Defining (reflexive) transitive closure on finite models

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Axiomatising (R)TC in FOL, modulo FIN

Let R be a binary relation on some domain. Use R^* for the reflexive transitive closure of R, i.e., the smallest binary relation S with $R \subseteq S$ that is reflexive and transitive. Use R^+ for the transitive closure of R, i.e., the smallest binary relation S with $R \subseteq S$ that is transitive. Use I for the identity relation on the domain. Let n range over natural numbers. Define R^n as follows, by induction:

$$\begin{array}{rcl} R^0 & := & I \\ R^{n+1} & := & R \circ R^n \end{array}$$

Here $\circ$ expresses relational composition. For finite domains we have that $R^* = \bigcup_{n \geq 0} R^n$, and that $R^+ = \bigcup_{n > 0} R^n$.

Assume the domain of discourse is finite (FIN). Introduce a ternary relation symbol C. Intended interpretation is as follows. C expresses:

$$\lambda xyz.\exists n, m \in \mathbb{N}(n > 0 \wedge xR^n yR^m z \wedge \forall k \in \mathbb{N}(k < n + m \rightarrow \neg xR^k z)).$$

This can be paraphrased as: y is at some finite non-zero distance n from x on some shortest R-path from x to z.

It follows, given FIN, that $\lambda xy.Cxyy$ expresses $R^+ - I$. Therefore, we can define reflexive transitive closure by means of a binary relation symbol T, as follows (all formulas universally closed).

$$Txy \leftrightarrow (x = y \vee Cxyy) \tag{DEF}$$

Now T expresses $I \cup (R^+ - I) = I \cup R^+ = R^*$.

Since $R^+ = R \circ R^*$, the following defines T' as transitive closure:

$$T'xy \leftrightarrow \exists z(Rxz \wedge Tzy) \tag{DEF'}$$

Clearly, $\lambda xy.Cxyu$ is irreflexive, for any choice of u. This is true in the intended interpretation of C because if there is an R-step from x to x, and an R-path $xR \cdots Ru$ from x to u, then the path $xRxR \cdots Ru$ that loops through x is longer than the path $xR \cdots Ru$ that avoids this loop. Irreflexivity of $\lambda xy.Cxyu$ is expressed by:

$$\neg Cxxu \tag{C1}$$

Also, $\lambda xy.Cxyu$ is transitive, for any u. For if $xR^n yR^m u$ is some shortest R-path from x to u, and $yR^k zR^p u$ is some shortest R-path from y to u, then $m = k + p$, and $xR^{n+k} zR^p u$ is some shortest R-path from x to u. This transitivity requirement is expressed by:

$$(Cxyu \wedge Cyzu) \to Cxzu \tag{C2}$$

Axiom C3 expresses that $(R^+ - I)$ is almost transitive:

$$(Cxyy \wedge Cyzz \wedge x \neq z) \to Cxzz \tag{C3}$$

Next, we want to say that $(R - I) \subseteq (R^+ - I)$. This is expressed by:

$$(Rxy \wedge x \neq y) \to Cxyy \tag{C4}$$

The next axiom expresses that if $(x, y) \in (R^+ - I)$ then it is always possible to make a first R-step on some shortest R-path from x to y.

$$Cxyy \to \exists z(Rxz \wedge Cxzy) \tag{C5}$$

Finally:

$$(Cxyz \wedge y \neq z) \to Cyzz \tag{C6}$$

This expresses that if y is somewhere along on a shortest R-path from x to z, and $y \neq z$, then $(y, z) \in (R^+ - I)$.

This turns out to be a complete first order theory for (reflexive) transitive closure on finite models.

Note: the finite domain constraint itself is *not* expressed by any first order axiom. In fact, it follows from the compactness theorem for first order logic that no first order sentence can express finiteness. For suppose FIN is a first order sentence expressing the finite domain constraint. Let L_n express that there are at least n objects. This is easily expressed in terms of equality. E.g., $\exists xyz(x \neq y \wedge x \neq z \wedge y \neq z)$ expresses that there are at least three objects. Then the infinite set of first order sentences $\{\text{FIN} \wedge L_n \mid n \in \mathbb{N}\}$ has the property that any finite subset of it has a (finite) model. By compactness, the whole set has a model. It is easily seen that a model of $\{L_n \mid n \in \mathbb{N}\}$ has to be infinite, and contradiction with the fact that FIN expresses finiteness.

Note that in the intended interpretation of C it holds that $Cxyx$ is false, for any x, y. This is derivable in the system, as follows. We assume $Cxyx$, and derive a contradiction. From $Cxyx$, with C1: $x \neq y$. From $Cxyx$ and $x \neq y$, with C6: $Cyxx$. From $Cyxx$ and $Cxyx$, with C2: $Cyyx$, and contradiction with C1.

It is easy to check that these axioms are sound for the intended interpretation. We will now show that the theory consisting of C1–6 defines (reflexive) transitive closure on finite models.

Theorem 1 *In all finite models of C1–6, the interpretation of T is the reflexive transitive closure of the interpretation of R and the interpretation of T' is the transitive closure of the interpretation of R.*

Proof. Let M be a finite model of C1–6. Use $[\![\cdot]\!]$ for relational interpretation in M. We show that $[\![R]\!]^* = [\![T]\!]$.

$[\![R]\!]^* \subseteq [\![T]\!]$. Let $[\![R]\!]^{\geq n}$ be given by:

$$[\![R]\!]^{\geq n} = \{(a,b) \mid (a,b) \in [\![R]\!]^n \wedge \forall m < n \ \ (a,b) \notin [\![R]\!]^m\}.$$

We show by induction that for each $n \in \mathbb{N}$, $[\![R]\!]^{\geq n} \subseteq [\![T]\!]$. Since the model is finite, this proves the claim. By DEF, $[\![T]\!]$ is reflexive, so $[\![R]\!]^{\geq 0} \subseteq [\![T]\!]$. Assume that for some $n \in \mathbb{N}$, $[\![R]\!]^{\geq n} \subseteq [\![T]\!]$. We show that $[\![R]\!]^{\geq n+1} \subseteq [\![T]\!]$. Let $(a,b) \in [\![R]\!]^{\geq n+1}$. Then $a \neq b$, and there is c in the domain with $a \neq c$,

$b \neq c$, $(a,c) \in [\![R]\!]$ and $(c,b) \in [\![R]\!]^{\geq n}$. From $(a,c) \in [\![R]\!]$ and $a \neq c$ it follows by C4 that $(a,c,c) \in [\![C]\!]$. By induction hypothesis it follows from $(c,b) \in [\![R]\!]^{\geq n}$ that $(c,b) \in [\![T]\!]$. Since $c \neq b$, by DEF, $(c,b,b) \in [\![C]\!]$. Since $a \neq b$ we can apply C3. This yields $(a,b,b) \in [\![C]\!]$, and therefore $(a,b) \in [\![T]\!]$ by DEF.

$[\![T]\!] \subseteq [\![R]\!]^*$. Let $(a,b) \in [\![T]\!]$. If $a = b$ then $(a,b) \in [\![R]\!]^*$ and done. So assume $a \neq b$. Then by DEF, $(a,b,b) \in [\![C]\!]$. From this, by C5, there is an a_1 with $(a,a_1) \in [\![R]\!]$ and $(a,a_1,b) \in [\![C]\!]$. By C1, $a \neq a_1$. Suppose $a_1 = b$. Then $(a,b) \in [\![R]\!]$ and done. Suppose $a_1 \neq b$. Then by C6, $(a_1,b,b) \in [\![C]\!]$, and from this it follows, by C5, that there is an a_2 with $(a_1,a_2) \in [\![R]\!]$ and $(a_1,a_2,b) \in [\![C]\!]$. By C1, $a_1 \neq a_2$. If $a = a_2$, then from $(a_1,a,b) \in [\![C]\!]$ and $(a,a_1,b \in [\![C]\!]$ it would follow by C2 that $(a_1,a_1,b) \in [\![C]\!]$, and contradiction with C1. So $a \neq a_2$. If $a_2 = b$ then $(a,b) \in [\![R]\!]^2$ and done. So assume $a_2 \neq b$. Then by C6, there is an a_2 with $(a_2,b,b) \in [\![C]\!]$. And so on. This creates a sequence $a = a_0, a_1, a_2, \ldots$, with the a_i all different. By finiteness of the domain, this process has to stop with $a_n = b$ for some $n \in \mathbb{N}$. It follows that $(a,b) \in [\![R]\!]^n$.

From $[\![R]\!]^* = [\![T]\!]$ it follows immediately with DEF' that $[\![T']\!] = [\![R]\!] \circ [\![R]\!]^* = [\![R]\!]^+$. □

First order logic cannot define transitive closure on arbitrary models. We also know that any first order theory with an infinite model has a countably infinite model. It follows that there are countably infinite models where the above axioms do not define reflexive transitive closure.

Here is an example. Let $\mathbb{N}$ be the natural numbers and a an object $\notin \mathbb{N}$. Consider the domain $\mathbb{N} \cup \{a\}$ and let $R = \{(n, n+1) \mid n \in \mathbb{N}\}$. Then $R^* = \{(n,m) \mid n,m \in \mathbb{N}, n \leq m\}$. Let

$$T = R^* \cup \{(n,a) \mid n \in \mathbb{N}\} \cup \{(a,a)\}.$$

Let

$$C = \lambda xyz.x(T - I)yTz.$$

It is not difficult to see that this is a model of the theory: all axioms are satisfied by this interpretation.

Special case: reflexive transitive closure of loopfree relations

The following result is from [1]. Consider the following theory.

$$Txx \tag{J1}$$

$$(Rxy \land Tyz) \to Txz \tag{J2}$$

$$(Txy \land x \neq y) \to \exists z (Rxz \land Tzy) \tag{J3}$$

A binary relation R is *loopfree* if R^+ is irreflexive.

Theorem 2 *If R is a* loopfree *binary relation on a finite domain D, then J1, J2, J3 defines R^*.*

Proof. Let M be a finite model of J1, J2, J3, and assume $[\![R]\!]$ is loopfree. We show that $[\![R]\!]^* = [\![T]\!]$.

$[\![R]\!]^* \subseteq [\![T]\!]$. We show with induction on n that $[\![R]\!]^n \subseteq [\![T]\!]$ for all n. This proves the claim. Clearly, $[\![R]\!]^0 \subseteq [\![T]\!]$, by J1. Assume (induction hypothesis) that $[\![R]\!]^n \subseteq [\![T]\!]$. We show that $[\![R]\!]^{n+1} \subseteq [\![T]\!]$. Let $(a,b) \in [\![R]\!]^{n+1}$. Then there is a c with $(a,c) \in [\![R]\!]$ and $(c,b) \in [\![R]\!]^n$. By induction hypothesis, it follows from $(c,b) \in [\![R]\!]^n$ that $(c,b) \in [\![T]\!]$. Hence, by J2, $(a,b) \in [\![T]\!]$.

$[\![T]\!] \subseteq [\![R]\!]^*$. Let $(a,b) \in [\![T]\!]$. Then either $a = b$, and $(a,b) \in [\![R]\!]^0$, and done, or $a \neq b$, and by J3 there is an a_1 with $(a,a_1) \in [\![R]\!]$ and $(a_1,b) \in [\![T]\!]$. By loopfreeness of $[\![R]\!]$, $a \neq a_1$. If $a_1 = b$ then $(a,b) \in [\![R]\!]^1$, and done. If $c \neq b$ then by J3 there is an a_2 with $(a_1,a_2) \in [\![R]\!]$ and $(a_2,b) \in [\![T]\!]$. By loopfreeness of $[\![R]\!]$, $a \neq a_2$ and $a_1 \neq a_2$. If $a_2 = b$ then done. Otherwise, by J3, there is an a_3 ... And so on. By the finiteness of the domain this process has to stop with some $a_n = b$. It follows that $(a,b) \in [\![R]\!]^n$. □

Note that the conjunction of J1, J2 and J3 is equivalent to:

$$Txy \leftrightarrow (x = y \lor \exists z (Rxz \land Tzy)) \tag{J}$$

Comparison

The present axiomatisation was inspired by the axioms for RTC in Claessen [2]. Claessen has the following axioms (tags are his):

$$Txx \tag{I1}$$

$$Rxy \rightarrow Txy \tag{I2}$$

$$(Txy \wedge Tyz) \rightarrow Txz \tag{I3}$$

$$(Txy \wedge x \neq y) \rightarrow R(x, s(x, y)) \tag{E1}$$

$$(Txy \wedge x \neq y) \rightarrow T(x, s(x, y)) \tag{E2}$$

$$(Txy \wedge x \neq y) \rightarrow C(x, s(x, y), y) \tag{E3}$$

plus (C1) and (C2). Here $s(\_, \_)$ is a binary function symbol that is added to the signature.

Although calculi C1–6 and I1–3, E1–3, C1–2 both use a ternary relation symbol C satisfying axioms C1 and C2, the interpretation of C in calculus C1–6 is much more constrained. As we saw, it follows from C1–6 that $\neg Cxyx$, for all x, y.

By contrast, the following is a model of I1–3, E1–3, C1–2:

$$\begin{array}{rcl} U & = & \{0,1\}, \\ R & = & \{(1,0),(1,1)\}, \\ s & = & \{(0,0,1),(0,1,1),((1,0,0),(1,1,0)\}, \\ C & = & \{(1,0,0),(1,0,1)\}, \\ T & = & \{(0,0),(1,0),(1,1)\} \end{array}$$

Clearly, this predicate C does *not* satisfy the intuition that was used above to motivate axioms C1–6, for we have that $(1, 0, 1)$ in C, while there is no R-path from 1 to 1 via 0.

I have briefly compared implementations of the two calculi in Alloy [3].

Here are some data for the calculus consisting of C1–6:

```
Executing "Check rtcFact for 2"
   Solver=sat4j Bitwidth=4 MaxSeq=2 Symmetry=20
   277 vars. 22 primary vars. 442 clauses. 5ms.
   No counterexample found. Assertion may be valid. 0ms.

Executing "Check rtcFact for 3"
   Solver=sat4j Bitwidth=4 MaxSeq=3 Symmetry=20
   907 vars. 57 primary vars. 1571 clauses. 11ms.
   No counterexample found. Assertion may be valid. 4ms.

Executing "Check rtcFact for 4"
   Solver=sat4j Bitwidth=4 MaxSeq=4 Symmetry=20
   2233 vars. 116 primary vars. 3872 clauses. 36ms.
   No counterexample found. Assertion may be valid. 42ms.

Executing "Check rtcFact for 5"
   Solver=sat4j Bitwidth=4 MaxSeq=5 Symmetry=20
   4018 vars. 205 primary vars. 7137 clauses. 86ms.
   No counterexample found. Assertion may be valid. 1260ms.

Executing "Check rtcFact for 6"
   Solver=sat4j Bitwidth=4 MaxSeq=6 Symmetry=20
   7141 vars. 330 primary vars. 12464 clauses. 243ms.
   No counterexample found. Assertion may be valid. 26153ms.

Executing "Check rtcFact for 7"
   Solver=sat4j Bitwidth=4 MaxSeq=7 Symmetry=20
   12118 vars. 497 primary vars. 20769 clauses. 571ms.
   No counterexample found. Assertion may be valid. 537403ms.
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And here are the data for the calculus consisting of I1–3, E1–3, C1–2:

```
Executing "Check rtcFact for 2"
   Solver=sat4j Bitwidth=4 MaxSeq=2 Symmetry=20
   341 vars. 26 primary vars. 453 clauses. 6ms.
   No counterexample found. Assertion may be valid. 1ms.
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```
Executing "Check rtcFact for 3"
   Solver=sat4j Bitwidth=4 MaxSeq=3 Symmetry=20
   1062 vars. 75 primary vars. 1591 clauses. 12ms.
   No counterexample found. Assertion may be valid. 5ms.

Executing "Check rtcFact for 4"
   Solver=sat4j Bitwidth=4 MaxSeq=4 Symmetry=20
   2641 vars. 164 primary vars. 4080 clauses. 34ms.
   No counterexample found. Assertion may be valid. 63ms.

Executing "Check rtcFact for 5"
   Solver=sat4j Bitwidth=4 MaxSeq=5 Symmetry=20
   5703 vars. 305 primary vars. 9189 clauses. 108ms.
   No counterexample found. Assertion may be valid. 1377ms.

Executing "Check rtcFact for 6"
   Solver=sat4j Bitwidth=4 MaxSeq=6 Symmetry=20
   9095 vars. 510 primary vars. 14421 clauses. 279ms.
   No counterexample found. Assertion may be valid. 25575ms.

Executing "Check rtcFact for 7"
   Solver=sat4j Bitwidth=4 MaxSeq=7 Symmetry=20
   15517 vars. 791 primary vars. 24469 clauses. 744ms.
   No counterexample found. Assertion may be valid. 2719276ms.
```

The tentative conclusion of this is that C1–6 scales up a bit better than I1–3, E1–3, C1–2. For domain sizes up to 6 there are no significant differences, but the check for domains up to size 7 was performed with the first calculus in less than one/fifth of the time it took with the second calculus.

References

[1] Thomas Baar. The definition of transitive closure with OCL. In *Fifth Amdreo Ershov International Conference, Perspectives of System Informatics*, volume 2890 of *LNCS*, pages 358–365. Springer, 2003.

[2] Koen Claessen. Expressing transitive closures for finite domains in pure first order logic. Unpublished draft, Chalmers University of Technology, May 2008.

[3] Daniel Jackson. *Software Abstractions; Logic, Language and Analysis*. MIT Press, 2006.