R$ is called an arc from i to j . A digraph D is an ordered pair $D = (V, R)$ of vertices and arcs. A topologically ordered acyclic digraph (TOAD) is a digraph $D = (V, R)$ such that every arc (i, j) in R satisfies $i < j$. It is well known that every acyclic digraph can be converted to a TOAD by permuting the labels of the vertices, and conversely every acyclic digraph can be obtained by permuting the labels of the vertices of a TOAD. The adjacency matrix $A = A(D) = A(V, R)$ of any digraph $D = (V, R)$ is an $n \times n$ matrix such that $a_{ij} = 1$ if $(i, j) \in R$, $a_{ij} = 0$ if $(i, j) \notin R$. It is also well known that (V, R) is a TOAD if and only if $A(V, R)$ is strictly upper triangular, i.e., $a_{ij} = 0$ whenever $i \geq j$. (See [4] for background on digraphs.)

The zeta function of any acyclic digraph D with adjacency matrix A is defined by $\zeta = I + A$, where I is the $n \times n$ identity matrix. ζ is the adjacency matrix of the digraph formed from D by adjoining loops to each vertex, i.e., by adjoining all the arcs (i, i) where $i \in V$. The Möbius inverse $\mu = \zeta^{-1}$ exists, because if P is a permutation matrix such that PAP^{-1} is strictly upper

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triangular, then $\det(I + A) = \det[P(I + A)P^{-1}] = \det(I + PAP^{-1}) = 1$. (Recall that for a permutation matrix P , $P^{-1} = P^T$, so PAP^{-1} is the matrix obtained by relabeling the indices of the rows and columns of A according to P .) (See [5; 2, Chapter 2; 3, Chapter 25] for background on Möbius inverses.)

Let S be the set of all strictly upper triangular $0-1$ $n \times n$ matrices, and let U be the set of all matrices PAP^T , where P is a permutation matrix and $A \in S$. The matrices in S are exactly the adjacency matrices of the set of all TOADs, and the matrices in U are exactly the adjacency matrices of the set of all acyclic digraphs.

A random acyclic digraph is specified by a probability distribution on U . Specifically, if \mathbf{A} denotes the random adjacency matrix of a random acyclic digraph \mathbf{D} , then for every $A \in U$, $p(A) = P\{\mathbf{A} = A\}$. The mean adjacency matrix of \mathbf{D} is $E(\mathbf{A}) = \sum_{A \in U} Ap(A)$. The mean Möbius inverse of \mathbf{D} is $E(\boldsymbol{\mu}) = \sum_{A \in U} (I + A)^{-1} p(A)$. Under natural conditions, stated in Theorem 2, $E(\boldsymbol{\mu}) = [I + E(\mathbf{A})]^{-1}$. This follows from a slightly more general result, stated as Theorem 1.

Let \mathbf{M} be a random $n \times n$ matrix (implicitly, a space of $n \times n$ matrices together with a probability measure on that space). Say that $\mathbf{M} = (m_{ij})$ has independent columns if and only if, for all j, k such that $1 \leq j < k \leq n$, the vector consisting of column j of \mathbf{M} and the vector consisting of column k of \mathbf{M} are independent. (Arbitrary dependence within any column is allowed.) Say that a random matrix has independent rows if its transpose has independent columns. If the rows or columns of \mathbf{M} are independent, so are those of PMP^T , for any permutation matrix P .

As usual, "a.s." means "almost surely."

For any deterministic matrix $M = (M_{ij})$, the skeleton of M is another deterministic matrix $H = (h_{ij})$ such that $h_{ij} = 1$ if $m_{ij} \neq 0$, $h_{ij} = 0$ if $m_{ij} = 0$. For any random matrix \mathbf{M} , define the *movie* of \mathbf{M} to be the random matrix \mathbf{H} formed by taking the skeleton of each realization of \mathbf{M} . For any random matrix \mathbf{M} , define the *still* of \mathbf{M} to be the deterministic matrix H defined by $h_{ij} = 0$ if $m_{ij} = 0$ a.s., $h_{ij} = 1$ if $P\{m_{ij} \neq 0\} > 0$. For example, if

$$M_1 = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 0 & 0 \\ 3 & 0 \end{pmatrix},$$

and $P\{\mathbf{M} = M_1\} = \frac{1}{4}$, $P\{\mathbf{M} = M_2\} = \frac{3}{4}$, then the movie

$$\mathbf{H} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{whenever } \mathbf{M} = M_1, \quad \mathbf{H} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \text{whenever } \mathbf{M} = M_2,$$

and the still

$$H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Though \mathbf{H} is acyclic a.s., the skeleton of $E(\mathbf{H})$, namely H , is not acyclic.

Define a deterministic matrix M to be nilpotent if there exists a positive integer k such that $M^k = 0$. It is well known that M is nilpotent if and only if the skeleton of M is in U , i.e., if and only if PMP^T is strictly upper triangular for some permutation matrix P . The previous example shows that it is possible to have \mathbf{M} be nilpotent a.s. while the still of \mathbf{M} is not nilpotent. However, if \mathbf{M} has independent rows or columns, such a possibility is excluded.

LEMMA. *Let \mathbf{M} be a complex-valued random matrix with independent rows or independent columns and such that \mathbf{M} is nilpotent a.s. Then the still of \mathbf{M} is nilpotent.*

Proof: Let $H = (h_{ij})$ be the still of \mathbf{M} . Then $P\{\mathbf{M} \text{ is nilpotent}\} = 1$ implies that for every k , $1 \leq k \leq n$, and for every set $\{i_1, \dots, i_k\}$ of k distinct elements of $V = \{1, \dots, n\}$,

$$P\{\mathbf{m}_{i_1 i_2} \mathbf{m}_{i_2 i_3} \cdots \mathbf{m}_{i_k i_1} \neq 0\} = 0.$$

Since the rows or columns of \mathbf{M} are independent,

$$0 = P\{\mathbf{m}_{i_1 i_2} \cdots \mathbf{m}_{i_k i_1} \neq 0\} = P\{\mathbf{m}_{i_1 i_2} \neq 0\} \cdots P\{\mathbf{m}_{i_k i_1} \neq 0\},$$

which implies that at least one factor on the right is 0. Therefore, at least one of $h_{i_1 i_2}, h_{i_2 i_3}, \dots, h_{i_k i_1}$ is 0. Since this is true for every set $\{i_1, \dots, i_k\}$ of k distinct elements of V , H is nilpotent. \square

Define the off-diagonal part of a random matrix \mathbf{A} to be the random matrix \mathbf{B} such that $\mathbf{b}_{ij} = \mathbf{a}_{ij}$ a.s. for all (i, j) with $i \neq j$, and $\mathbf{b}_{ii} = 0$ a.s. for all $i \in V$.

THEOREM 1. *Let \mathbf{M} be a complex-valued random matrix such that*

- (i) *the expectation $E(\mathbf{M})$ exists;*
- (ii) *the off-diagonal part of \mathbf{M} is a.s. nilpotent, i.e., the movie of the off-diagonal part of \mathbf{M} is a.s. nilpotent;*
- (iii) *$\mathbf{m}_{ii} = c_i$ a.s., where $c_i \neq 0$ is a nonzero constant;*
- (iv) *\mathbf{M} has independent columns or \mathbf{M} has independent rows.*

Then $E(\mathbf{M}^{-1})$ exists and $E(\mathbf{M}^{-1}) = [E(\mathbf{M})]^{-1}$.

Proof: By the Lemma, the still of the off-diagonal part of \mathbf{M} is nilpotent, and therefore so is the expectation of the off-diagonal part of \mathbf{M} . Hence $E(\mathbf{M})$ is nonsingular.

Let $K = (k_{ij})$ have elements $\delta_{ij} c_i$, where δ_{ij} is Kronecker's delta, $\delta_{ii} = 1$, $\delta_{ij} = 0$ if $i \neq j$. Then $\mathbf{H} = K^{-1} \mathbf{M}$ has all diagonal elements equal to 1 a.s. Let $I - \mathbf{H} = \mathbf{L}$. Then \mathbf{L} has a.s. the same movie as the off-diagonal part of \mathbf{M} and is a.s. nilpotent, so a.s. $\mathbf{L}^n = 0$. Therefore, $(I - \mathbf{L})^{-1} = I + \mathbf{L} + \mathbf{L}^2 + \cdots + \mathbf{L}^{n-1}$ a.s.

Hence a.s.

$$\begin{aligned} \mathbf{M}^{-1} &= (\mathbf{KH})^{-1} = \mathbf{H}^{-1}\mathbf{K}^{-1} = (\mathbf{I} - \mathbf{L})^{-1}\mathbf{K}^{-1} \\ &= (\mathbf{I} + \mathbf{L} + \mathbf{L}^2 + \cdots + \mathbf{L}^{n-1})\mathbf{K}^{-1}, \end{aligned}$$

so if $E(\mathbf{M}^{-1})$ exists, it must be

$$E(\mathbf{M}^{-1}) = [\mathbf{I} + E(\mathbf{L}) + E(\mathbf{L}^2) + \cdots + E(\mathbf{L}^{n-1})]\mathbf{K}^{-1}.$$

Now for $k = 2, \dots, n-1$,

$$(\mathbf{L}^k)_{ij} = \sum_{i_1=1}^n \sum_{i_2=1}^n \cdots \sum_{i_{k-1}=1}^n \mathbf{L}_{i,i_1} \mathbf{L}_{i_1,i_2} \cdots \mathbf{L}_{i_{k-1},j}.$$

Because \mathbf{L} is a.s. nilpotent, the only terms on the right that are not a.s. 0 are those in which $i, i_1, i_2, \dots, i_{k-1}, j$ are all distinct. Then, since \mathbf{L} has independent columns or rows (inherited from \mathbf{M} and \mathbf{H}),

$$\begin{aligned} E[(\mathbf{L}^k)_{ij}] &= \sum_{\{i, i_1, \dots, i_{k-1}, j\} \text{ all distinct}} E(\mathbf{L}_{i,i_1} \mathbf{L}_{i_1,i_2} \cdots \mathbf{L}_{i_{k-1},j}) \\ &= \sum_{\{i, i_1, \dots, i_{k-1}, j\} \text{ all distinct}} E(\mathbf{L}_{i,i_1}) E(\mathbf{L}_{i_1,i_2}) \cdots E(\mathbf{L}_{i_{k-1},j}); \end{aligned}$$

hence $E(\mathbf{L}^k) = [E(\mathbf{L})]^k$ if $E(\mathbf{L})$ exists, and $E(\mathbf{L}) = \mathbf{I} - \mathbf{K}^{-1}E(\mathbf{M})$ does exist by (i). Thus $E(\mathbf{M}^{-1})$ exists and equals

$$\begin{aligned} E(\mathbf{M}^{-1}) &= \{\mathbf{I} + E(\mathbf{L}) + [E(\mathbf{L})]^2 + \cdots + [E(\mathbf{L})]^{n-1}\}\mathbf{K}^{-1} \\ &= [\mathbf{I} - E(\mathbf{L})]^{-1}\mathbf{K}^{-1} = [\mathbf{K}(\mathbf{I} - E(\mathbf{L}))]^{-1} \\ &= [E(\mathbf{M})]^{-1}. \quad \square \end{aligned}$$

By contrast with Theorem 1, if \mathbf{X} is a nondegenerate random variable such that $\mathbf{X} > 0$ a.s. and $E(\mathbf{X})$ and $E(\mathbf{X}^{-1})$ exists, then $[E(\mathbf{X})]^{-1} < E(\mathbf{X}^{-1})$. [Since $f(x) = x^{-1}$ is strictly convex on $(0, \infty)$, the inequality follows by Jensen's inequality.] The matrix equality obtained in Theorem 1 differs from the scalar inequality because, of course, the 1×1 case of the matrix \mathbf{M} is a.s. a constant, not a nondegenerate scalar random variable; for a constant scalar or degenerate random variable \mathbf{X} , $[E(\mathbf{X})]^{-1} = E(\mathbf{X}^{-1}) = \mathbf{X}^{-1}$ a.s.

THEOREM 2. *Suppose a random acyclic digraph has adjacency matrix \mathbf{A} with independent columns or independent rows. Then $E(\mathbf{A})$ exists and the mean Möbius inverse is $E[(\mathbf{I} + \mathbf{A})^{-1}] = [\mathbf{I} + E(\mathbf{A})]^{-1}$.*

Proof: $E(\mathbf{A})$ exists because the elements of \mathbf{A} are drawn from $\{0,1\}$, so $\zeta = I + \mathbf{A}$ satisfies hypothesis (i) of Theorem 1. The off-diagonal part of the zeta matrix $\zeta = I + \mathbf{A}$ is just the adjacency matrix \mathbf{A} , so $\zeta = I + \mathbf{A}$ satisfies (ii), (iii) because $\zeta_{ii} = 1$ a.s., and (iv) by assumption. The conclusion of Theorem 2 then follows from Theorem 1. \square

Example of Theorem 2 (The cascade model [1]): Suppose $\mathbf{a}_{ij} = 0$ a.s. if $i \geq j$, while $\mathbf{a}_{ij} = 1$ with probability p and $\mathbf{a}_{ij} = 0$ with probability $q = 1 - p$, independently for all (i, j) with $i < j$, where $0 < p < 1$. Then $E(\mathbf{a}_{ij}) = pJ_{(i < j)}$, where $J_{(i < j)} = 1$ if $i < j$, $J_{(i < j)} = 0$ if $i \geq j$. Let $M = (m_{ij}) = E(\mu) = E[(I + \mathbf{A})^{-1}] = [I + E(\mathbf{A})]^{-1}$. Then it is easy to check that

$$m_{ij} = \begin{cases} 0 & \text{if } i > j, \\ 1 & \text{if } i = j, \\ -p(1-p)^{j-i-1} & \text{if } i < j. \end{cases}$$

For example, if $n = 4$, then

$$E(\mathbf{A}) = \begin{pmatrix} 0 & p & p & p \\ 0 & 0 & p & p \\ 0 & 0 & 0 & p \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$E(\mu) = [I + E(\mathbf{A})]^{-1} = \begin{pmatrix} 1 & -p & -p(1-p) & -p(1-p)^2 \\ 0 & 1 & -p & -p(1-p) \\ 0 & 0 & 1 & -p \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In the ecological interpretation of the cascade model [1] the elements of V represent groups of organisms called trophic species, $\mathbf{a}_{ij} = 1$ means species j eats species i , and $\mathbf{a}_{ij} = 0$ means species j does not eat species i . The TOAD specified by \mathbf{A} is called a food web. Let $x^T = (x_1, \dots, x_n)$ and $y^T = (y_1, \dots, y_n)$ be row vectors such that $y^T = x^T(I + \mathbf{A})$, i.e., y_j is the sum of x_j plus all the x_i such that j eats i according to \mathbf{A} . Then $y^T(I + \mathbf{A})^{-1} = x^T$. Now suppose y^T is fixed, e.g., y^T can be measured directly with negligible error. Then $E(x^T) = y^T E[(I + \mathbf{A})^{-1}] = y^T M$ provides a way of estimating the mean of x^T from measurements of y^T and the average structure of the food web; the latter may be derived from the cascade model in the absence of more detailed data.

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