Supplementary material for
"Approximating attractors of Boolean networks by iterative CTL model checking"

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1 Proofs for the propositions

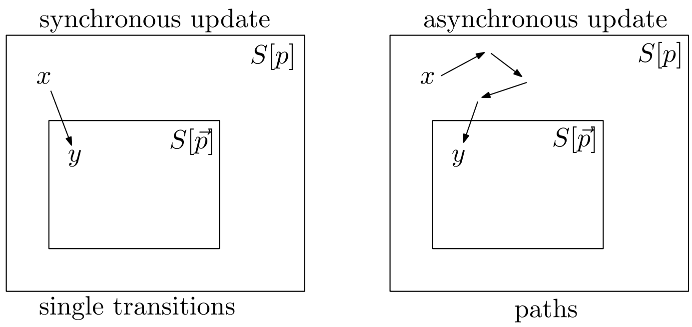


Figure 1: Since there every $x \in S[p]$ there is $y \in S[\vec{p}]$ such that there is a path from x to y there can not be an attractor that intersect $S[p] \setminus S[\vec{p}]$.

Proposition 1 (Fig. 1)**.** *If p is a trap space and $A \subseteq S[p]$ an attractor of $(S, \rightarrow)$ then $A \subseteq S[\vec{p}]$.*

Proof. The percolation $\vec{p}$ of a trap space p is defined by iterative substitution (see Sec. 3.1 in main text), i.e., by a sequence of trap spaces

$$p = p_0, p_1, p_2 \ldots, p_K = \vec{p}$$

where each pair p_k, p_{k+1} is a single percolation step and K the first index that satisfies $p_K = p_{K+1}$. Witout loss of generality we can assume that $K = 1$ because the statement is trivially true for $K = 0$ and will follow for $K > 1$ by induction. Hence, let p be a trap space whose percolation is achieved by a single step.

Synchronous update: Any state in the subspace p will reach the subspace $\vec{p}$ by a single transition because $f_v(x) = \vec{p}(v)$ holds for any v in the domain of

$\vec{p}$ (by definition of $\vec{p}$). Since $\vec{p}$ is a trap space this implies that there can not be a SCC in between p and $\vec{p}$, i.e., intersecting $S[p] \setminus S[\vec{p}]$.

Asynchronous update: For any state x in the subspace p and any variable v that is fixed in $\vec{p}$ there is a transition to some state y such that $\vec{p}(v) = y(v)$. Since this argument can be repeated for y there is a path from x to the subspace $\vec{p}$ (of at most $|D_{\vec{p}} \setminus D_p|$ transitions). As before, since $\vec{p}$ is a trap space there can be no attractor in between p and $\vec{p}$. □

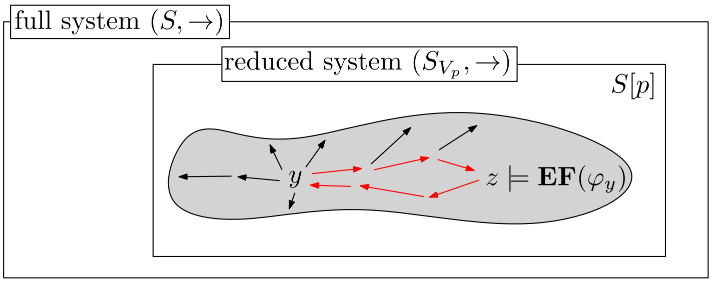


Figure 2: Iff all states z that are reachable from y satisfy $\mathbf{EF}(\varphi_y)$ then y belongs to an attractor $A \subseteq S[p]$.

Proposition 2 (Attractor State, Fig. 2)**.** *Let p be a trap space and $x \in S[p]$. The state x belongs to an attractor $A \subseteq S[p]$ of $(S, \rightarrow)$ iff*

$$TS = (S_{V_p}, \rightarrow, \{y\}) \models \mathbf{AG}(\mathbf{EF}(\varphi_y))$$

where $y \in S_{V_p}$ is the projection of $x \in S_V$ onto V_p, i.e., $y(v) := x(v)$ for all $v \in V_p$.

Proof. Let p be a trap space and $x \in S[p]$ with $x \in A$ for some attractor $A \subseteq [p]$. Since A is an attractor it is an inclusion-wise minimal trap set (by definition) and must therefore be strongly connected because otherwise it would contain a smaller trap set. Hence any state in A, and therefore any state reachable from x, has a path back to x. With respect to the reduced system $(S_{V_p}, \rightarrow)$ this means that any state $z \in S_{V_p}$ that is reachable from the projection y satisfies $\mathbf{EF}(\varphi_y)$. Since the states reachable from y are referenced by $\mathbf{AG}$ it follows that $\mathbf{AG}(\mathbf{EF}(\varphi_y))$ is true for y. So the transition system $(S_{V_p}, \hookrightarrow)$ with initial states $\{y\}$ satisfies $\models \mathbf{AG}(\mathbf{EF}(\varphi_y))$.

Let p be a trap space such that $TS = (S_{V_p}, \hookrightarrow, \{y\}) \models \mathbf{AG}(\mathbf{EF}(\varphi_y))$ where $y \in S_{V_p}$ is the projection of some state $x \in S_V$ onto V_p. Then all states reachable from y ($\mathbf{AG}$) have a path back to y ($\mathbf{EF}(\varphi_y)$ and hence y belongs to a strongly connected component A' (all states of A' are connected via y). A' must also be a trap set because the connectedness holds for every state reachable from y. Hence A' is an attractor. Note that $A' \subseteq S_{V_p}$ so far, but given p we can position A' in S_V, call it A, by assigning values to the variables D_p according to p such that $A \subseteq S_V$ is an attractor of $(S, \rightarrow)$ and $x \in A$. □

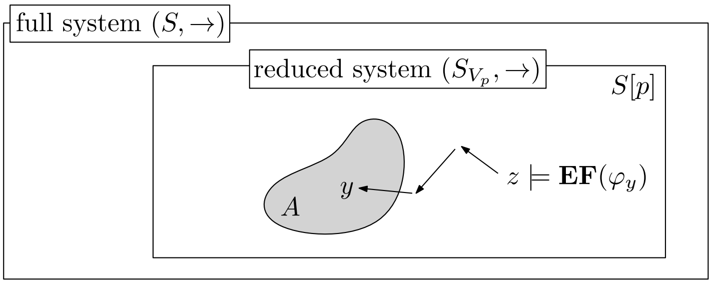


Figure 3: Iff for every state $z \in S_{V_p}$ there is a path to y then A is be the unique attractor of $S[p]$.

Proposition 3 (Univocality, Fig. 3)**.** *Let p be a trap space and $x \in A$ such that $A \subseteq S[p]$ is an attractor of $(S, \to)$. p is univocal in $(S, \to)$ iff*

$$TS = (S_{V_p}, \to, S_{V_p}) \models \mathbf{EF}(\varphi_y)$$

where $y \in S_{V_p}$ is the projection of $x \in S_V$ onto V_p.

Proof. If p is univocal in $(S, \to)$ then A is the only attractor of $(S, \to)$ and $x \in A$ can be reached from every state in S_{V_p}. Hence the transition system $(S_{V_p}, \to)$ with initial states S_{V_p} satisfies $\mathbf{EF}(\varphi_y)$.

If the transition system $TS = (S_{V_p}, \to, S_{V_p})$ satisfies $\mathbf{EF}(\varphi_y)$ then y belongs to the unique attractor $A' \subseteq S_{V_p}$ of $(S_{V_p}, \to)$. As in the previous proof we can use p to position A' in the original transition system $(S, \to)$ and this set A will be the unique attractor $A \subseteq S[p]$ and $x \in A$ holds. □

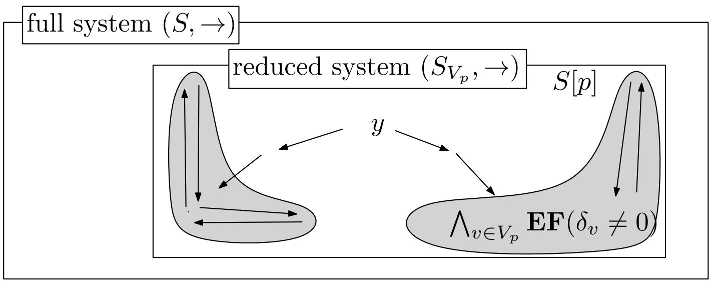


Figure 4: The attractors of a trap space p are faithful iff for every $y \in S_{V_p}$ and $v \in V_p$ there is a path to a state z that satisfies $z \models \delta_v \neq 0$.

Proposition 4 (Faithfulness, Fig. 4)**.** *A trap space p is faithful in $(S, \to)$ iff*

$$TS = (S_{V_p}, \to, S_{V_p}) \models \bigwedge_{v \in V_p} \mathbf{EF}(\delta_v \neq 0).$$

Proof. Let p be faithful and $x \in S_{V_p}$ arbitrary. We want to prove that

$$x \models \bigwedge_{v \in V_p} \mathbf{EF}(\delta_v \neq 0). \tag{1}$$

Since p is faithful, every attractor $A \subseteq S[p]$ satisfies $Sub(A) = p$. Let A be an attractor of $S[p]$ that is reachable from x. Since $Sub(A) = p$ there are $x_1, x_2 \in A$ such that $x_1(v) \neq x_2(v)$ for every $v \in V_p$. Since x_1, x_2 belong to A there is a path between x_1 and x_2 and hence a transition in which the activity of $v \in V_p$ changes. Let $x_1' \to x_2'$ be such that $x_1'(v) \neq x_2'(v)$. Hence $\delta_v(x_1') \neq 0$. Since A is reachable from x and x_1' from x it follows that $x \models \mathbf{EF}(\delta_v \neq 0)$. Since $v \in V_p$ was chosen arbitrarily, Eq. 1 holds.

For the other direction let the transition system $(S_{V_p}, \to)$ with initial states S_{V_p} be such that Eq. 1 holds for every $x \in S_{V_p}$. The equation therefore holds in particular for every $x \in A$ where A is an attractor of $S[p]$. Hence, for every $v \in V_p$ and attractor A there is $y \in A$ such that $\delta_v(y) \neq 0$ and hence a transition $y \to y'$ such that $y(v) \neq y'(v)$. Hence $Sub(A) = p$ and so p is faithful. □

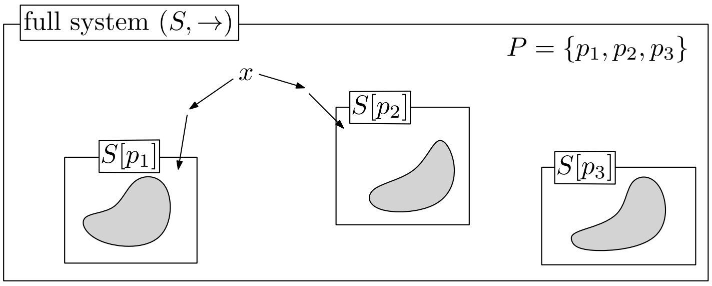


Figure 5: The trap spaces $P := \{p_1, p_2, p_3\}$ are complete iff for every initial state x there is a path to some trap space $p \in P$.

Proposition 5 (Completeness, Fig. 5)**.** *A set of trap spaces P is complete in $(S, \to)$ iff*

$$TS = (S, \to, S) \models \bigvee_{p \in P} \mathbf{EF}(\varphi_p).$$

Proof. Let P be a complete set or trap spaces of $(S, \to)$ and $x \in S$ arbitrary. We want to show that

$$x \models \bigvee_{p \in P} \mathbf{EF}(\varphi_p). \tag{2}$$

Let A be an arbitrary attractor that is reachable from x. Since P is complete there is $p \in P$ such that $A \subseteq S[p]$. Since there is a path from x to A it follows that $x \models \mathbf{EF}(\varphi_p)$ and therefore Eq. 2 holds.

For the other direction note that if Eq. 2 holds for all $x \in S$ that it holds in particular for all states of every attractor. But if for every attractor A there is a $p \in P$ such that there is a path from A to $S[p]$ then $A \subseteq S[p]$ and P is complete. □

Proposition 6 (Refinement of Complete Sets, Fig. 6)**.** *Let $P \subseteq S_F^\star$ be complete in $(S, \to)$ and $p \in P$ some trap space. If $Q \subseteq S_{F_p}^\star$ is complete in $(S_{V_p}, \to)$ then $P' := (P \setminus \{p\}) \cup \{q \sqcap p \mid q \in Q\}$ is complete in $(S, \to)$.*

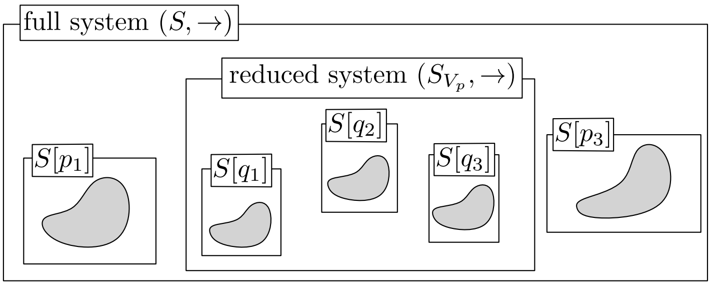
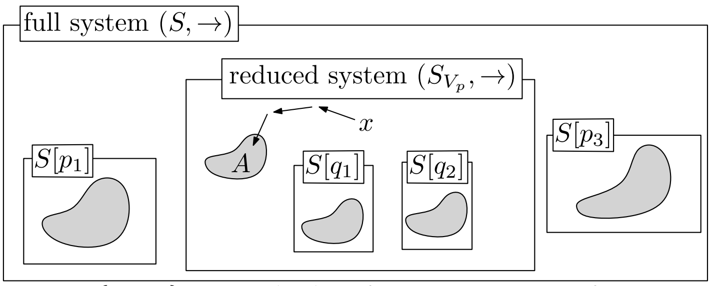


Figure 6: Refinement works by replacing a trap space p by some set of trap spaces that is complete in S_{V_p}.

Proof. Let P be a complete set of trap spaces of $(S, \to)$ and $p \in P$ arbitrary. Consider the reduced system (F_p, V_p) and its trap spaces $S^\star_{F_p}$ and let $Q \subseteq S^\star_{F_p}$ be complete in $(S_{V_p}, \to)$. Note that we defined subspaces as mappings $p : D_p \to \mathbb{B}$. Hence, although a trap space q of (V_p, F_p) is well-defined when considered as a subspace of (V, F), we need to intersect it with p to assign values to the variables that are implicitly fixed in q when considered as a subspace of (V_p, F_p). The completeness of P' then follows from the completeness of Q in $(S_{V_p}, \to)$ because the dynamics inside p is identical with the dynamics of the reduced system (V_p, F_p). □



$Q = \{q_1, q_2\}$ $\quad$ $\min(S^\star_F) = \{p_1, p_2, p \sqcap q_1, p \sqcap q_2\}$

Figure 7: .

Proposition 7 (Failure Criterion, Fig. 7)**.** *If there is a trap space p such that $\min(S^\star_{F_p})$ is not complete in $(S_{V_p}, \to)$ then $\min(S^\star_F)$ is not complete in $(S, \to)$.*

Proof. Suppose p is such that $Q := \min(S^\star_{F_p})$ is not complete in $(S_{V_p}, \to)$. The main observation is that $P := \{p \sqcap q \mid q \in \min(S^\star_{F_p})\} \subseteq \min(S^\star_F)$. That is, if the subspace Q are positioned correctly within $(S, \to)$, i.e., intersected with p, then they are also minimal trap spaces of (V_p, F_p). The statement then follows because if Q is not complete in $(S_{V_p}, \to)$ then there is a state $x \in S[p]$ that can not reach any trap space in P. But, since p is a trap space x must reach some attractor A which is therefore outside of P and hence outside of $\min(S^\star_F)$ which implies that $\min(S^\star_F)$ is not complete in $(S, \to)$. □

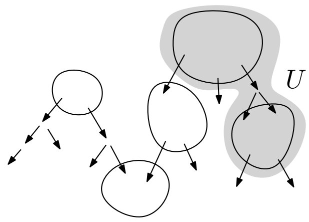


Figure 8: A schematic drawing of the interaction graph, enclosed are SCCs, and an autonomous set U.

Proposition 8 (Fig. 8)**.** *Let U be autonomous and $Q := \min(S^\star_{F_{|U}})$ the minimal trap spaces of the restriction $(U, F_{|U})$.*

(a) If Q is complete in $(S_U, \to)$ then Q is also complete in $(S, \to)$.
(b) If Q is not complete in $(S_U, \to)$ then $\min(S^\star_F)$ is not complete in $(S, \to)$.

Proof. **Observations:** The dynamics in the restricted and full transition systems can be related to each other. For any path $(y_0, y_1, \dots, y_k)$ of $(S_U, \to)$ and any $x_0 \in S[y_0]$ there is a path $(x_0, x_1, \dots, x_k)$ of $(S, \to)$ such that $x_i(u) = y_i(u)$ for all $u \in U$ and $1 \le i \le k$. Also, for any path $(x_0, x_1, \dots, x_k)$ of $(S, \to)$ there is a unique path $(y_0, y_1, \dots, y_r)$ in $(S_U, \to)$ with $r \le k$, $x_0 \in S[y_0]$ and $x_k \in S[y_r]$ that describes the projected dynamics. It follows that a trap space q of $(U, F_{|U})$ is also a trap space of (V, F) because otherwise we could consider the projection of the path that proves that q is not a trap space in (V, F) and deduce that q is not a trap space in $(U, F_{|U})$, a contradiction. Hence Q is a set of trap spaces of (V, F).

Proof of (a): Let Q be complete in $(S_U, \to)$ and $x \in S$ an arbitrary state. We want to show that there is a path from x to some $q \in Q$. Let y be the projection of x onto U. Since Q is complete there is a path $(y_0, y_1, \dots, y_k)$ such that $y_0 = y$ and $y_k \in S[q]$ for some $q \in Q$. By the observations above there is therefore a path $(x_0, x_1, \dots, x_k)$ with $x_0 = x$ and $x_k \in S[q]$. Hence Q is complete in $(S, \to)$.

Proof of (b): The main observation is that since U is autonomous and since $Q = \min(S^\star_{F_{|U}})$ it follows that for any $p \in \min(S^\star_F)$ there is $q \in Q$ such that $p \le q$. If Q is not complete in $(S_U, \to)$ then there is $y \in S_U$ that can not reach any $q \in Q$. Any x whose projection on U is equal to y can therefore not reach any $q \in Q$ in $(S, \to)$. Hence it can not reach any $p \in \min(S^\star_F)$ (because for any p there is a $q \in Q$ with $q \le p$). Hence $\min(S^\star_F)$ is not complete in $(S, \to)$. □

Proposition 9 (Fig. 8)**.** *Let $U \subseteq V$. The following statements are equivalent:*

(a) U is a minimal autonomous set of $(V, \to)$.
(b) U is autonomous and $U \in SCCs(V, \to)$.

Proof. **(a) ⇒ (b):** Let U be minimal and autonomous in $(V, \to)$. We need to show that U is strongly connected. Let $u, v \in U$ be arbitrary. If there is no path from u to v then u is not above v and so $Above(v)$ is a proper autonomous subset U, a contradiction to minimality. Hence, there is a path from u to v and so U is stronlgy connected.

(b) ⇒ (a): Let U be autonomous and strongly connected. We need to show that U does not contain a smaller autonomous set. Assume there is $U' \subset U$ with $U' \neq U$ and U' is autonomous. Let $u \in U \setminus U'$. Since U is strongly connected there is a path from u to any $u' \in U'$. Hence u is above u' and so $u \in U'$ which contradicts $u \in U \setminus U'$. Hence such U' does not exist and U is minimal. □

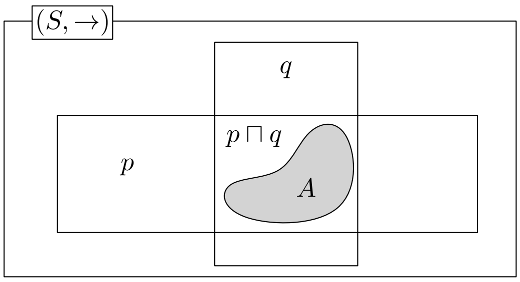


Figure 9: For every attractor A there are $p \in P$ and $q \in Q$ such that $A \subseteq S[p]$ and $A \subseteq S[q]$. Hence p and q are consistent and $A \subseteq S[p \sqcap q]$.

Proposition 10 (Fig. 9)**.** *If $P, Q \subseteq S_F^\star$ are complete in $(S, \to)$ then $P \sqcap Q := \{p \sqcap q \mid p \in P, q \in Q : p$ and q are consistent$\}$ is also complete in $(S, \to)$.*

Proof. Let A be an attractor of $(S, \to)$. Since P and Q are complete there are $p \in P$ and $q \in Q$ such that $A \subseteq S[p]$ and $A \subseteq S[q]$. Hence, p and q are consistent and $(p \sqcap q) \in P \sqcap Q$. Hence $P \sqcap Q$ is complete in $(S, \to)$. □

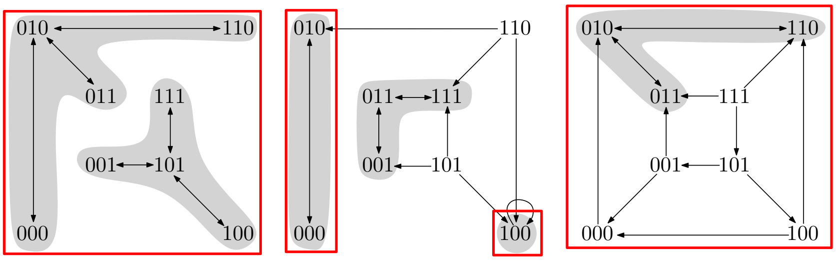
Proposition 11. *Let $(Z, \rhd)$ be the condensation graph of a constant-free network (V, F). A set $U \subseteq V$ is minimal and autonomous iff $U \in Z$ and $Lay(U) = 1$.*

Proof. Let U be minimal and autonomous. It follows from Prop. 9 that $U \in SCCs(V, \to)$. We need to show that $Lay(U) = 1$. If $Lay(U) > 1$ then $Above(U) \supseteq U$ with $Above(U) \neq U$ which contradicts U being autonomous.

For the other direction assume that $U \in Z$ and $Lay(U) = 1$. We will again use Prop. 9. Note that $Z = SCCs(V, \to)$. Also, U is autonomous because if $Above(U) \supset U$ with $U \neq Above(U)$ then $Lay(U) > 1$, i.e., there would have to be an SCC above U. Note that the last deduction uses the fact that (V, F) is constant-free. □

2 Update Functions

The update functions for the three Boolean networks are given in Fig. 10.



(a) Not univocal (b) Not complete (c) Not faithful

Figure 10: The asynchronous STGs of the three Boolean networks given in Fig. 1 of the main text.

$$\begin{aligned} f_1 &:= \overline{v_1}\,\overline{v_2}v_3 + \overline{v_1}v_2\overline{v_3} + v_1\overline{v_2}\,\overline{v_3} + v_1v_2v_3 \\ f_2 &:= \overline{v_1}\,\overline{v_2}\,\overline{v_3} + \overline{v_1}v_2v_3 + v_1\overline{v_2}v_3 + v_1v_2\overline{v_3} \\ f_3 &:= \overline{v_1}\,\overline{v_2}v_3 + \overline{v_1}v_2\overline{v_3} + v_1\overline{v_2}\,\overline{v_3} + v_1v_2v_3 \end{aligned} \tag{a}$$

$$\begin{aligned} f_1 &:= \overline{v_1}\,v_2v_3 + v_1\overline{v_2}\,\overline{v_3} \\ f_2 &:= \overline{v_1}\,\overline{v_2} + v_1v_3 \\ f_3 &:= \overline{v_1}\,v_3 + v_1v_2 \end{aligned} \tag{b}$$

$$\begin{aligned} f_1 &:= \overline{v_1}\,v_2\overline{v_3} \\ f_2 &:= \overline{v_1} + \overline{v_3} \\ f_3 &:= \overline{v_1}\,v_2\overline{v_3} \end{aligned} \tag{c}$$