

CDM

Automaticity

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1 Properties of Rat

2 Synchronous Relations

3 Model Checking Automatic Structures

Wurtzelbrunft remembers the Banach quote about analogies and immediately concludes:

Every result about regular languages carries over, *mutatis mutandis*, to rational relations.

After all, it's just about the same Kleene algebra we are working in, so what could possibly change? For example, we should be able to come up with a nice machine model, figure out how to determinize and minimize these devices, and so on.

Fortunately, life is so much more interesting than that.

Some results do indeed carry over, almost verbatim. But others are plain false and one has to be very careful not to jump at conclusions.

Consider the binary rational relations

$$A = \left(\begin{smallmatrix} a \\ c \end{smallmatrix}\right)^* \left(\begin{smallmatrix} b \\ \varepsilon \end{smallmatrix}\right)^* \quad B = \left(\begin{smallmatrix} a \\ \varepsilon \end{smallmatrix}\right)^* \left(\begin{smallmatrix} b \\ c \end{smallmatrix}\right)^*$$

Then

$$A \cap B = \left\{ \left(\begin{smallmatrix} a^i b^i \\ c^i \end{smallmatrix}\right) \mid i \geq 0 \right\}$$

It is easy to see that the intersection cannot be recognized by a finite state transducer, essentially for the same reasons that $\{a^i b^i \mid i \geq 0\}$ fails to be regular.

Exercise

Prove that $A \cap B$ really fails to be rational.

Rational relations are closed under union by definition: we allow nondeterminism.

So the last result shows that we fail to have closure under intersection and complement.

Remember that we ultimately want to tackle first-order logic over simple structures, so this looks like a total fiasco. Indeed, we will have to adjust our definitions in a while.

But for the time being, let's stick with rational relations.

Disregarding state complexity, in the world of regular languages, there is no difference between NFAs and DFAs: nondeterminism does not increase the power of the machines.

One might wonder if there is some notion of deterministic rational relation and a corresponding deterministic transducer.

The basic idea is simple: there should be at most one computation on all inputs.

Unfortunately, the technical details are a bit messy (use of endmarkers) and we'll skip this opportunity to inflict mental pain on the student body.

Consider the binary rational relations

$$A = \left(\begin{smallmatrix} aa \\ b \end{smallmatrix} \right)^* \quad B = \left(\begin{smallmatrix} a \\ bb \end{smallmatrix} \right)^*$$

It is clear that both A and B are deterministic rational relations.

Now consider

$$A \cup B = \left\{ \left(\begin{smallmatrix} a^i \\ b^j \end{smallmatrix} \right) \mid i = 2j \vee j = 2i \right\}$$

For the union, your intuition should tell you that nondeterminism is critical: initially, we don't know which type of test to apply. This indicates that determinization is not going to work in general for rational relations (which is to be expected since we already know that complementation fails in general).

While we have to give up on negation and intersection, it is still the case that a great many natural relations on words turn out to be rational:

- prefix, factor, suffix
- orders: subsequence, order, split, lexicographic, length-lex
- homomorphic image, substitution image
- concatenation
- successor, predecessor, addition

Example

If $K \subseteq \Sigma^*$ and $L \subseteq \Gamma^*$ are regular, then $K \times L$ is rational.

Example

If $\rho \subseteq \Sigma^* \times \Gamma^*$ is rational, then $\text{spt}(\rho) \subseteq \Sigma^*$ and $\text{rng}(\rho) \subseteq \Gamma^*$ are regular.

Example

Recall the definition of **shuffle**:

$$\begin{aligned}\varepsilon \parallel y &= y \parallel \varepsilon = \{y\} \\ xa \parallel yb &= (x \parallel yb) a \cup (xa \parallel y) b.\end{aligned}$$

So $x \parallel y$ is the set of all possible interleavings of the letters of x and y (preserving relative order). The map $(x, y) \mapsto x \parallel y$ is rational.

There are several useful ways to order words over an alphabet that all turn out to be rational.

The **subsequence order** on words is defined by $u = u_1 \dots u_n$ precedes $v = v_1 v_2 \dots v_m$ if there exists a strictly increasing sequence $1 \leq i_1 < i_2 < \dots i_n \leq m$ of positions such that $u = v_{i_1} v_{i_2} \dots v_{i_n}$.

Subsequence order is interesting since it does not depend on any given order on the alphabet.

A famous theorem by Higman shows that this order does not admit infinite anti-chains.

Consider the binary relation $<_{\text{len}}$ on Σ^* defined by

$$x <_{\text{len}} y \iff |x| < |y|.$$

We obtain a strict pre-order called **length order**; the corresponding classes of indistinguishable elements are words of the same length.

Given an ordered alphabet Σ consider the binary relation $<_s$ on Σ^* defined by

$$x <_s y \iff \exists a < b \in \Sigma, u, v, w \in \Sigma^* (x = uav \wedge y = ubw)$$

This produces another strict pre-order, the so-called **split order**; this time indistinguishable words are prefixes of one another.

Again assume an ordered alphabet Σ . The **lexicographic order** is a mix of prefix order and split order:

$$x <_{\ell} y \iff x \sqsubset y \vee x <_s y$$

Here $x \sqsubset y$ means that x is a proper prefix of y .

Lexicographic order is a total order, there are no indistinguishable elements. And it is relative robust when it comes to looking up words in ordinary languages.

For algorithmic purposes, length-lex order (see next slide) is much better suited.

Another important way of ordering words is the product order of length order and lexicographic order, the so-called **length-lex order**.

$$x <_{\ell\ell} y \iff x <_{\text{len}} y \vee (|x| = |y| \wedge x <_{\ell} y)$$

Length-lex order is easily seen to be a well-order and there are many algorithms on strings that are naturally defined by induction on length-lex order.

Needless to say, length-lex order is also rational.

Proposition

All the order relations on the last few slides are rational.

Exercise

Construct rational expressions that prove the proposition.

Construct transducers that prove the proposition.

Proposition

The relation $x = y^{\text{op}}$ fails to be rational.

This is easy to see by using a standard “pumping argument:” a transducer for this relation would have to remember arbitrarily long prefixes of the input.

Exercise

Give a careful proof of the proposition.

Usually one thinks of concatenation as a binary operation. Since we want to avoid functions, we can also model it as a ternary relation γ :

$$\gamma(x, y, z) \iff x \cdot y = z$$

Proposition

Concatenation is rational.

Proof. For simplicity assume $\Sigma = \{a, b\}$

$$\gamma = (a:\varepsilon:a + b:\varepsilon:b)^* \cdot (\varepsilon:a:a + \varepsilon:b:b)^*$$



Consider the ternary relation α on $\mathbf{2}$ defined by

$$\alpha(x, y, z) \iff \text{bin}(x) + \text{bin}(y) = \text{bin}(z)$$

where $\text{bin}(x)$ is the numerical value of x assuming the LSD is first (reverse binary).

Proposition

Binary addition in reverse binary is rational.

Proof. The kindergarten algorithm for addition shows that α is rational. $\square$

Warning: there is no analogous result for multiplication (for reverse binary encoding; but beware of exotic encodings).

Here is a central result: rational relations are closed under composition. Suppose we have two binary relations $\rho \subseteq \Sigma^* \times \Gamma^*$ and $\sigma \subseteq \Gamma^* \times \Delta^*$. Their composition $\tau = \rho \circ \sigma \subseteq \Sigma^* \times \Delta^*$ is defined to be the binary relation

$$x \tau y \iff \exists z (x \rho z \wedge z \sigma y)$$

Theorem (Elgot, Mezei 1965)

If both ρ and σ are rational, then so is their composition $\rho \circ \sigma$.

Assume we have transducers $\mathcal{A}$ and $\mathcal{B}$ for ρ and σ , respectively. We may safely assume that the labels in $\mathcal{A}$ have the form a/ε or ε/b where $a \in \Sigma$, $b \in \Gamma$; likewise for $\mathcal{B}$. Add self-loops labeled ε/ε everywhere.

We construct a product automaton $\mathcal{C}$ with transitions

$$(p, q) \xrightarrow{a/c} (p', q')$$

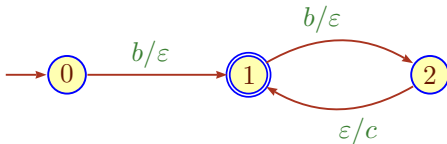
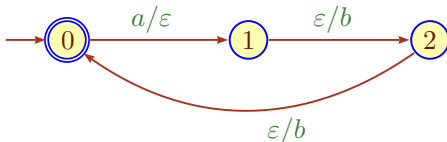
whenever there are transitions $p \xrightarrow{a/b} p'$ and $q \xrightarrow{b/c} q'$ in $\mathcal{A}$ and $\mathcal{B}$, respectively, for some $a \in \Sigma_\varepsilon$, $b \in \Gamma_\varepsilon$ and $c \in \Delta_\varepsilon$.

Initial and final states in $\mathcal{C}$ are $I_1 \times I_2$ and $F_1 \times F_2$. It is a labor of love to check that $\mathcal{C}$ accepts x/z if, and only if, $x \rho y$ and $y \sigma z$ for some $y \in \Gamma^*$. $\square$

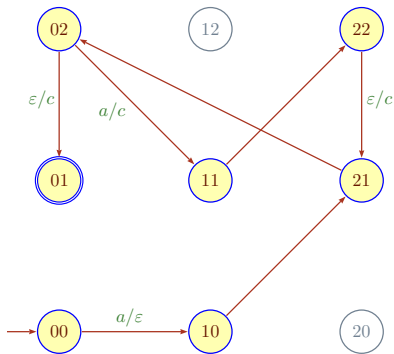
Let $\rho = \left(\begin{smallmatrix} a \\ b \end{smallmatrix} \right)^*$ and $\sigma = \left(\begin{smallmatrix} b \\ \varepsilon \end{smallmatrix} \right) \left(\begin{smallmatrix} b \\ c \end{smallmatrix} \right)^*$; thus

$$\rho \circ \sigma = \left(\begin{smallmatrix} a \\ c \end{smallmatrix} \right) \left(\begin{smallmatrix} a \\ cc \end{smallmatrix} \right)^* = \left\{ \left(\begin{smallmatrix} a^{i+1} \\ c^{2i+1} \end{smallmatrix} \right) \mid i \geq 0 \right\}$$

Here are the two machines, without the ε/ε self-loops.



And here is the accessible part of the product. Unlabeled edges are supposed to be ε/ε .



Of course, there is a “better” transducer, but this is the one obtained by blind application of the algorithm.

Here is another important closure property. Suppose ρ is a k -ary relation on words. We define the **projection** of ρ to be

$$\rho'(x_2, \dots, x_k) \iff \exists z \rho(z, x_2, \dots, x_k)$$

Lemma

Whenever ρ is rational, so is its projection ρ' .

Proof.

In a transducer for ρ , erase the first track in the k -track alphabet:

$$p \xrightarrow{a_1:a_2:\dots:a_k} q \quad \rightsquigarrow \quad p \xrightarrow{a_2:\dots:a_k} q$$

Done!



Note that the use of the term *projection* is slightly different here from the standard use: $x \mapsto x_i$.

Clearly, rational relations contain ordinary projections in this sense.

So, we are really dealing with a clone, except that this time we have a clone of relations rather than a clone of functions (recall the section on computability).

And while we are talking about bad terminology and notation . . .

One might wonder what happens when we move to the transitive reflexive closure $\text{tcl}(\rho)$. Recall that

$$\text{tcl}(\rho) = \bigsqcup_k \rho^{\circ k}$$

where $\rho^{\circ k}$ indicates the standard iterate, the k -fold composition of ρ with itself: $\rho \circ \rho \circ \dots \circ \rho$.

Mental Health Warning: Unfortunately, the transitive closure is often written ρ^* , in direct clash with the standard notation for the Kleene star of a relation.

Alas, the two are quite incompatible. For example, let ρ be lexicographic order. Clearly, $\text{tcl}(\rho) = \rho$.

But $ab \rho^* aabb$ since $a \rho aa$ and $b \rho bb$. So Kleene star clobbers the order completely.

Theorem

The transitive closure $\text{tcl}(\rho)$ of a rational relation is semidecidable.

Proof.

By definition $x \text{ tcl}(\rho) y$ iff $\exists k (x \rho^{\circ k} y)$.

Obviously, $\rho^{\circ k}$ is primitive recursive, uniformly in k .

So we are conducting an unbounded search over a primitive recursive relation; semidecidability follows. $\square$

What would happen if we add tcl to the closure operations that produce the rational relations?

Theorem

Adding tcl to the closure operations produces precisely all semidecidable relations.

Proof.

It is clear that every rational is primitive recursive. The transitive closure of a rational relation is thus no more than semidecidable. Moreover, the operations of union, concatenation and Kleene star preserve semidecidability; lastly, the transitive closure of a semidecidable relation is again semidecidable.

For the opposite direction, we use the old trick of coding configurations of a Turing machine as words of the form $\Gamma^* Q \Gamma^*$, assumed to be disjoint.

$$x_m x_{m-1} \dots x_1 p a y_2 \dots y_n$$

Then the next configuration could look like

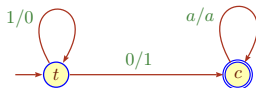
$$x_m x_{m-1} \dots x_1 b q y_2 \dots y_n$$

For the most part, we just copy the tape symbols, but there is a little bit of hanky panky right next to the state symbol.

A transducer can easily handle this type of update operation. Hence, transitive closures are enough to produce all semidecidable relations.



Most transducers define relations rather than functions, here is one that does.



Theorem (Schützenberger 1975)

It is decidable whether a transducer is single-valued.

The argument is tricky, and it took 25 years to find a polynomial algorithm for this.

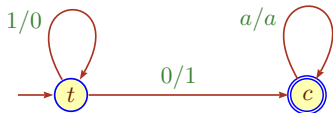
If we write natural numbers as binary string, arithmetical operations turn into transductions; simple operations turn into rational transductions.

One needs to be a bit careful about the way the naturals are represented as strings: we need to fix a **numeration system**. Here are a few considerations:

- choice of base
- LSD first or last (reverse radix or plain radix)
- empty string denotes zero
- leading/trailing zeros

A reasonable convention would be the following **numeration system** $\mathcal{N}$: write numbers in reverse binary (LSD first), the empty string is not allowed, neither are trailing zeros.

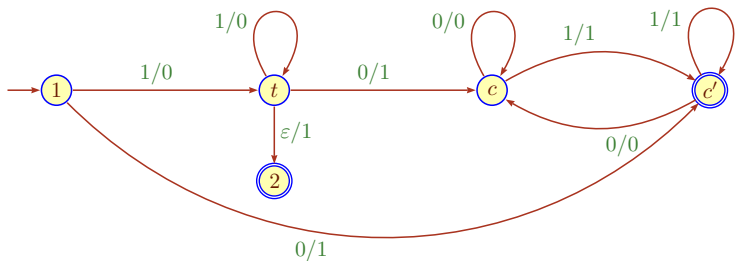
The key component for the successor transduction is the following machine:



Here t stands for toggle, c for copy. Alas, this transducer allows for trailing zeros. Much worse, it implements a cyclic counter: $1^k \mapsto 0^k$.

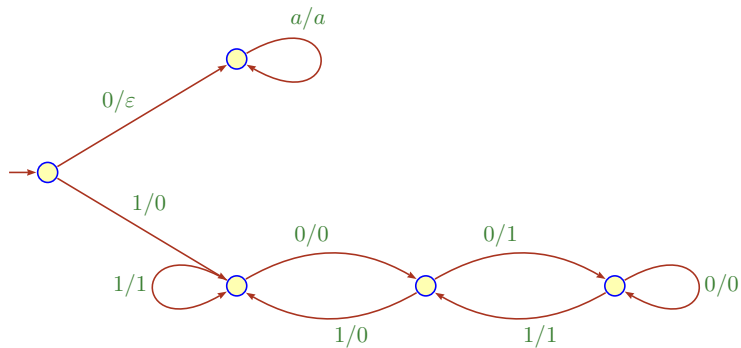
To fix things, it can help to write down a list of specifications for a transducer that is compliant with the numeration system $\mathcal{N}$. We need for any binary string x :

$$\begin{array}{lll}
 0x & \rightsquigarrow & 1x \\
 11^k & \rightsquigarrow & 00^k 1 \\
 11^k 0x & \rightsquigarrow & 00^k 1x
 \end{array}$$



This version is obtained by a bit of surgery on the basic machine, and is compliant with our numeration system $\mathcal{N}$.

For correctness, one can show by induction that it implements the specifications from the last slide.

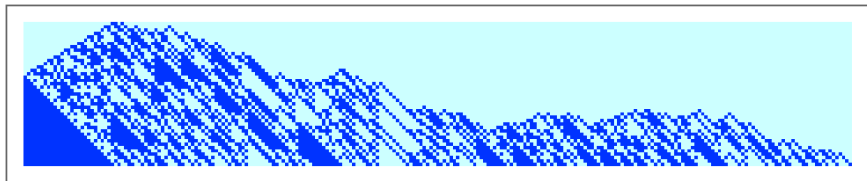
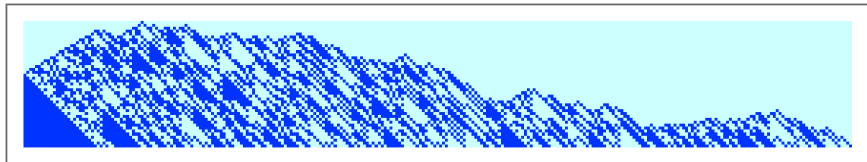


Recall the infamous Collatz conjecture:
The following program halts for all $x \geq 1$.

```
while( x > 1 )           // x positive integer
  if( x even )
    x = x/2;
  else
    x = 3 * x + 1;
```

If we write x in reverse binary, and right-pad with 00, the transducer on the last slide computes one execution of the loop body.

So iterating the composition of the trivial map $x \mapsto x00$ and the transducer leads to an open problem in number theory.



The lower part of the Collatz transducer is a special case of a more general problem: multiply by a fixed constant m and add another fixed constant a . We assume the numbers are written in reverse binary.

Roughly, one can organize the construction of a transducer into 2 phases.

1. Write the multiplication in terms of repeated additions of terms $2^i x$ (just a right shift).
2. Then handle the addition of a .
3. This produces a raw transducer that works “in essence,” conveniently ignoring issues of padding or trailing zeros.
4. Lastly, deal with all the actual details of the numeration system.

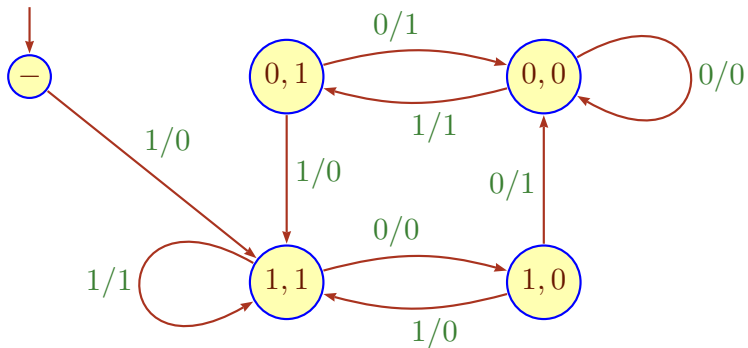
Getting everything correct right from the start is hard, it's much easier to work in stages.

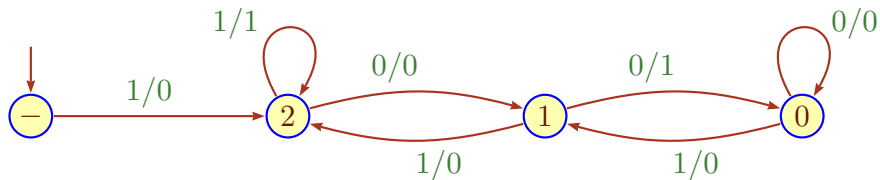
As always, the key is to pick the right state set. We can add the strings x and $1x$ to get multiplication by 3. Here is the odd case:

$$\begin{array}{r|cccccccccccc}
 x & 1 & x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & 0 & 0 & 0 & 0 & \dots \\
 2x+1 & 1 & 1 & x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & 0 & 0 & 0 & \dots \\
 \hline
 3x+1 & 0 & x_1 & y_2 & y_3 & y_4 & y_5 & y_6 & y_7 & y_8 & 0 & 0 & \dots
 \end{array}$$

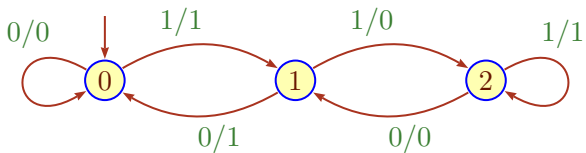
So we really have to deal with addition, using the standard add-digits and keep-track-of-carries approach. But note that there is only one input, and we have to remember the current input bit for the next step.

This suggests states for the form $(c, b) \in \mathbf{2} \times \mathbf{2}$: c is the carry, b the last bit.





A moment's thought reveals that the states $(0, 1)$ and $(1, 0)$ have the same behavior; we can merge them to get a smaller machine.



The key part is the raw “multiply-by-3” transducer.

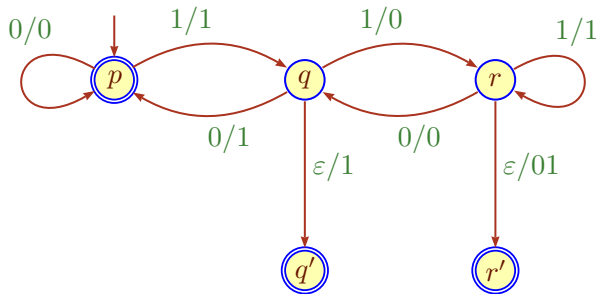
To get around padding, one sometimes augments transducers with initial and final output maps $\text{inp} : Q \rightarrow \Gamma^*$ and $\text{outp} : Q \rightarrow \Gamma^*$.

We then redefine our notion of acceptance: instead of $u:v$ obtained directly by a run from p to q , we declare the following 2-track word to be accepted:

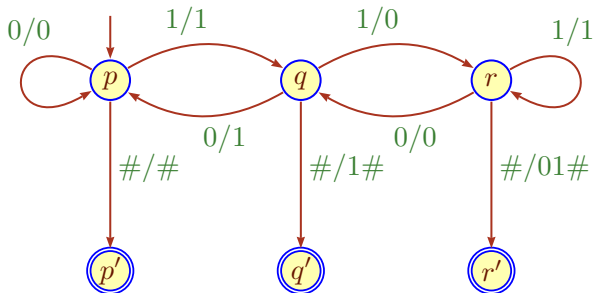
$$u : \text{inp}(p) \, v \, \text{outp}(q)$$

Essentially, we allow systematic padding, both at the beginning and at the end.

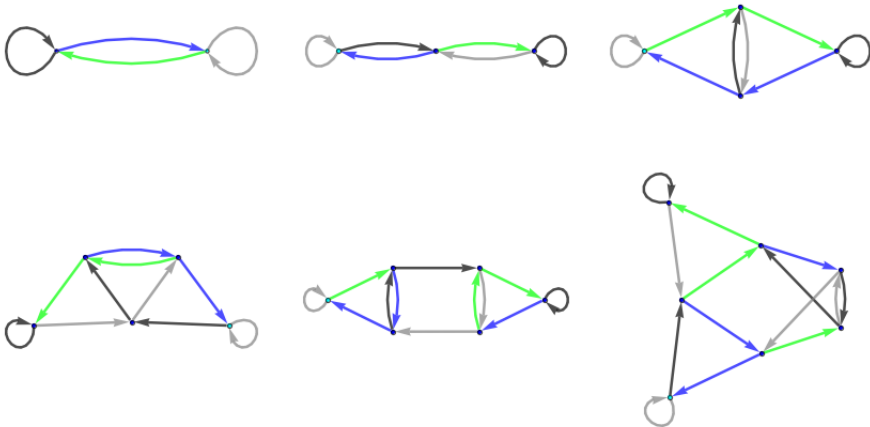
For full-fledged transducers this makes no real difference, we could simply add corresponding transitions with ε -labels. For limited classes of transducers, such as alphabetic ones, this convention is very convenient.



Here the output function is given by $p \rightsquigarrow \varepsilon$, $q \rightsquigarrow 1$ and $r \rightsquigarrow 01$ and handles the carry.



Lastly, a machine that assumes that every track has a special endmarker $\#$. Note that this machine is clearly deterministic, the endmarkers tell us when the end of the input has been reached.



Some raw transducers for various small multipliers.

Life should be much easier with **length-preserving** transductions:

$$x \tau y \Rightarrow |x| = |y|$$

In fact, let's only consider the functional case: we are just iterating a map $y = \tau(x)$. Clearly, if τ is length-preserving, then all orbits must be finite (in fact they cannot be longer than $|\Sigma|^{|x|}$). Still, computational hardness is lurking nearby.

Theorem

For length-preserving transductions, transitive closure is PSPACE-complete in general.

It is clear that the map $x \mapsto x^{\text{op}}$ cannot be rational.

But iteration of a length-preserving transduction can be used to “compute” x^{op} as follows.

Define a new alphabet $\Gamma = \Sigma \cup \{\bar{a} \mid a \in \Sigma\}$.

There is a length-preserving rational function τ such that $\tau(\varepsilon) = \varepsilon$ and

$$\tau(auv) = u\bar{a}v$$

where $au \in \Sigma^*$ and $v \in \overline{\Sigma}^*$. Let f be the “unbar” homomorphism $f(\bar{a}) = f(a) = a$. Then

$$x^{\text{op}} = f(x \text{ tcl}(\tau) \cap \overline{\Sigma}^*) = \{f(z) \mid x \text{ tcl}(\tau) z \wedge z \in \overline{\Sigma}^*\}$$

1 Properties of Rat

2 **Synchronous Relations**

3 Model Checking Automatic Structures

Rational relations in general are just a little too powerful for our purposes, they don't have nice closure properties (the way recognizable languages do). We need to scale back a bit.

One sledge-hammer restriction is to insist that all the relations are **length-preserving**. In this case we have $\rho \subseteq (\Sigma \times \Gamma)^*$, so our multi-words are actually words over the product alphabet $\Sigma \times \Gamma$. These can be checked by an ordinary FSM over a standard 2-track alphabet:

x_1	x_2	$\dots$	x_n
y_1	y_2	$\dots$	y_n

Nothing new here, a length-preserving relation is rational iff it is recognizable as a language over $\Sigma \times \Gamma$.

There is one particularly simple type of transducer that is often useful to recognize length-preserving relations. In a **Mealy machine**, the transitions are described by a function

$$\delta : Q \times \Sigma \longrightarrow \Gamma \times Q.$$

The idea is that transitions are labeled by pairs in $\Sigma \times \Gamma$, so each input letter is transformed into an output letter (alphabetic transducers).

And, the transitions are deterministic.

For example, the raw transducer that implements the successor function modulo 2^k on words of length k in reverse binary is a Mealy machine.

Alas, length-preserving relations are bit too restricted for our purposes. To deal with words of different lengths, first extend each component alphabet by a **padding symbol** $\#$: $\Sigma_{\#} = \Sigma \cup \{\#\}$ where $\# \notin \Sigma$.

The alphabet for 2-track words is $\Delta_{\#} = \Sigma_{\#} \times \Gamma_{\#}$.

This pair of padded words is called the **convolution** of x and y and is written $x^{\#} : y$.

$$x^{\#} : y =$$

x_1	x_2	$\dots$	x_n	$\#$	$\dots$	$\#$
y_1	y_2	$\dots$	y_n	y_{n+1}	$\dots$	y_m

Another example of bad terminology, convolutions usually involve different directions.

Note that we are not using all of $\Delta_{\#}^*$ but only the recognizable subset coming from convolutions. In other words, $\#$ can only appear as a suffix, and in exactly one track. For example,

a	$\#$	b	$\#$
a	b	a	a

a	b	b	$\#$	$\#$
a	b	a	b	$\#$

are not allowed.

As always, a similar approach clearly works for k ary relations, just use

$$\Delta_{\#} = \Sigma_{1,\#} \times \Sigma_{2,\#} \times \dots \times \Sigma_{k,\#}$$

Exercise

Show that the collection of all convolutions forms a recognizable language.

Here is an idea going back to Büchi and Elgot in 1965.

Definition

A relation $\rho \subseteq \Sigma^* \times \Gamma^*$ is **synchronous** or **automatic** if there is a finite state machine $\mathcal{A}$ over $\Delta_{\#}$ such that

$$\mathcal{L}(\mathcal{A}) = \{ x^{\#}y \mid x,y \in \rho \} \subseteq \Delta_{\#}^*$$

k -ary relations are treated similarly.

Note that this machine $\mathcal{A}$ is just a language recognizer, not a transducer: since we pad, we can read one symbol in each track at each step.

In a sense, synchronous relations are the most basic examples of transductions that are not entirely trivial.

By contrast, one sometimes refers to arbitrary rational relations as asynchronous.

- Equality and inequality are synchronous.
- Lexicographic order is synchronous.
- The prefix-relation is synchronous.
- The ternary addition relation is synchronous.
- The suffix-relation is not synchronous.
- The relations “ x is a factor of y ” and “ x is a (scattered) subword of y ” are not synchronous.

Intuitively, the difference between arbitrary transductions and synchronous ones is that, for the latter, one can build a 2-track machine whose heads can move independently, but are never further than some fixed distance d apart.

Bounded head distance is already enough: essentially, we could then force phantom heads to move in lockstep by remembering the last d symbols and the actual head positions.

So the critical difference is when the two heads move arbitrarily far away from each other.

Our motivation for synchronous relations was taken from length-preserving relations: it is plausible that two words of the same length should be processed in lock-step fashion. The justification for this idea is the following result.

Theorem (Elgot, Mezei 1965)

Any length-preserving rational relation is already synchronous.

The proof is quite messy, we'll skip.

For intuition, think about the gap between the two heads during a computation and the way it interacts with the length-preserving requirement.

Claim

Given two k -ary synchronous relations ρ and σ on Σ^ , the following relations are also synchronous:*

$$\rho \sqcup \sigma \quad \rho \sqcap \sigma \quad \rho - \sigma$$

The proof is very similar to the argument for recognizable languages: one can effectively construct the corresponding automata using the standard product machine idea.

This is a hugely important difference between general rational relations and synchronous relations: the latter do form an effective Boolean algebra, but we have already seen that the former are not closed under intersection (nor complement).

Synchronous relations are not closed under concatenation (or Kleene star). For example, let

$$\rho = \begin{pmatrix} a \\ \varepsilon \end{pmatrix}^*$$
$$\sigma = \begin{pmatrix} b \\ b \end{pmatrix}^*$$

Then both ρ and σ are synchronous, but $\rho \cdot \sigma$ is not (the dot here is concatenation, not composition): recognizing words in $\rho \cdot \sigma$ comes down to counting. On the other hand, $\sigma \cdot \rho$ is fine.

Exercise

Prove all examples and counterexamples.

On the upside, synchronous relations are closed under composition.

Suppose we have two binary relations $\rho \subseteq \Sigma^* \times \Gamma^*$ and $\sigma \subseteq \Gamma^* \times \Delta^*$.

Theorem

If both ρ and σ are synchronous relations, then so is their composition $\rho \circ \sigma$.

Exercise

Prove the theorem.

More good news: synchronous relations are closed under projections.

Lemma

Whenever ρ is synchronous, so is its projection ρ' .

The argument is verbatim the same as for general rational relations: we erase a track in the labels.

Again, this will generally produce a nondeterministic transition system even if we start from a deterministic one. If we also need complementation to deal with logical negation, we may have to deal with exponential blow-up.

1 Properties of Rat

2 Synchronous Relations

3 **Model Checking Automatic Structures**

To simplify matters, suppose we are looking at a structure over the alphabet $\mathbf{2}$ with just one binary relation representing a function:

$$\mathfrak{C} = \langle \mathbf{2}^+, \rightarrow \rangle$$

Concretely, think about elementary cellular automata operating on finite words, say, with periodic boundary conditions.

Note that $\rightarrow$ is length-preserving, so there will not be any problems with synchronicity.

$$\forall x, y, z (x \rightarrow y \wedge x \rightarrow z \Rightarrow y = z)$$

$$\forall x, y, z (x \rightarrow y \wedge z \rightarrow y \Rightarrow x = z)$$

$$\forall x \exists y (y \rightarrow x)$$

$$\exists x, y, z (x \rightarrow y \wedge y \rightarrow z \wedge z \rightarrow x \wedge x \neq y)$$

$$\forall x \exists y, z ((y \rightarrow x \wedge z \rightarrow x \wedge y \neq z) \wedge \forall u (u \rightarrow x \Rightarrow u = y \vee u = z))$$

What is the meaning of these formulae?

So suppose we have the finite state machines describing $\mathfrak{C} = \langle \mathbf{2}^+, \rightarrow \rangle$ and some FO sentence Φ in the language $\mathcal{L}(\rightarrow)$

As always, we may assume that quantifiers use distinct variables and that the formula is in prenex-normal-form[†], say:

$$\Phi = \exists x_1 \forall x_2 \forall x_3 \dots \exists x_k \varphi(x_1, \dots, x_k)$$

The matrix $\varphi(x_1, \dots, x_k)$ is quantifier-free, so all we have there is Boolean combinations of atomic formulae.

[†]This is actually a bad idea for efficiency reasons, but it simplifies the discussion of the basic algorithm.

In our case, there are only two possible atomic cases:

- $x_i = x_j$
- $x_i \rightarrow x_j$

Given an assignment for x_i and x_j (i.e., actual strings) we can easily test these atomic formulae using two synchronous transducers $\mathcal{A}_=$ and $\mathcal{A}_{\rightarrow}$.

So $\varphi(x_1, \dots, x_k)$ defines a k -ary relation over 2^+ , constructed from $\rightarrow$ and $=$ using Boolean operators. The first step is to build a finite state machine that recognizes this relation.

Our matrix is the quantifier-free formula

$$\varphi(x_1, x_2, \dots, x_k)$$

containing exactly the displayed free variables. In order to recognize the k -track words that satisfy φ , we construct a k -track machine by induction on the subformulae of φ .

The atomic pieces read from two appropriate tracks and check $\rightarrow$ or $=$.

Note that there is a bureaucratic problem: the atomic machines are 2-track, but the machine for the matrix is usually k -track for some $k > 2$.

More precisely, use superscripts to indicate the number of tracks of a machine as in $\mathcal{A}_{\rightarrow}^{(2)}$ and $\mathcal{A}_{=}^{(2)}$.

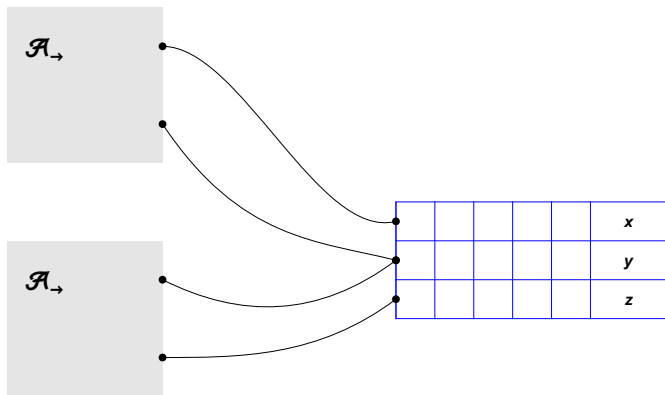
Let $m \leq n$. We need an embedding operation

$$\text{emb}_t^{(n)} : m\text{-track} \longrightarrow n\text{-track}$$

where $t = t_1, \dots, t_m$, $t_i \in [n]$, all distinct.

So $\text{emb}_t^{(n)}(\mathcal{A}^{(m)}) = \mathcal{B}^{(n)}$ means that track i of $\mathcal{A}^{(m)}$ is identified with track t_i in $\mathcal{B}^{(n)}$. The other tracks are free (all possible transitions). This does not affect the state set, but it can cause potentially very large alphabets and, correspondingly, large numbers of transitions in the embedded automaton[†].

[†]One of the reasons why state complexity alone is not really a good measure of the size of an automaton, one needs to add the number of transitions.



A product machine to check $x \rightarrow y \wedge y \rightarrow z$.

Slightly more generally, we can combine any two 2-track machines $\mathcal{A}_i^{(2)}$ and construct the product machine

$$\mathcal{B} = \text{emb}_{1,2}^{(3)}(\mathcal{A}_1^{(2)}) \times \text{emb}_{2,3}^{(3)}(\mathcal{A}_2^{(2)})$$

$\mathcal{B}$ checks for strings $x:y:z$ such that $\mathcal{A}_1$ recognizes $x:y$ and $\mathcal{A}_2$ recognizes $y:z$.

And so on for any number of embedded automata. Note that the product machine construction can produce uncomfortably large state sets.

Suppose $\varphi = \psi_1 \wedge \psi_2$ with corresponding machines $\mathcal{A}_{\psi_1}$ and $\mathcal{A}_{\psi_2}$. We can use a product machine construction to get $\mathcal{A}_{\varphi}$.

Disjunctions are even easier: just take the disjoint union, there is really no way to get around nondeterminism here.

But negations are potentially expensive: we have to determinize first.

At any rate, we wind up with a composite automaton $\mathcal{A}_{\varphi}$ that recognizes the relation defined by the matrix:

$$\mathcal{L}(\mathcal{A}_{\varphi}) = \{ u_1:u_2:\dots:u_k^{\#} \mid \mathcal{C} \models \varphi(u_1, u_2, \dots, u_k) \}$$

There is a natural dual to embeddings: **projections**.

Let $m \leq n$. We have a projection operation

$$\text{prj}_t^{(n)} : n\text{-track} \longrightarrow m\text{-track}$$

where $t = t_1, \dots, t_{n'}$, $n' \leq n$, $t_i \in [n]$, all distinct, $m = n - n'$.

So $\text{prj}_t^{(n)}(\mathcal{A}^{(n)}) = \mathcal{B}^{(m)}$ means that, for all transitions in $\mathcal{A}^{(n)}$, the tracks t_i of the transition labels have been erased, producing $\mathcal{B}^m$. The state set is unaffected.

It is fine to have $n = n'$, in which case it is understood that we are left with an unlabeled digraph (with special initial and final nodes).

It remains to deal with all the quantifiers in the prefix of Φ . First consider a single existential quantifier, say

$$\exists x \psi(x)$$

We have a machine $\mathcal{A}_\psi^{(n)}$ that has a track t for variable x .

Simply erase the x -track from all the transition labels.

In other words, $\text{prj}_t^{(n)}(\mathcal{A}^{(n)})$ corresponds exactly to existential quantification over variable x .

Alas, for universal quantifiers we have to use the old equivalence $\forall \equiv \neg \exists \neg$.

This is all permissible, since projections and negations do not disturb automaticity—though they may increase the machine size substantially.

Recall the machine checking $x \rightarrow y \wedge y \rightarrow z$.

$$\mathcal{B} = \text{emb}_{1,2}^{(3)}(\mathcal{A}_{\rightarrow}) \times \text{emb}_{2,3}^{(3)}(\mathcal{A}_{\rightarrow})$$

Projecting away the y -track

$$\mathcal{B}' = \text{prj}_2^{(n)}(\mathcal{B})$$

produces a machine that recognizes $x:z$ such that $\exists y (x \rightarrow y \wedge y \rightarrow z)$.

Similarly we can handle $f^k(x) = z$ for any fixed value of k . However, the size of the machine is only bounded by m^k .

In the process of removing quantifiers, we lose one track at each step and get intermediate machines $\mathcal{B}_{\varphi,\ell}$

$$\mathcal{L}(\mathcal{B}_{\varphi,\ell}) = \{ u_1:u_2:\dots:u_\ell^\# \mid \mathcal{C} \models \varphi_\ell(u_1, u_2, \dots, u_\ell) \}$$

for $\ell \leq k$. In the end $\ell = 0$, and we are left with an unlabeled transition system $\mathcal{B}_{\varphi,0}$. This transition system has a path from I to F iff the original sentence Φ is valid.

So the final test is nearly trivial (DFS anyone?), but it does take a bit of work to construct the right machine.

Why does this all work, fundamentally? It is all a direct consequence of various closure properties:

$\cup$	union
$\cap$	intersection
$\neg$	complement
$\exists$	homomorphism
emb	inverse homomorphism

Needless to say, all the closures are effective: we have algorithms to construct all the corresponding machines.

- $\forall$ and $\exists$ are linear if we allow nondeterminism.
- $\wedge$ is at most quadratic via a product machine construction.
- $\neg$ is potentially exponential since we need to determinize first.
- $\forall$ well ...

So this is a bit disappointing: we may run out of computational steam even when the formula is not terribly large. Universal quantifiers, in particular, can be a major problem.

A huge amount of work has gone into streamlining this and similar algorithms to deal with instances that are of practical relevance.

Let's figure out the details on how to determine the existence of a 3-cycle in $\mathcal{C}$. The obvious formula to use is this:

$$\Phi \equiv \exists x, y, z (x \rightarrow y \wedge y \rightarrow z \wedge z \rightarrow x \wedge x \neq y \wedge x \neq z \wedge y \neq z)$$

The first part ensures that there is a cycle, and the second part prevents the cycle from being shorter than 3.

Perfectly correct, but note the following. Suppose the basic machine $\mathcal{A}_{\rightarrow}$ that checks $\rightarrow$ has m states. Then the first part of the formula produces a machine of possibly m^3 states. The non-equal part blows things up further to at least $8m^3$ states.

We could replace Φ by any equivalent formula, which would be useful if we could find a smaller formula. It seems hard to get around the m^3 part, checking for each inequality doubles the size of the machine, so we get something 8 times larger than the machine for the raw 3-cycle. It is better to realize that since $\rightarrow$ is functional, the last formula is equivalent to

$$\exists x, y, z (x \rightarrow y \wedge y \rightarrow z \wedge z \rightarrow x \wedge x \neq y)$$

Exercise

Figure out how to deal with k -cycles for arbitrary k .

So, based on the better formula, we use the 3-track alphabet $\mathbf{2}^3 = \mathbf{2} \times \mathbf{2} \times \mathbf{2}$ plus padding to recognize

$$\{u:v:w^\# \mid u \rightarrow v \rightarrow w \rightarrow u \wedge u \neq v\}$$

Let $\mathcal{A}_{i,j} = \text{emb}_{i,j}^{(3)}(\mathcal{A}_{\rightarrow}^{(2)})$. Also, let $\mathcal{D}_{\neq}^{(2)}$ be the machine that checks for inequality and $\mathcal{D} = \text{emb}_{1,2}^{(3)}(\mathcal{D}_{\neq}^{(2)})$.

We can now concoct a 3-track product machine for the conjunctions:

$$\mathcal{B} = \mathcal{A}_{1,2} \times \mathcal{A}_{2,3} \times \mathcal{A}_{3,1} \times \mathcal{D}$$

where $\mathcal{A}_{\rightarrow,i,j}$ tests if the word in track i evolves to the word in track j .

So we get a machine $\mathcal{B}$ that is roughly cubic in the size of $\mathcal{A}_{\rightarrow}$ (disregarding possible savings for accessibility).

Once $\mathcal{B}_3$ is built, we erase all the labels and are left with a digraph (since φ has no universal quantifiers there is no problem with negation).

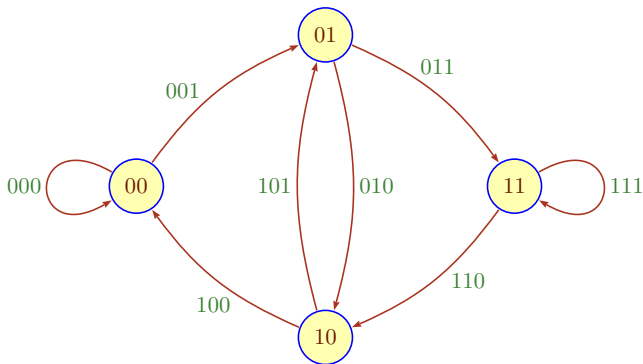
This digraph has a path from an initial state to a final state if, and only if, there is a 3-cycle under $\rightarrow$.

Note, though, how the machines grow if we want to test for longer cycles: the size of $\mathcal{B}_k$ is bounded only by m^k , where m is the size of $\mathcal{A}_{\rightarrow}$, so this will not work for long cycles. And, we need several products with $\mathcal{D}_{i,j}$, each at least doubling the size of the product.

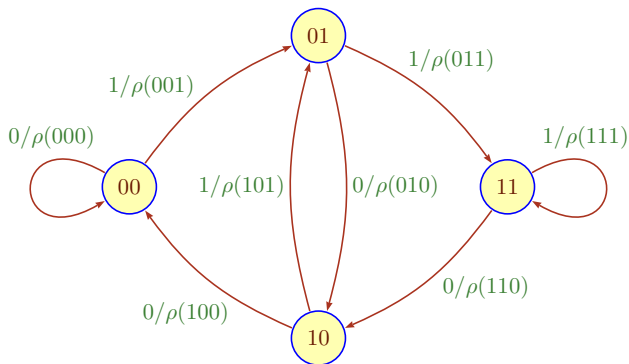
What would the basic one-step automaton $\mathcal{A}_{\rightarrow}$ for an elementary cellular automaton look like?

It turns out to be a little easier if we first consider configurations over $2^{\mathbb{Z}}$. As usual, the finite case is often harder than the infinite scenario.

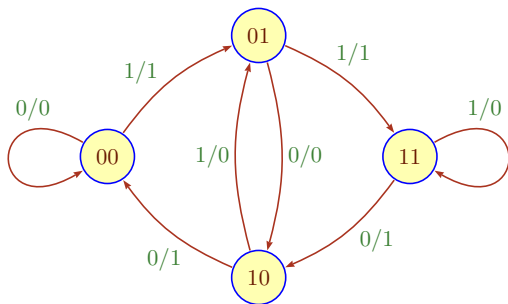
First, an automaton that corresponds to sliding a window of length 2 across the configuration. The states will naturally be 2^2 , and the edges corresponds to just having seen 3 bits in a row.



Each configuration in $2^{\mathbb{Z}}$ corresponds to exactly one biinfinite path in this automaton. And every biinfinite path corresponds to a configuration (at least if we are a bit relaxed about where the origin is).



If we replace the edge labels xyz by $xyz/\rho(xyz)$, where ρ is the local rule, we get a transducer that corresponds to the global map. All states are initial and final, we are interested in biinfinite runs.



A rather civilized transducer: a partial DFA over the alphabet 2^2 . It remains deterministic even if we project away either one of the tracks.

To define the global map G_f of a cellular automaton on finite configurations we need to deal with the endpoints: a priori they have no left/right neighbors.

- Cyclic boundary conditions: assume the configuration wraps around.
- Fixed boundary conditions: assume there are two phantom bits 0 pre/appended.

So for $x = x_1x_2 \dots x_n$ we apply the local map f to n many 3-blocks:

$$\begin{array}{ll} \text{CBC} & x_nx_1x_2 \quad x_1x_2x_3 \quad \dots \quad x_{n-1}x_nx_1 \\ \text{FBC} & 0x_1x_2 \quad x_1x_2x_3 \quad \dots \quad x_{n-1}x_n0 \end{array}$$

that

We need to modify the transducer for $2^{\mathbb{Z}}$ to work for plain 2^n . Say, we use fixed boundary conditions. The central problem is this: we are scanning two words

$$u:v = \begin{array}{|c|c|c|c|} \hline u_1 & u_2 & \dots & u_n \\ \hline v_1 & v_2 & \dots & v_n \\ \hline \end{array}$$

But a synchronous transducer must read the letters in pairs, both read heads move in lockstep.

We need to check whether $v_1 = \rho(0, u_1, u_2)$, and we do not know u_2 after scanning just the first bit pair.

It seems that some kind of look-ahead is required (**memory** versus **anticipation**), but synchronous automata don't do look-ahead, they live in the here-and-now. Looks like we are sunk.

If we drop the synchronicity condition, there is no problem: it easy to see that $\rightarrow$ is rational. And $\rightarrow$ is clearly length-preserving.

But remember the theorem by Elgot and Mezei:

Rational and length-preserving implies synchronous.

So our relation must be synchronous. Of course, that's not enough: we need to be able to construct the right transducer, not just wax poetically about its existence.

Exercise

Show that $\rightarrow$ is rational.

Nondeterminism saves the day: we can guess what x_2 is and then verify in the next step.

Automaton $\mathcal{A}_{\rightarrow}$ uses state set $Q = \{\perp, \top\} \cup \mathbf{2}^3$.

$\perp$ is the initial state, $\top$ the final state and the transitions are given by

$$\perp \xrightarrow{a/e} 0ab \quad e = \rho(0, a, b)$$

$$abc \xrightarrow{c/e} bcd \quad e = \rho(b, c, d)$$

$$abc \xrightarrow{c/e} \top \quad e = \rho(b, c, 0)$$

So, this is more complicated than the plain de Bruijn transducer for $\mathbf{2}^{\mathbb{Z}}$.

input	state	condition
—	$\perp$	—
$u_1:v_1$	$0\ u_1u_2$	$v_1 = \rho(0u_1u_2)$
$u_2:v_2$	$u_1u_2u_3$	$v_2 = \rho(u_1u_2u_3)$
$u_3:v_3$	$u_2u_3u_4$	$v_3 = \rho(u_3u_3u_4)$
	$\vdots$	
$u_{n-1}:v_{n-1}$	$u_{n-2}u_{n-1}u_n$	$v_n = \rho(u_{n-1}u_n0)$
$u_n:v_n$	$\top$	—

A successful computation on input $u_1u_2 \dots u_n:v_1v_2 \dots v_n$.

Define a 3-track machine that checks whether x and y both evolve to z ; then project away the z -track.

$$\mathcal{A} = \text{prj}_3^{(3)} \left(\text{emb}_{1,3}^{(3)}(\mathcal{A}_{\rightarrow}) \times \text{emb}_{2,3}^{(3)}(\mathcal{A}_{\rightarrow}) \right)$$

Then

$$\mathcal{L}(\mathcal{A}) = \{ x:y \mid \widehat{\rho}(x) = \widehat{\rho}(y) \}$$

So we only need to check

$$\mathcal{L}(\mathcal{A} \times \mathcal{A}_{\neq}) = \emptyset$$

to verify that the global map $\widehat{\rho}$ is injective.

For biinfinite configurations the last approach translates into a nice algorithm for reversibility testing.

Write $\mathcal{B}_{\rightarrow}$ for the ordinary de Bruijn automaton with edges 2^2 and labels $ab \xrightarrow{\rho(a,b,c)} bc$.

But then the ordinary full product automaton $\mathcal{B}_{\rightarrow}^2 = \mathcal{B}_{\rightarrow} \times \mathcal{B}_{\rightarrow}$ is the same as $\mathcal{A}$. There is no need for the embedding/projection mechanism.

To check that this machine only accepts strings $x: x \in 2^{\mathbb{Z}} \times 2^{\mathbb{Z}}$ it suffices to check that the only non-trivial SCC in $\mathcal{B}_{\rightarrow}^2$ is the diagonal (a subgraph isomorphic to $\mathcal{B}_{\rightarrow}$).

State-explosion is a major issue with our approach, it may well happen that some of the (intermediate) machines are so large that they cannot be handled.

One way of keeping the machines small is to rewrite the formula under consideration into an equivalent one that produces smaller machines. Typical example: checking for 3-cycles. One also should avoid prenex-normal-form like the plague and try to handle projections early.

If the outermost block of quantifiers is universal, the last check can be more naturally phrased in terms of Universality rather than Emptiness. In this case one should try to use Universality testing algorithms without complementation (e.g., the antichain method that avoids direct determinization).

We can easily augment our decision machinery by using additional predicates so long as these predicates are themselves synchronous.

This can be useful as a shortcut: instead of having a large formula that defines some property (which formula is then translated into a potentially large automaton), we just build the automaton directly from scratch and in an optimal way.

Interestingly, this trick can also work for properties that are not even definable in FOL. We can extend the expressibility of our language and get smaller machines for the logic part that way.

We can base a surjectivity test directly on the definition:

$$\forall x \exists z (z \rightarrow x)$$

Unfortunately, the universal quantifier up front means that we have to check whether a certain regular language is all of 2^* , a task that could be exponential.

Here is a trick: define **almost equality** ($x \stackrel{*}{=} y$) to mean that configurations x and y differ in only finitely many places.

Claim: Almost equality is not definable by any first-order formula.

However, it is known that the global map is surjective iff it satisfies the following modified injectivity condition:

$$\forall x, y, z (x \rightarrow z \wedge y \rightarrow z \wedge x \stackrel{*}{=} y \Rightarrow x = y)$$

Trick: While $\stackrel{*}{=}$ is not first-order definable over $\langle \mathbf{2}^{\mathbb{Z}}; \rightarrow \rangle$, it is a synchronous property.

Hence we can work over the larger structure $\langle \mathbf{2}^{\mathbb{Z}}; \rightarrow, \stackrel{*}{=} \rangle$, and, after negation, we only have to worry about a Σ_1 statement. All we need is a product construction followed by projections.