COMPLEMENTS AND TRANSITIVE CLOSURES *

R.L. GRAHAM

Bell Telephone Laboratories, Inc., Murray Hill, N.J. 07974, USA

D.E. KNUTH

Stanford University, Stanford, Calif. 94305, USA

T.S. MOTZKIN

University of California at Los Angeles, Los Angeles, Calif. 90024, USA

Abstract. The complement of the transitive closure of the complement of a transitive relation is transitive. We prove this fact in three ways, analyze the underlying structure and consider various refinements and applications.

§ 1. Preliminary remarks

The purpose of this note is to explore the interaction between two fundamental operations on binary relations. If R is a relation on a set A, the *complement* R^- is defined to be $(A \times A) - R$, and the transitive hull or *transitive closure* R^+ is defined to be the smallest transitive relation containing R. When $(a, b) \in R$ we write aRb. The *composition* $R \circ S$ of two relations R and S is defined to be $\{(a, c) \mid aRb$ and bSc for some $b\}$. It is well known that $R^+ = R \cup R \circ R \cup R \circ R \circ R \cup \ldots = \{(a, b) \mid$ there exist $a_0, a_1, \ldots, a_n$ for some $n \geq 1$ such that $a = a_0, a_{i-1} R a_i$ for $1 \leq i \leq n$, and $a_n = b\}$.

If $R \subseteq S$ it is obvious that $R^- \supseteq S^-$ and $R^+ \subseteq S^+$. In particular we always have

$$(1) \qquad R^{-+-} \subseteq R ,$$

since $R^- \subseteq R^{-+}$. Another immediate consequence of the definitions is

(2) $R^+ - R \subseteq R \circ R^+ = R^+ \circ R$.

By putting these facts together we can derive a less obvious property:

Lemma 1. $R^+ \circ R^{+-+-} \subseteq R^{+-+-}$.

Proof. The stated relation is false if and only if there exist a, b, c such that aR^+b, $bR^{+-+-}c$, and $aR^{+-+}c$. By (1), bR^+c; hence aR^+c, i.e. $(a, c) \in R^{+-+} - R^{+-}$. By (2), there exists an element d such that $aR^{+-}d$ and $dR^{+-+}c$. But now if bR^+d, we have aR^+d, contradicting $aR^{+-}d$; and if $bR^{+-}d$, we have $bR^{+-+}c$, contradicting $bR^{+-+-}c$.

Theorem 1. *If R is any binary relation, $R^{+-+-+} = R^{+-+-}$. Therefore at most 10 relations can be generated from R by taking complements and transitive closures, namely*

(3)
$$R\ ,R^+\ ,R^{+-}\ ,R^{+-+}\ ,R^{+-+-}\ ,$$
$$R^-, R^{-+}, R^{-+-}, R^{-+-+}, R^{-+-+-} .$$

Proof. By the lemma and (1), $R^{+-+-} \circ R^{+-+-} \subseteq R^+ \circ R^{+-+-} \subseteq R^{+-+-}$, i.e., R^{+-+-} is transitive. The 10 relations in (3) are now the only possibilities, since $R^{--} = R$ and $R^{++} = R^+$.

   Theorem 1 is analogous to the well-known "Kuratowski closure and complement problem" [4, 6]; Kuratowski proved in his Ph. D. dissertation that a subset of a topological space generates at most 14 sets under the operations of complementation and (topological) closure.

   The following relation on five elements generates all 10 of the distinct possibilities in Theorem 1, hence the result is "best possible":

(4a)

00011	00111	11000	11000	00111
01011	01111	10000	11000	00111
R = 00011,	R^+ = 00111,	R^{+-} = 11000,	R^{+-+} = 11000,	R^{+-+-} = 00111,
00001	00111	11000	11000	00111
00110	00111	11000	11000	00111

(4b)

$$
\begin{array}{ccccc}
11100 & 11100 & 00011 & 00011 & 11100 \\
10100 & 11100 & 00011 & 00011 & 11100 \\
R^- = 11100, \; R^{-+} = 11100, \; R^{-+-} = 00011, \; R^{-+-+} = 00011, \; R^{-+-+-} = 11100, \\
11110 & 11110 & 00001 & 00011 & 11100 \\
11001 & 11101 & 00010 & 00011 & 11100
\end{array}
$$

We shall see below that this is the "simplest" relation R which generates all 10 possibilities. The first example of such a relation on five elements was found by Garey [2]. Note that the operation of transposition (often called the converse or *inverse* relation) commutes with complementation and transitive closure; hence at most 20 relations can be generated from a given one under the operations of complementation, closure and inverse. The example in (4), together with the transposes of each matrix, shows that 20 is best possible.

§ 2. The underlying structure

Let us now look at the 10 relations in (3) more closely, so that we can understand what they represent.

If R is not connected, so that $R \subseteq B \times B \cup (A-B) \times (A-B)$ with B and $A-B$ nonempty, the situation is degenerate. For in this case $R^- \supseteq B \times (A-B) \cup (A-B) \times B$, and $R^{-+} = A \times A$; R^{-+-} is empty. Similarly $R^{+-+} = A \times A$, so (3) contains at most 6 different relations. (In fact there are exactly 6 if and only if R is not transitive, when R is not connected.) Therefore the only interesting cases arise when R and R^- are connected.

In general, we can define two important equivalence relations based on a given relation R. Let us write

$$a \leftrightarrow b(R)$$

if $a = b$, or aR^+b and bR^+a. This relation is obviously reflexive, symmetric and transitive, so it partitions A into equivalence classes; in fact, regarding R as a directed graph with an arc from a to b if and only if aRb, these classes are precisely the *strong components*.

Another, somewhat coarser, equivalence

$$a \Longleftrightarrow b(R)$$

is defined to mean that either $a \leftrightarrow b(R)$ or $a \leftrightarrow b(R^{+-})$. Since $a \leftrightarrow b(R)$ and $b \leftrightarrow c(R^{+-})$ imply $a \leftrightarrow c(R^{+-})$, it is not difficult to verify that $\Longleftrightarrow$ is an equivalence relation; let us call the associated classes the *weak components*.

Note that $aR^{+-}b$ and $bR^{+-}c$ and $aR^{+}c$ implies $bR^{+-}a$ and $cR^{+-}b$. Hence any *minimum-length* chain $a = a_0 R^{+-} a_1 R^{+-} ... R^{+-} a_n = b$ of R^{+-} relations between two elements a and b will also be a chain $b = a_n R^{+-} ... R^{+-} a_1 R^{+-} a_0 = a$ in the opposite direction, whenever $n \geq 2$. This makes it easy to prove a slightly "stronger" property of the weak components:

Lemma 2. *Let R^M be the symmetric relation $\{(a, b) \mid aR^{+-}b \text{ and } bR^{+-}a\}$. Then $a \Longleftrightarrow b(R)$ if and only if either $a \leftrightarrow b(R)$ or $aR^{M+}b$.*

The importance of the equivalence relations $\leftrightarrow$ and $\Longleftrightarrow$ is due to the fact that R^+ defines a *partial order* on the strong components, and a *total order* on the weak components. Indeed, the strong components constitute the *finest* partition of A which is partially ordered by R^+, and the weak components constitute the finest partition which is *totally* ordered by R^+. In order to see this, let π be any partition which is totally ordered by R^+, and suppose that a and b are elements of different blocks of π although $a \Longleftrightarrow b(R)$. We may assume that $aR^+ b$ and $bR^{+-}a$; hence by Lemma 2 we must have $aR^{M+}b$. But this implies that a and b must belong to the *same* partition of π, contradicting our assumption. In other words, each block of π must be a union of weak components.

The total ordering property allows us to write

$$a < b(R)$$

if $a \nLeftrightarrow b(R)$ and aR^+b. Every weak component is made up of one or more strong components; we shall call a weak component *simple* if it consists of just one strong component, and we shall call a component *trivial* if it consists of a single element.

These definitions are illustrated in fig. 1, where a relation R on 15 points is shown as a directed graph. The 9 strong components are enclosed in dotted lines, and the 4 weak components are separated by straight horizontal lines. Only one of the weak components is simple and they are all nontrivial; 5 of the strong components are trivial.

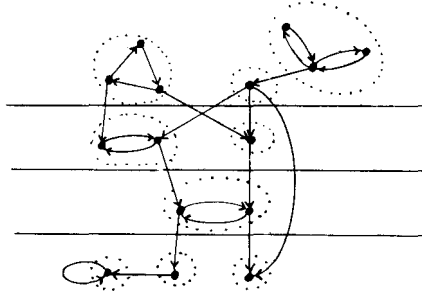We have defined the strong and weak components in such a way that

Fig. 1. Strong and weak components of a relation.

they are unchanged when R is replaced by R^+. Let us now observe what happens when R is replaced by the relation R^{+-}: All arcs within non-trivial strong components disappear, and there are paths between any two strong R-components of a single weak R-component. If $a < b(R)$, we have $bR^{+-}a$ by definition, hence all points belonging to *different* weak components are joined in the graph for R^{+-} by an arc from the larger element to the smaller. It follows that elements of different weak R-components belong to different weak R^{+-}-components. Conversely, if a and b belong to the *same* weak R-component, and if this component is simple and nontrivial, then a and b must be unrelated in R^{+-+}; on the other hand if this component is not simple it is easy to see that $a \leftrightarrow b(R^{+-})$.

These observations allow us to characterise R^{+-+} completely:

Theorem 2. *For $a \neq b$, $aR^{+-+}b$ if and only if a and b are in the same nonsimple weak R-component or $b < a(R)$. Also, $aR^{+-+}a$ if and only if a is in a nonsimple weak R-component, or a is in a trivial weak R-component and aR^-a.*

Hence, for $a \neq b$, $aR^{+-+-}b$ if and only if a and b both belong to the same simple weak R-component or $a < b(R)$. Also, $aR^{+-+-}a$ if and only if a is in a simple nontrivial weak R-component, or a is in a trivial weak R-component and aRa. This relation is clearly transitive, so we have found the structure underlying Theorem 1.

§3. Free relations

Most relations R seem to generate a complete set of fewer than 10 relations; at least, the authors spent six or seven frustrating hours before finding a single example such as (4), since we had not yet discovered Theorem 2. Let us now determine the structure of "free relations" which generate all 10 distinct possibilities.

So far we have seen connections between R and R^{+-}; there is also an interesting relation between the components of R and R^-:

Lemma 3. *Every nonsimple weak R-component is contained in some simple weak R^--component.*

Proof. Let a and b belong to the same nonsimple weak R-component with $a \neq b$. If $a \nleftrightarrow b(R)$, we have $a \leftrightarrow b(R^{+-})$, i.e., $aR^{+-+}b$ and $bR^{+-+}a$. But $R^{+-+} \subseteq R^{-+}$ so that $aR^{-+}b$ and $bR^{-+}a$, i.e., $a \leftrightarrow b(R^-)$. If $a \leftrightarrow b(R)$ there is an element c in the same weak R-component but not in the same strong R-component (since the weak component is non-simple) and again $a \leftrightarrow b(R^-)$ since $a \leftrightarrow c(R^-)$ and $b \leftrightarrow c(R^-)$. Hence a and b belong to the same strong R^--component.

If the weak R^--component containing a and b were not simple, we could use the same argument to show that it is contained in a simple weak R-component, since $R^{--} = R$; but that would be absurd.

Let us say that a weak R-component W contains an *arc* if there exist elements $a, b \in W$ such that aRb.

Consider the following four conditions on a relation R:

    (I). R has a nonsimple weak component containing an arc.

    (II). R^- has a nonsimple weak component containing an arc.

    (III). Some simple nontrivial weak R-component intersects some simple nontrivial weak R^--component.

    (III'). The weak R-components are not the same as the weak R^--components.

Theorem 3. *A relation R is free if and only if R satisfies* (I), (II) *and* (III), *or* (I), (II) *and* (III').

Proof. ($\Rightarrow$). In order for R to be free we must certainly have

    (i) $R^{+-} \neq R^{+-+}$,

(ii) $R^{-+-} \neq R^{-+-+}$,

(iii) $R^{+-+-} \neq R^{-+-+}$.

Let us examine these in detail.

Since $aR^{+-}b$ is equivalent to $aR^{+-+}b$ whenever a and b lie in different weak R-components, or if a and b lie in the same strong R-component of a simple weak R-component, condition (i) can hold only if there is a nonsimple weak R-component. Theorem 2 tells us that $aR^{+-+}b$ holds for all a and b within such a component. Thus condition (i) is equivalent to the existence of a nonsimple weak R-component containing elements a, b such that $aR^+ b$, and this is equivalent to (I).

Of course, (ii) is just (i) with R replaced by R^-. Hence, (ii) holds if and only if (II) holds.

Suppose (iii) holds. Since $R^{-+-+} \subseteq R^{+-+-+} = R^{+-+-}$, we must have

$$(5) \qquad aR^{+-+-}b \quad \text{and} \quad aR^{-+-+-}b \quad \text{for some } a \text{ and } b \, .$$

If $a \neq b$, then by Theorem 2 we have: a and b are in the same simple weak R-component or $a < b(R)$, and a and b are in the same simple weak R^--component or $a < b(R^-)$. If $a = b$, then by Theorem 2 we have: a is in a simple nontrivial weak R-component or a is in a trivial weak R-component and aRa, and a is in a simple nontrivial weak R^--component or a is in a trivial weak R^--component and aR^-a.

Since we cannot have both $a < b(R)$ and $a < b(R^-)$, property (5) holds if and only if at least one of the following is true:

(1). There exists a simple weak R-component not contained in a weak R^--component.

(2). There exists a simple weak R^--component not contained in a weak R-component.

(3). Some simple nontrivial weak R-component intersects some simple nontrivial weak R^--component.

(4). There exists an element a in a trivial weak R-component and a simple nontrivial weak R^--component, with aRa.

(5). There exists an element a in a trivial weak R^--component and a simple nontrivial weak R-component, with aR^-a.

Note that by Lemma 3, we may delete the word "simple" in the first two of these conditions. These first two conditions are then exactly equivalent to (III'). Moreover, if they fail to hold, then so do the final two conditions listed. We are left with the third condition which is, of course, identical to (III).

In summary, we have now shown that (i) $\Longleftrightarrow$ (I), (ii) $\Longleftrightarrow$ (II) and (iii) $\Longleftrightarrow$ (III) or (III$'$), and the necessity of the conditions has been established.

($\Leftarrow$). Assume that (I), (II) and either (III) or (III$'$) hold. To show that R is free, we must prove that all 10 expressions R, R^+, R^{+-}, R^{+-+}, R^{+-+-}, R^-, R^{-+}, R^{-+-}, R^{-+-+}, R^{-+-+-} are distinct. Table 1 indicates the various reasons behind the 45 necessary inequalities.

<div align="center">

Table 1
Summary of 45 cases

</div>

	$\emptyset$	$+$	$+-$	$+-+$	$+-+-$	$-$	$-+$	$-+-$	$-+-+$	$-+-+-$
$\emptyset$										
$+$	(III)									
$+-$	*	*								
$+-+$	*	*	(I)							
$+-+-$	(I)	(I)	*	*						
$-$	*	*	(III)	(I)	*					
$-+$	*	(Ī)	(III)	(III)	(Ī)	(III)				
$-+-$	(III)	(III)	(Ī)	(Ī)	(III)	*	*			
$-+-+$	(II)	(III)	(ĪĪ)	(Ī)	(III)	*	*	(II)		
$-+-+-$	*	(ĪĪ)	(III)	(III)	(Ī)	(II)	(II)	*	*	

An entry of (I), (II) or (III) indicates that condition (I), (II) or (III) (or (III$'$)) is used in establishing the corresponding inequality. For example, the $(\emptyset,+-+-)$ entry is (I), where, of course, $\emptyset$ denotes R itself. If $R = R^{+-+-}$, then

$$R^{+-} = (R^{+-+-})^{+-} = (R^{+-+-+})^-$$

$$= (R^{+-+-})^- \qquad \text{by Theorem 1}$$

$$= R^{+-+},$$

which contradicts (I).

An entry of ∗ denotes that the corresponding inequality follows from the fact that A is nonempty so that no relation equals its complement. For example, the (+,+−+) entry is ∗. If $R^+ = R^{+-+}$ then

$$R^{+-+-} = (R^{+-+})^{-+-} = (R^{+-+-+})^- = (R^{+-+-})^- \quad \text{by Theorem 1}$$

$$= R^{+-+},$$

which contradicts the nonemptiness of A.

The entries $(\bar{\text{I}})$, $(\bar{\text{II}})$ indicate that the argument needed uses more than Theorem 1. For example, the (+−+, −+−+) entry is $(\bar{\text{I}})$. By (I), R has a nonsimple weak component. Let a and b belong to this component with $a \neq b$. By Lemma 3, a and b are in a simple R^--component. By Theorem 2, $aR^{+-+}b$, $aR^{-+-+-}b$, i.e. $R^{+-+} \neq R^{-+-+}$.

The (−+,+) entry is also $(\bar{\text{I}})$, since $R^{-+} = R^+$ implies $R^{-+-+} = R^{+-+}$, and the latter is impossible as we have just seen. The reader should have little difficulty in verifying the remaining entries, thus completing the proof of the theorem.

With this result, we may now justify the claim made earlier for (4).

Theorem 4. *A relation on less than 5 elements always generates less than* 10 *relations under complementation and transitive closure.*

Proof. Suppose R is free and A has ≤ 4 elements. By Theorem 3, (I) and (II) imply that R and R^- must each have a nonsimple weak component. By Lemma 3, these components must be disjoint. Hence A must have 4 elements. It is easily seen, though, that in this case (III) and (III′) must both fail, contradicting the freeness of R.

It can be shown, in fact, that all free relations on 5 elements must have at least 10 ordered pairs. Thus (4) is minimal in a strong sense.

§4. Extensions and applications

Suppose $R \subseteq T$, where T is a total order relation. T may be reflexive, irreflexive, or partly reflexive; the "diagonal" elements are immaterial in the following discussion. We can consider complements with respect

to T instead of $A \times A$; thus, let $R^\Delta = T - R$. For this case, the analog of Lemma 1 does not hold:

$$R = R^+ = \begin{matrix} 0011 \\ 0000 \\ 0001 \\ 0000 \end{matrix}, \quad T = \begin{matrix} 0111 \\ 0011 \\ 0001 \\ 0000 \end{matrix}, \quad R^{+\Delta+\Delta} = \begin{matrix} 0000 \\ 0000 \\ 0001 \\ 0000 \end{matrix}, \quad R^+ \circ R^{+\Delta+\Delta} = \begin{matrix} 0001 \\ 0000 \\ 0000 \\ 0000 \end{matrix}.$$

On the other hand, the analog of Theorem 1 is true:

Theorem 5. *In terms of the above notation, $R^{+\Delta+\Delta+} = R^{+\Delta+\Delta}$.*

Proof. Assume that $R^{+\Delta+\Delta}$ is not transitive. There must be elements a, b, c such that $aR^{+\Delta+\Delta}b$, $bR^{+\Delta+\Delta}c$ and $aR^{+\Delta+}c$ (since aTc). Hence for some $n \geq 1$ we have elements $a_0, a_1, ..., a_n$ such that $a = a_0$, $a_0R^{+\Delta}a_1$, $a_1R^{+\Delta}a_2, ..., a_{n-1}R^{+\Delta}a_n$, $a_n = c$.

If $b = a_j$ for some j, we would have $aR^{+\Delta+}b$, a contradiction; hence the fact that T is a total order implies that there is some j such that $a_{j-1}Tb$ and bTa_j. Now $a_{j-1}R^+b$ (since $a_{j-1}R^{+\Delta}b$ would imply that $aR^{+\Delta+}b$) and similarly bR^+a_j; hence $a_{j-1}R^+a_j$, a contradiction.

The proof of this theorem makes essential use of the hypothesis that T is a total order. If T were merely assumed to be a partial order containing R, we could not prove Theorem 5, because of the following simple counterexample:

$$R = \begin{matrix} 0010 \\ 0000 \\ 0001 \\ 0000 \end{matrix}, \quad T = \begin{matrix} 0111 \\ 0001 \\ 0001 \\ 0000 \end{matrix}, \quad R^{+\Delta+\Delta} = R \neq R^+.$$

Another common operation of interest is the *reflexive closure* $R^I = R \cup I$ where I is the equality relation. It is not difficult to prove that $R^{I-I} = R^{-I}$ and $R^{+-I-+} = R^{-I-+}$. A somewhat less evident identity is $R^{+-+I-+-} = R^{-I-+-+}$; the reader will find it instructive to prove this. By using identities such as these, it is possible to establish the analog of Theorem 1 for the three operations $^+$, $^-$ and ^{I}. We state this without proof.

Theorem 1'. *At most* 42 *relations can be generated from a relation R by taking complements, transitive closures and reflexive closures. These are indicated in fig.* 2.
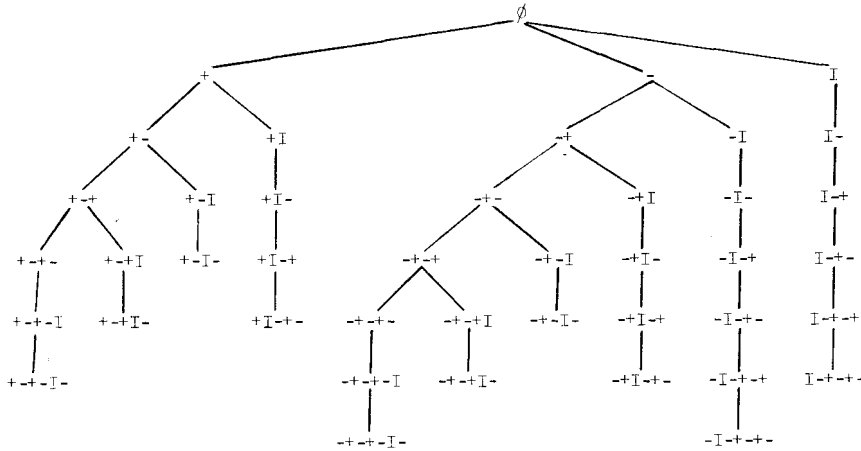

Fig. 2. Independent relations using $^+$, $^-$ and ^{I}.

The following relation R generates 42 distinct relations under $^+$, $^-$ and ^{I}:

$$
R = \begin{matrix}
000011101 \\
001011101 \\
000011101 \\
000111101 \\
000111101 \\
000101101 \\
000111101 \\
111111111 \\
000000000
\end{matrix}
$$

M.R. Garey [2] has recently considered the operation of "transitive reduction", the smallest relation whose transitive closure is the same as R^+. He has shown that any finite relation leads to at most 34 different relations under repeated application of complementation, transitive reduction and transitive closure, and that this bound actually can be attained.

It is possible to consider other operations on relations and ask similar questions, e.g., the difunctional closure $R^D = (R \circ R^T)^+ \circ R$, where R^T is

the converse of R (cf. [5], [7]), but this will not be done here.

The original application which led to the above theorems was the following: Let R be a transitive relation; find the largest transitive relation contained in R whose complement with respect to $A \times A$ is transitive. By Theorem 1, the answer is simply R^{-+-}. Or, let R be an irreflexive partial ordering contained in the irreflexive total ordering T; find the largest partial ordering contained in R whose complement with respect to T is a partial ordering. By Theorem 4, the answer is $R^{\Delta+\Delta}$.

The latter result applies also to permutations: If $p_1 p_2 ... p_n$ is a permutation of $\{1, 2, ..., n\}$, an *inversion* is a pair of indices (i, j) such that $i < j$ and $p_i > p_j$. Write iVj if (i, j) is an inversion; then V is transitive, and so is its complement V^Δ with respect to $T = \{(i, j) \mid i < j\}$. Conversely it is not difficult to show ([1] pp. 114–117) that there is a unique permutation $p_1 p_2 ... p_n$ whose inversions correspond in this way to a relation $V \subseteq T$, whenever V and V^Δ are transitive. If R is a transitive subset of T, the relation $V = R^{\Delta+\Delta}$ is the largest subset of R which corresponds to a permutation. The corresponding permutation therefore has the maximum number of inversions, among all permutations whose inversions are contained in R.

If we call a relation *closed* when it is transitive, and *open* when its complement is transitive, then the closure R^+ is the smallest closed relation containing R and the "interior" R^{-+-} is the largest open relation contained in R. In these terms, Theorem 1 asserts that the interior of the closure is closed; dually, the closure of the interior is open.

A result somewhat similar to Theorem 5 has been proved by Guilbaud and Rosenstiehl [3], who discovered that $(R \cup S)^{+\Delta}$ is transitive whenever $R^{+\Delta}$ and $S^{+\Delta}$ are both transitive. The same result holds for $^-$ in place of $^\Delta$. We have been unable to find any other work closely related to the above theorems, in spite of the fact that the operation of transitive closure has been known and applied for so many years. For example, E. Schröder failed to discover any of the theorems of this paper in his "exhaustive" study of identities involving binary relations [8]; he would have dearly loved to know that, in his notation, $a_{00};(a_{00})_{11} \nleq (a_{00})_{11}$ and $((a_{00})_{11})_{00} = (a_{00})_{11}$!

References

[1] C. Berge, Principes de combinatoire (Dunod, Paris, 1968).

[2] M.R. Garey, personal communication.

[3] G. Guilbaud and P. Rosenstiehl, Analyse algébrique d'un scrutin, Math. Sci. Humaines 4 (1960) 9–33.

[4] C. Kuratowski, Sur l'opération $\bar{A}$ de l'Analysis Situs, Fund. Math. 3 (1922) 182–199.

[5] J. Lambek, Goursat's theorem and the Zassenhaus lemma, Canad. J. Math. 10 (1957) 45–56.

[6] E. Langford, Characterization of Kuratowski 14-sets, Am. Math. Monthly 74 (4) (1971) 362–367.

[7] J. Riguet, Quelques propriétés des relations difonctionelles, Comt. Rend. Acad. Sci. Paris 230 (1950) 1999–2000.

[8] E. Schröder, Vorlesungen über die Algebra der Logik. 3: Algebra und Logik der Relative (Teubner, Leipzig, 1895) 346–404.