Shapes of dependencies in reaction systems ♻️⛓⛓🌼

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Structure 🧬 vs behaviour 🏃‍♀️

- What are the consequences of structural restrictions on the behaviour of RS?

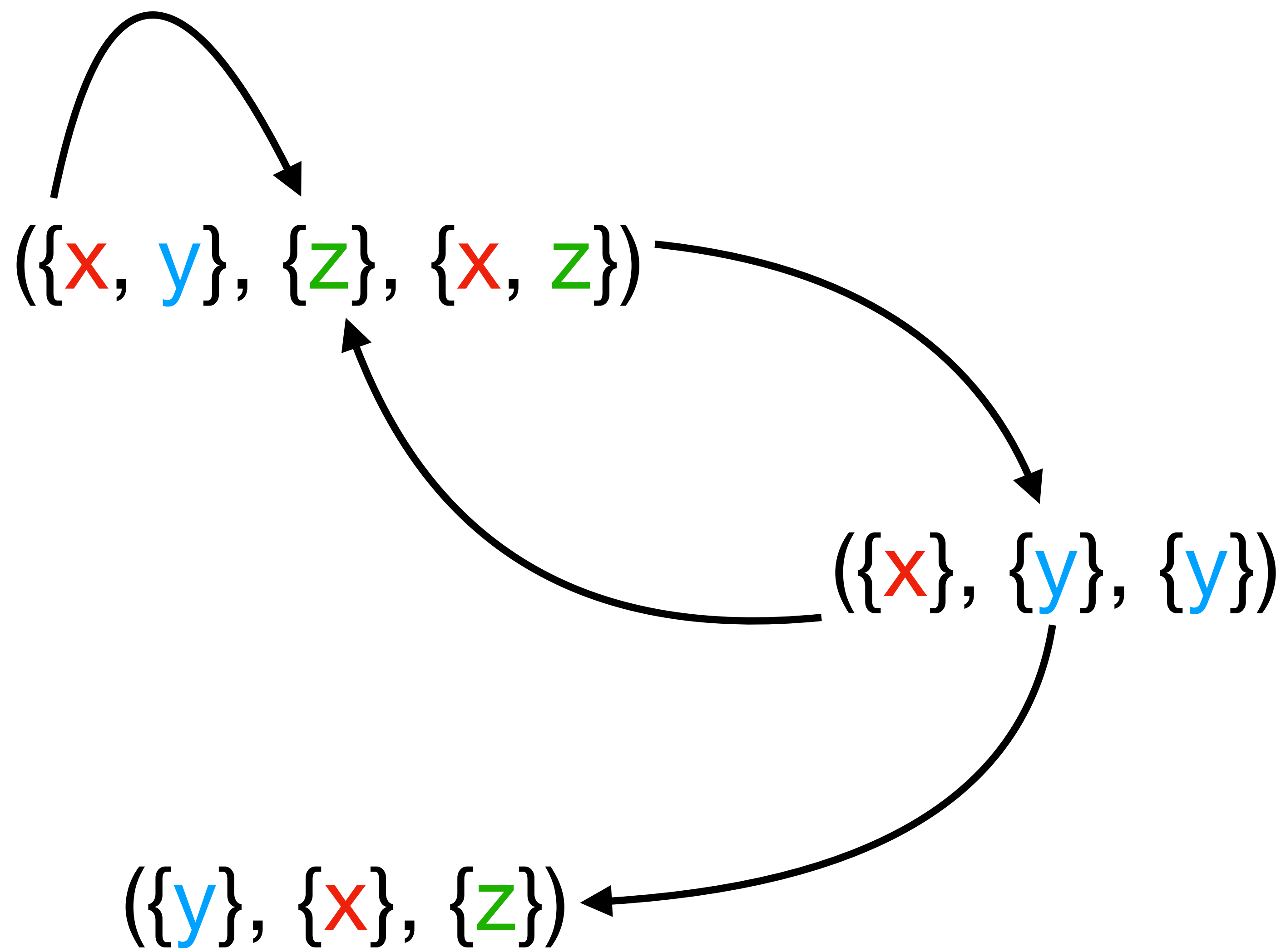
- Example: minimal RS cannot compute all result functions

- But, for each RS $\mathcal{A}$ there exists a minimal RS $\mathcal{B}$ such that $\mathrm{res}_{\mathcal{A}}^{k}(T) = \mathrm{res}_{\mathcal{B}}^{2k}(T)$ for all $k \in \mathbf{N}$ and state T of $\mathcal{A}$

Positive dependency graph 🧬

- Vertices = set of reactions A
- There is an oriented edge $a \rightarrow b$ iff at least one product of reaction a is a reactant of reaction b

Positive dependency graph 🧬

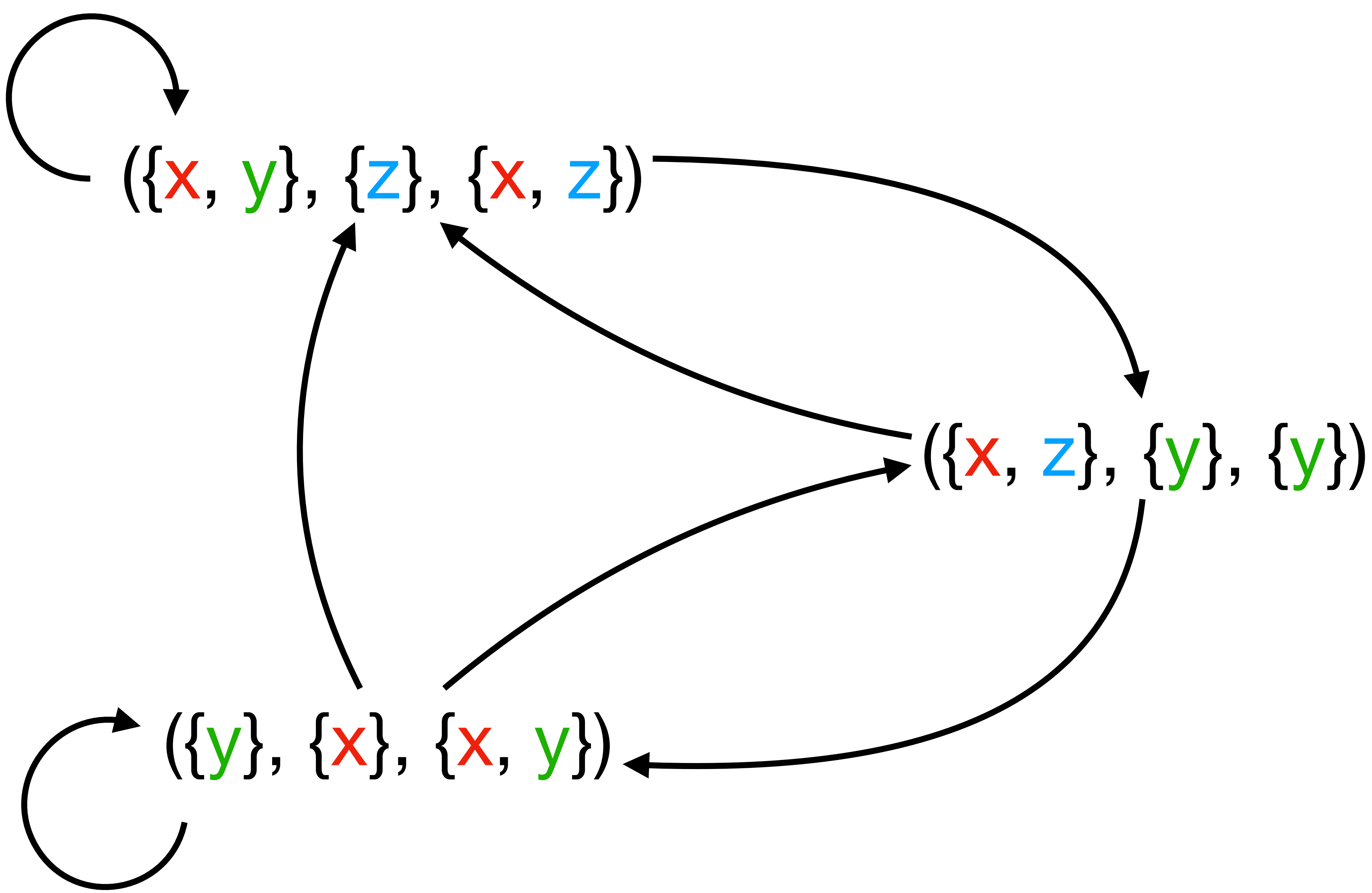


Self-sustaining cycle ♻️

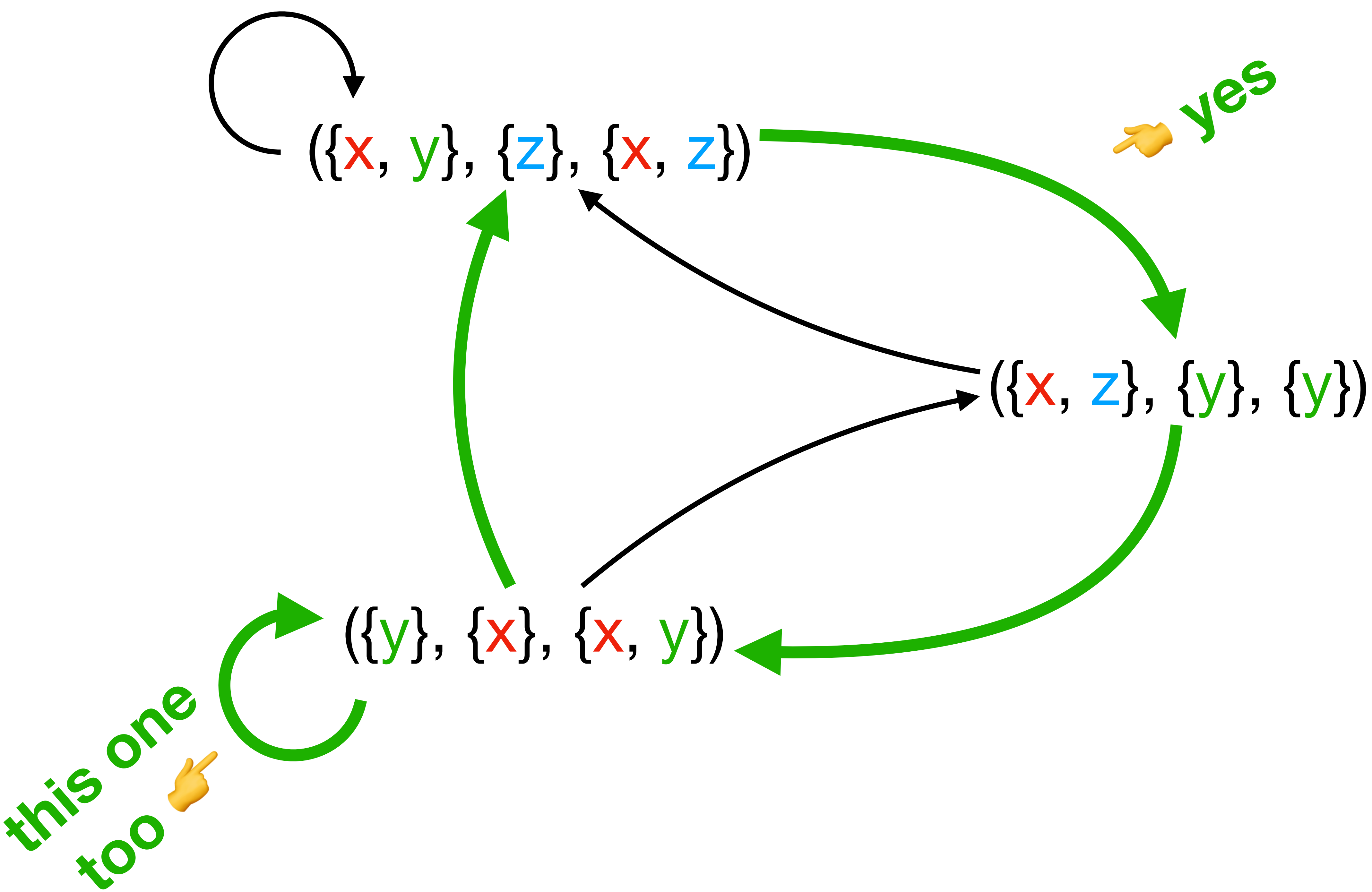
A path in the (positive) dependency graph
such that for each edge $a \rightarrow b$ we have:

- Reaction a produces all reactants of b: $R_b \subseteq P_a$
- Reaction a doesn't produce any inhibitor for b: $P_a \cap I_b = \varnothing$

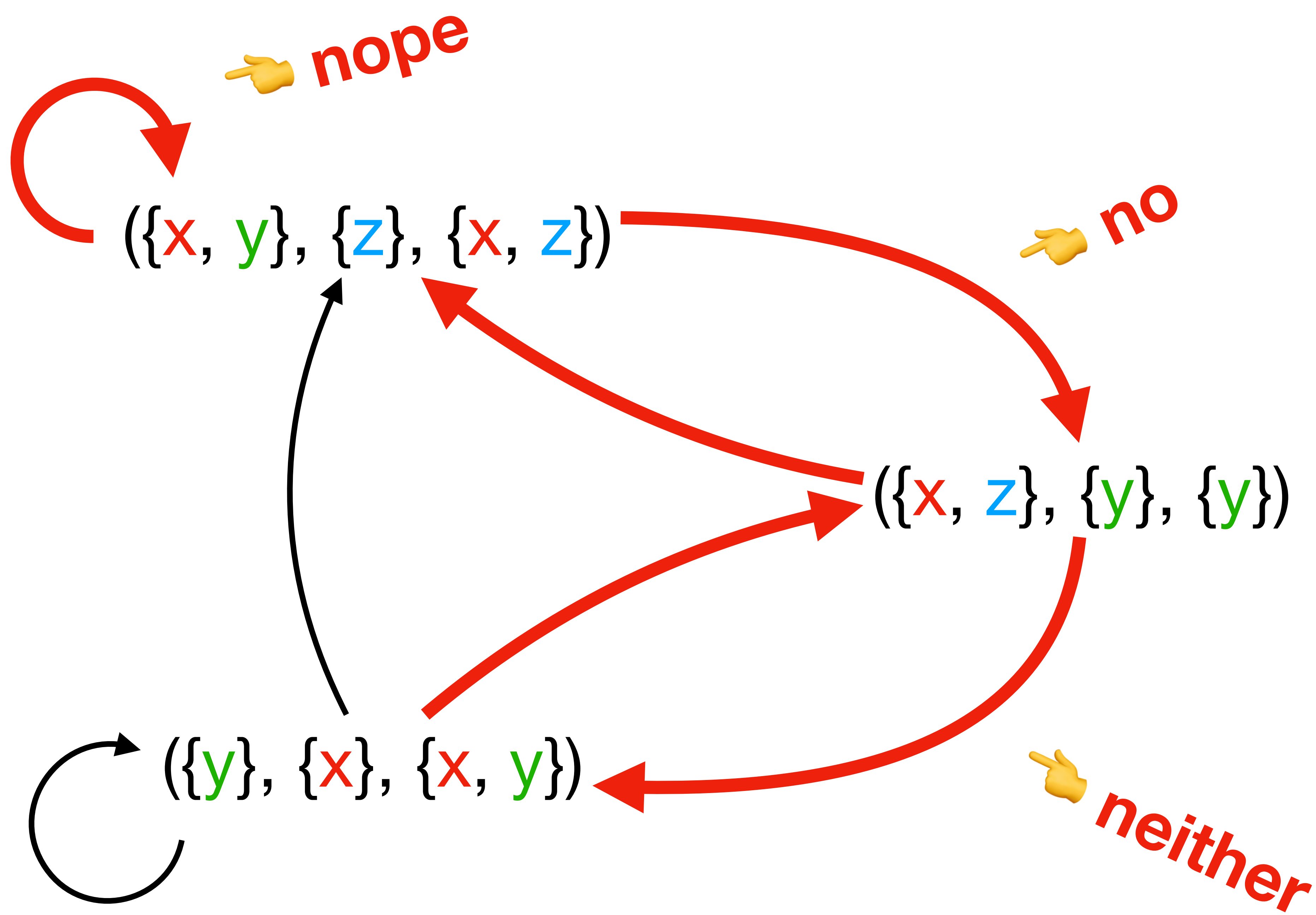
Self-sustaining cycle ♻️



Self-sustaining cycle ♻️



Self-sustaining cycle ♻️

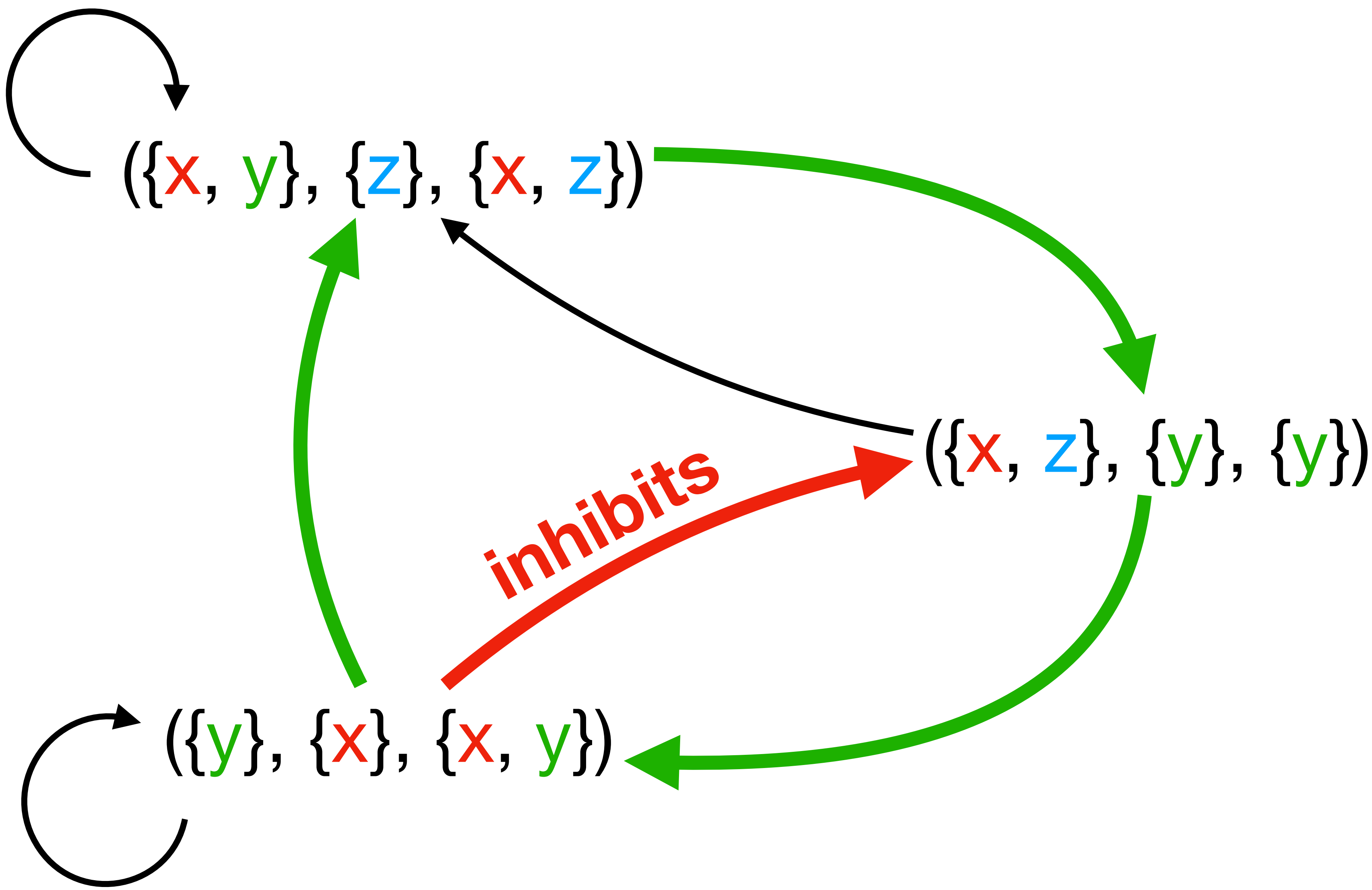


Non self-inhibiting reactions 🧬

A set of reactions $\{a_1, a_2, \ldots, a_n\}$ such that no reaction produces inhibitors for any other reaction in the set:
$P_i \cap P_j = \varnothing$ for all i, j belonging to the set

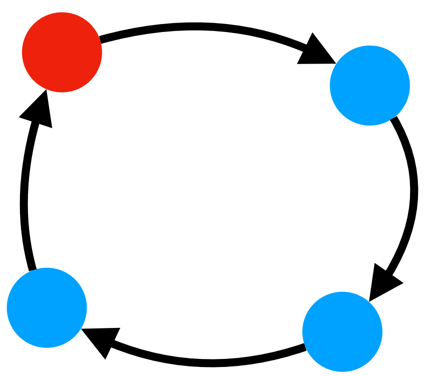
Otherwise, the set is called self-inhibiting

Self-sustaining but also self-inhibiting cycle 🧬



Simple cyclical dependencies ♻️

RS with a single self-sustaining, non self-inhibiting dependency cycle



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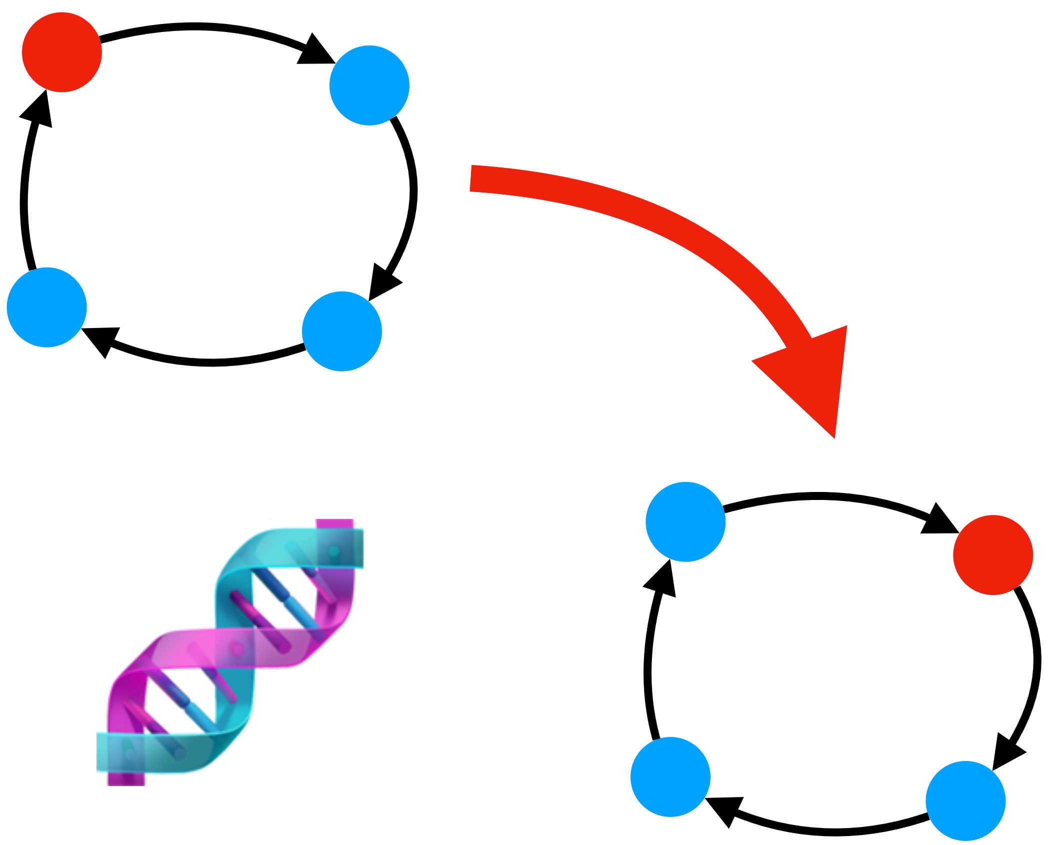

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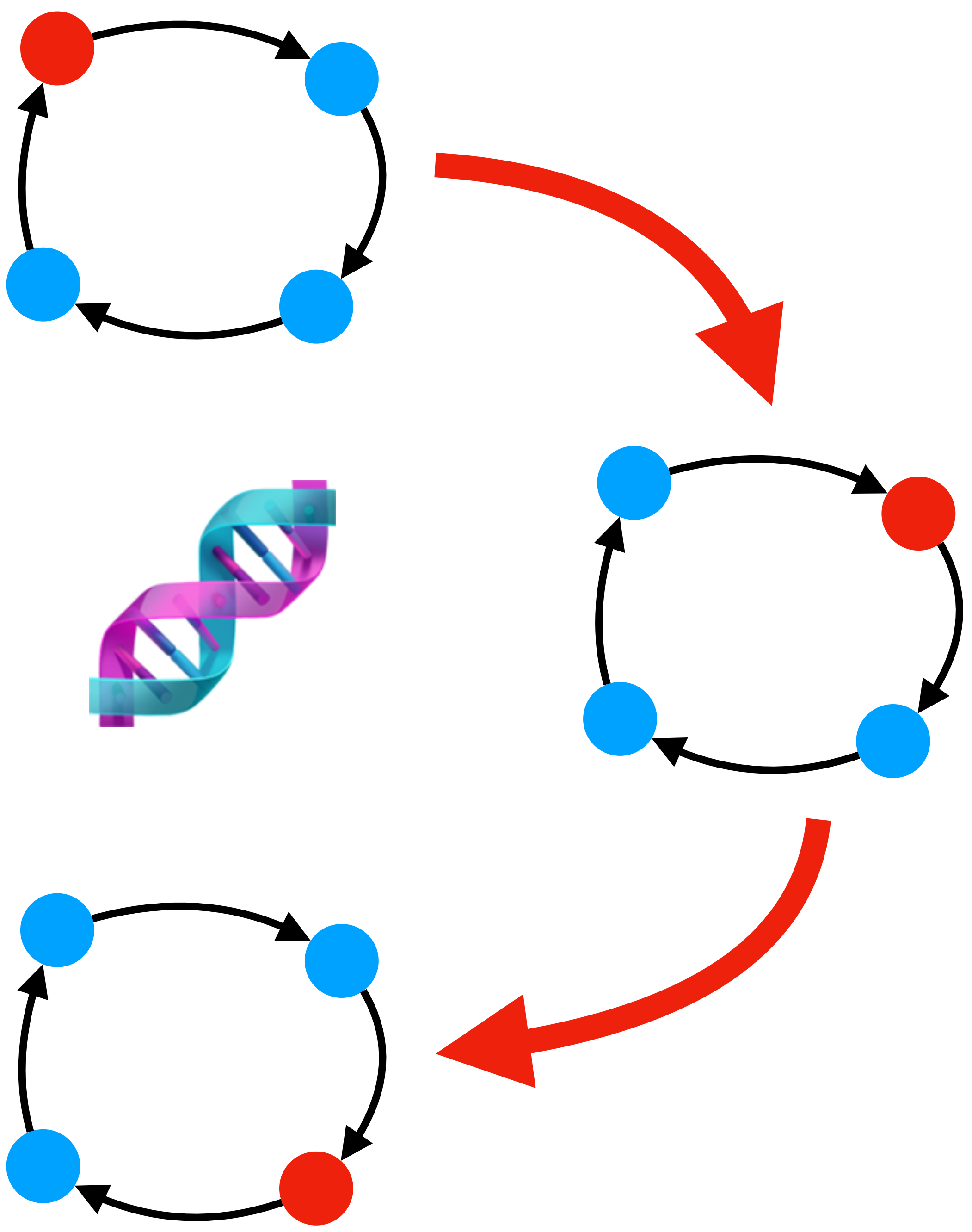

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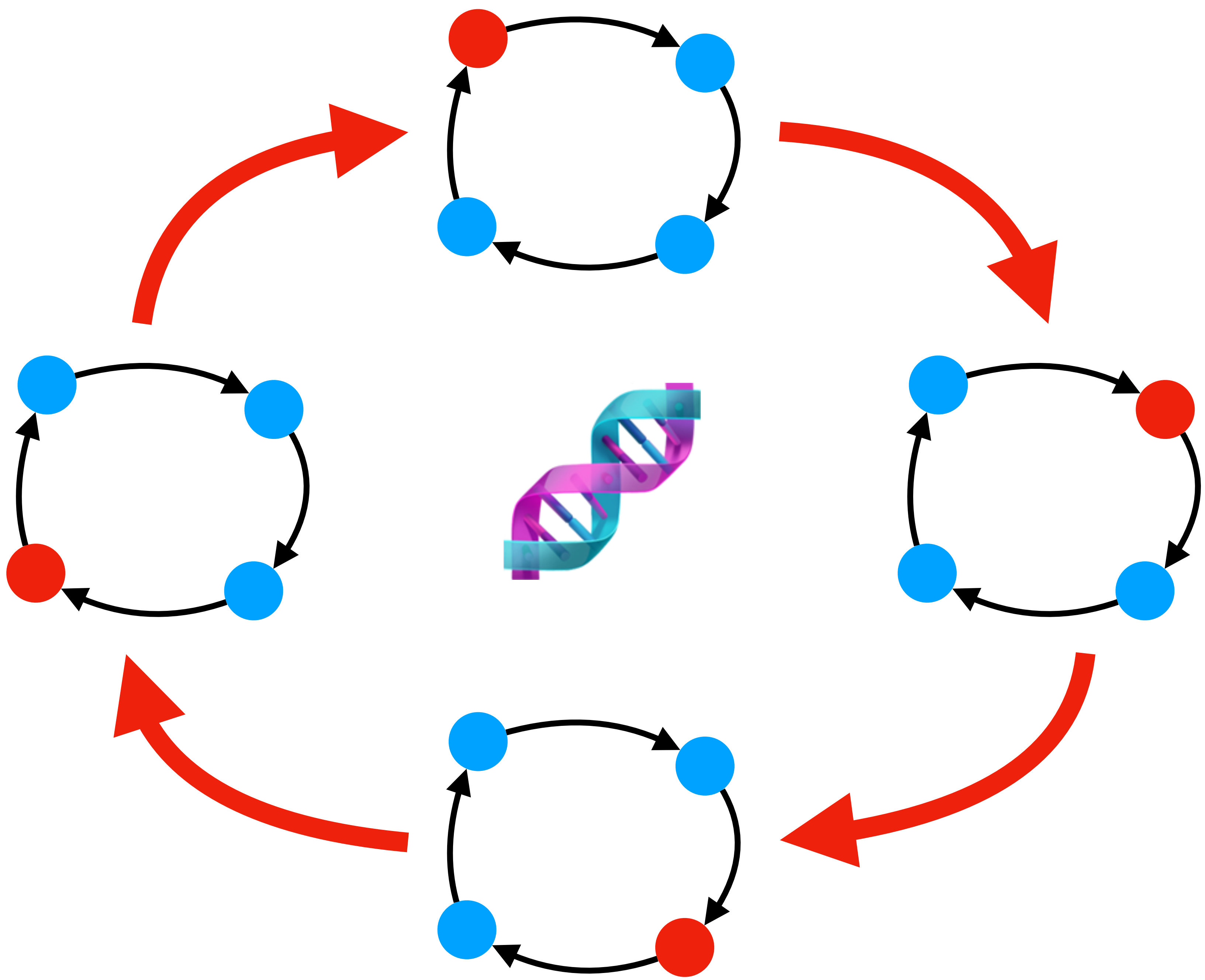

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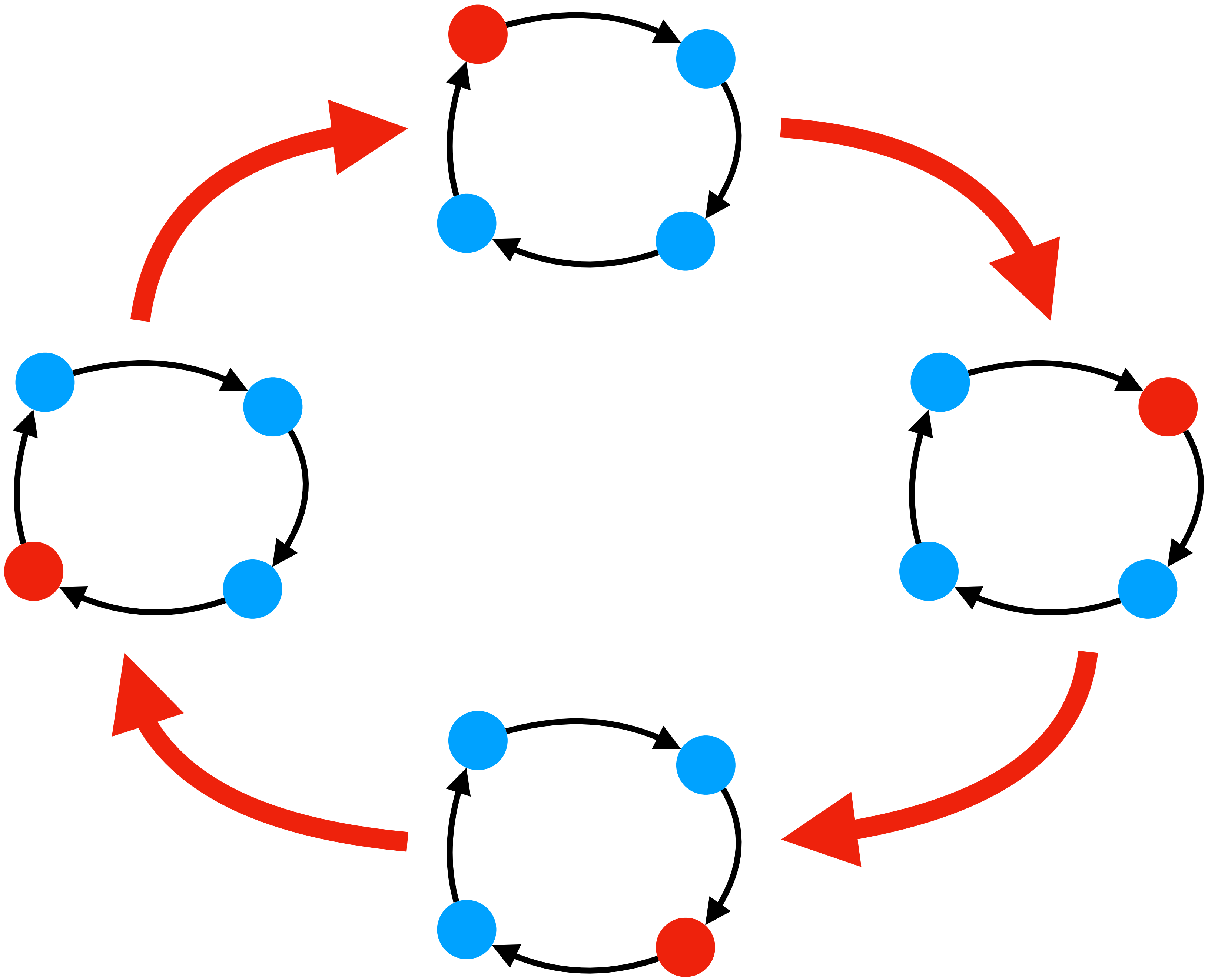

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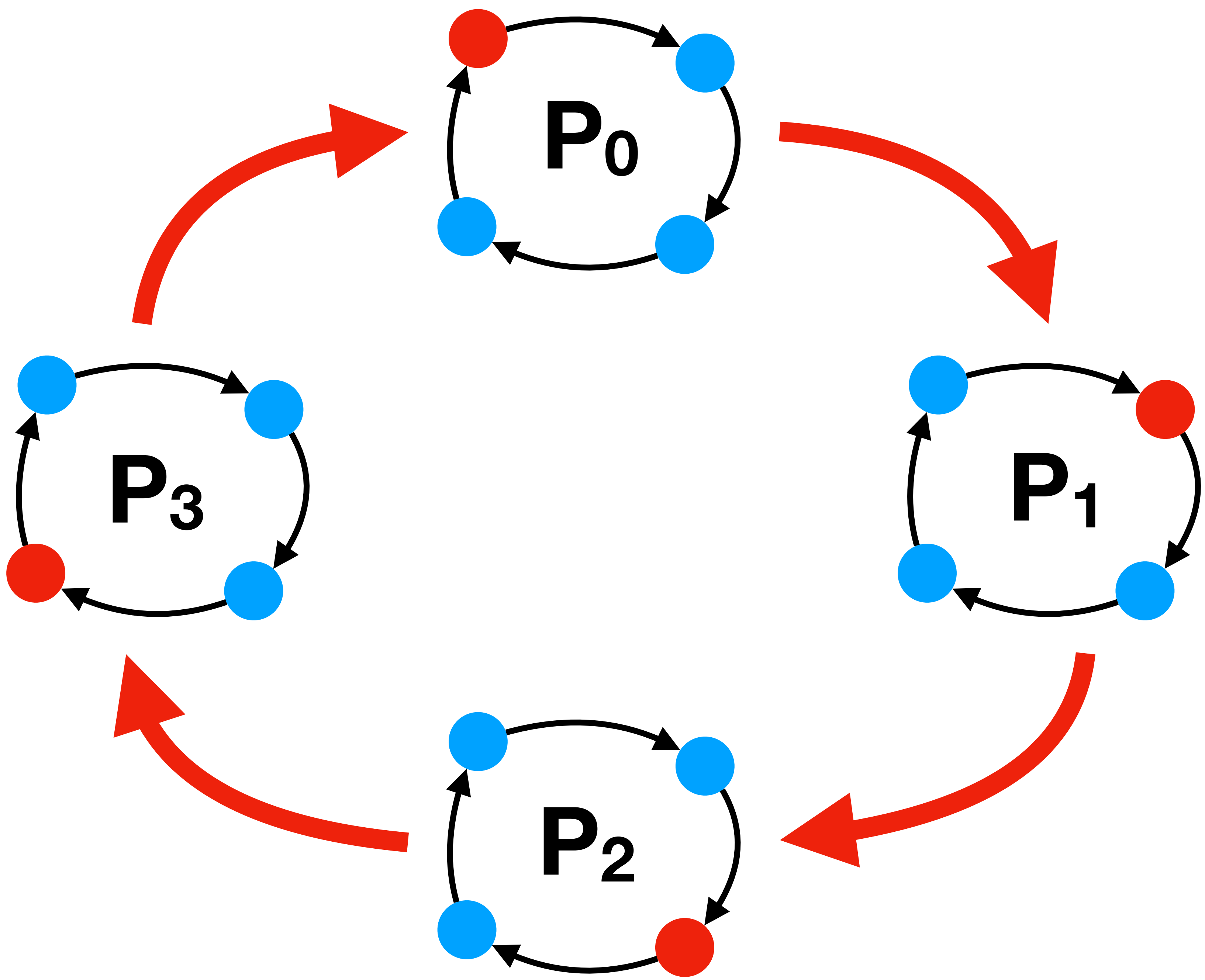


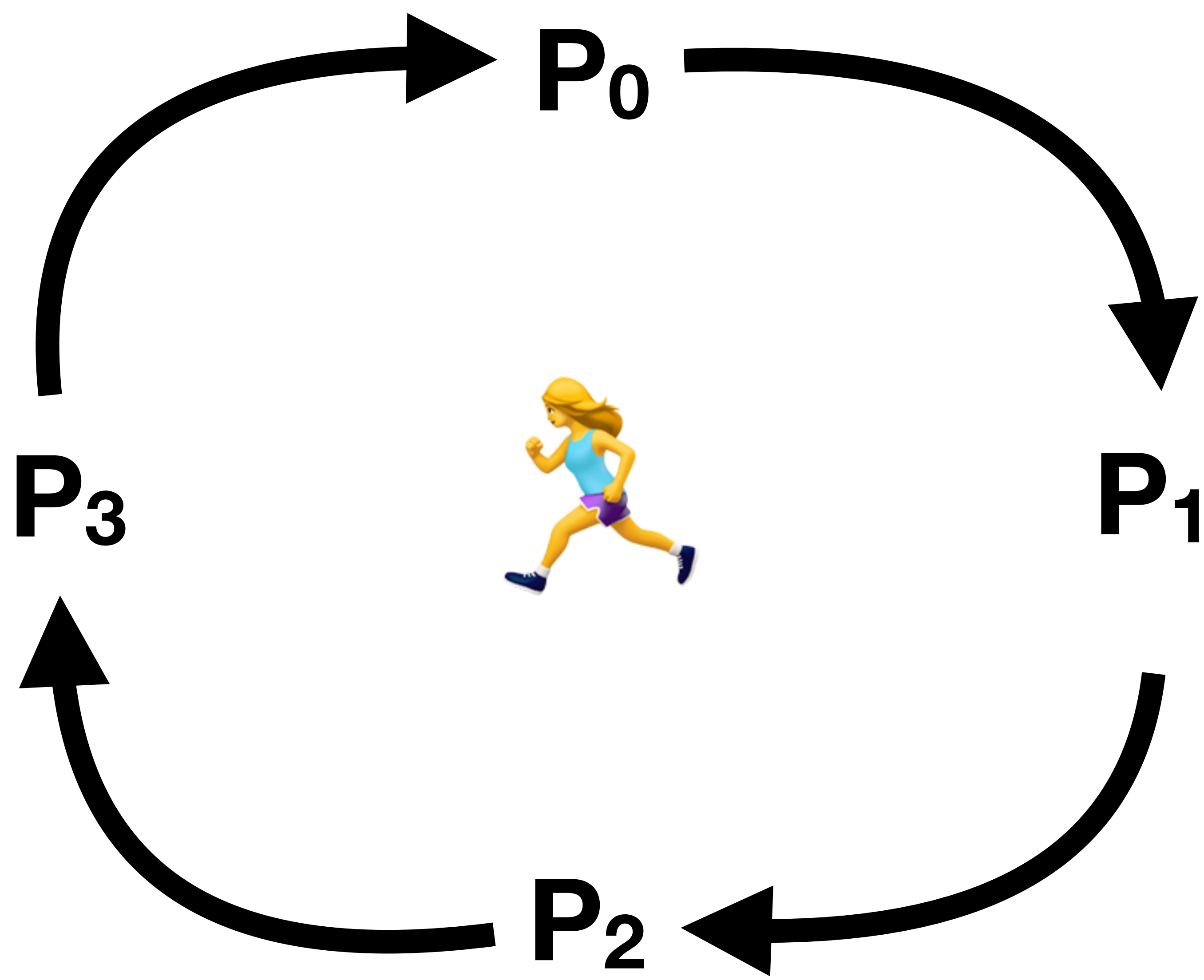
RS with a single self-sustaining, non self-inhibiting dependency cycle

P_0

P_3 P_1

P_2

RS with a single self-sustaining, non self-inhibiting dependency cycle



Rotations and cycles

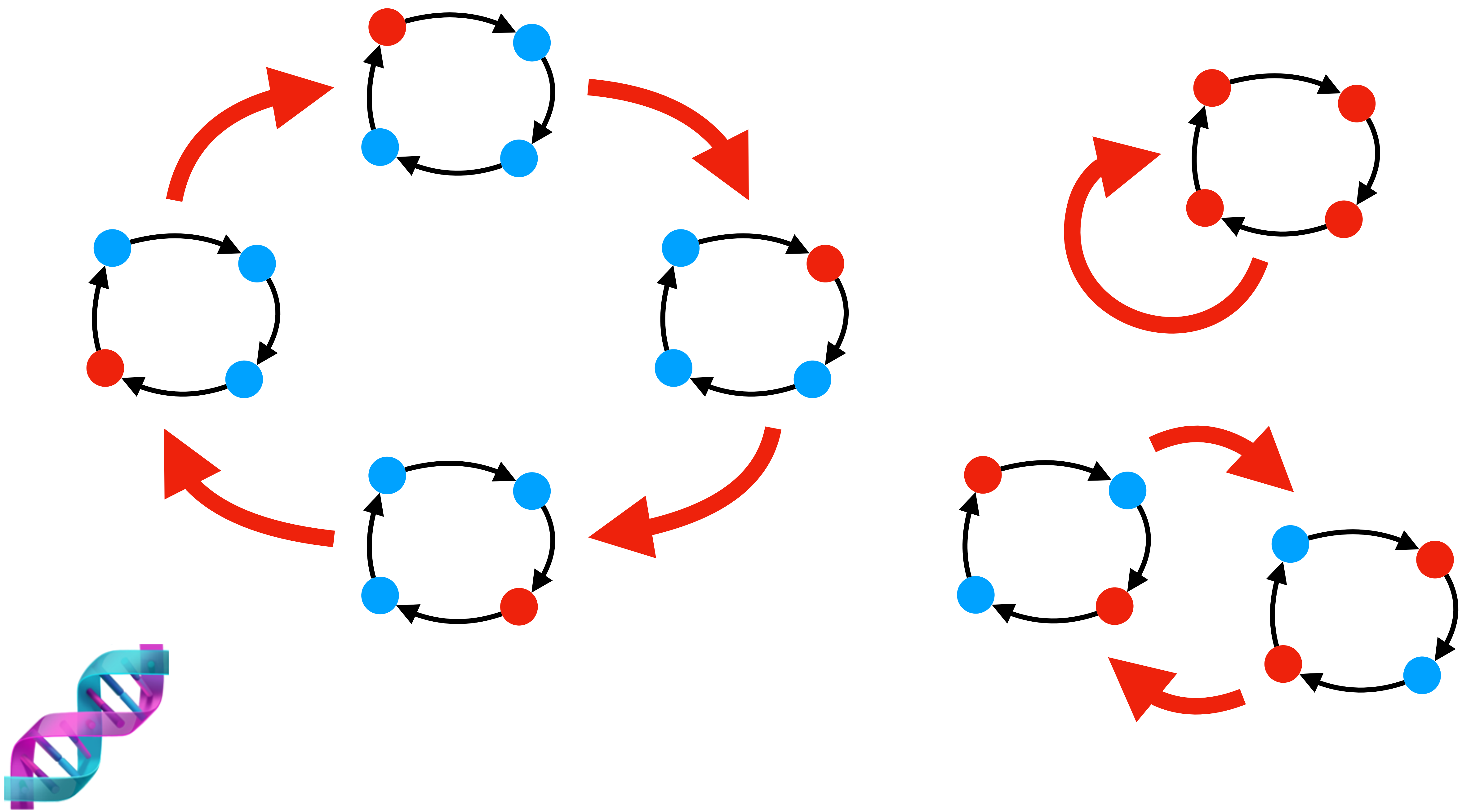
The rotations of active reactions along the (unique) cycle in the dependency graph 🧬 starting from a given configuration correspond to transitions in the graph of the dynamics 🏃‍♀️

♻️ Theorem

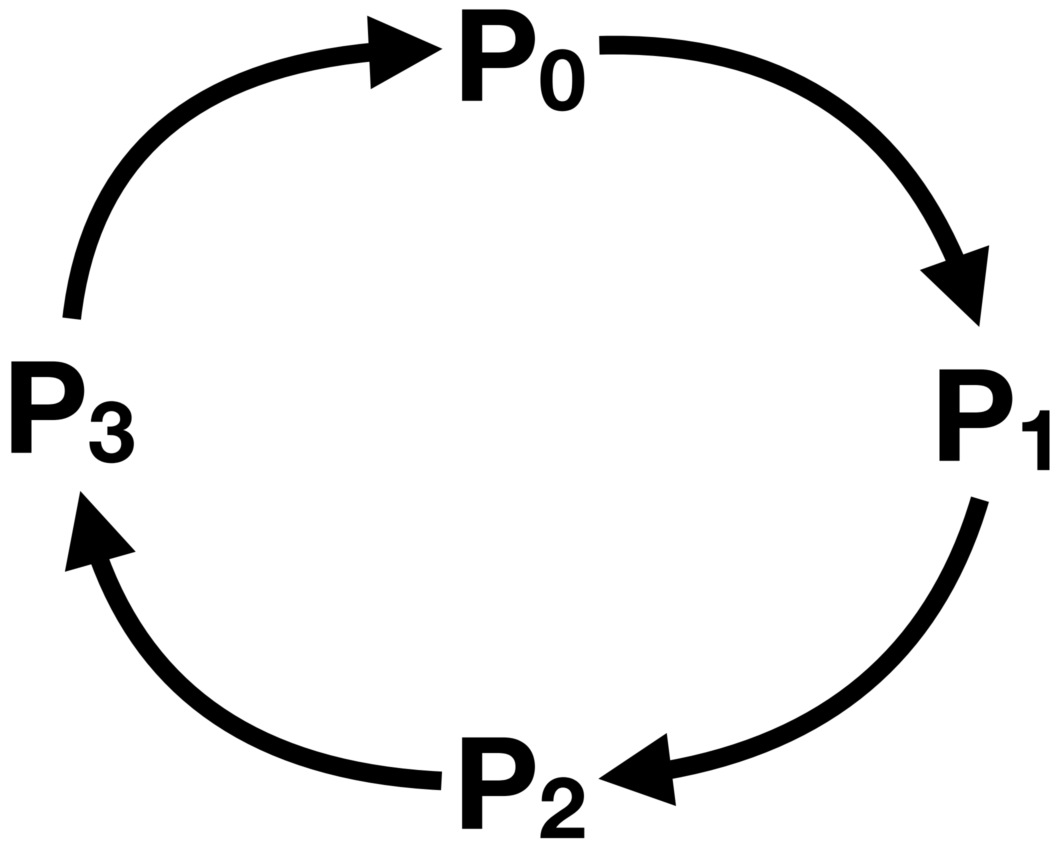
🧬 **IF** the dependency graph of a RS consists only one self-sustaining, non-self-inhibiting cycle of length n

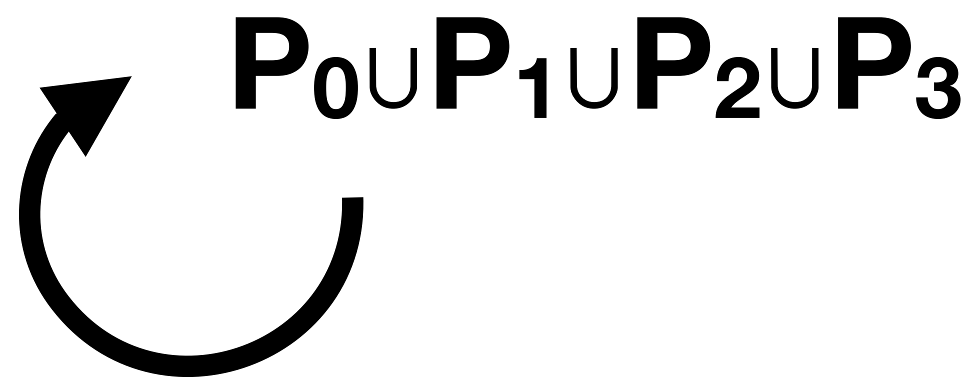
🏃‍♀️ **THEN** the dynamics of the RS only contains cycles of length dividing n, and there is at least one such cycle for each divisor of n

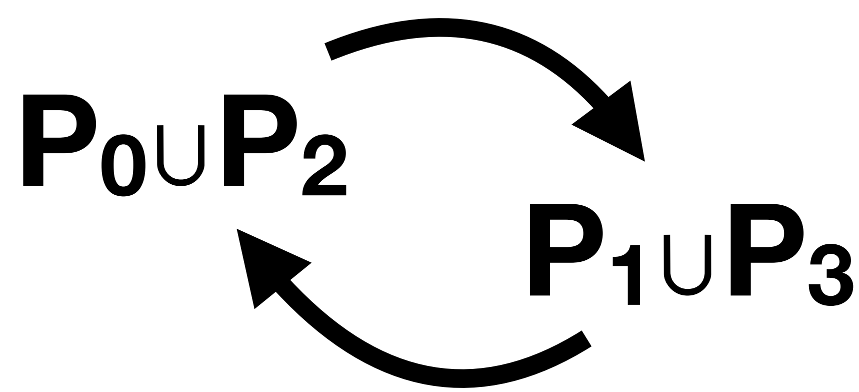
Length of the cycles



Length of the cycles







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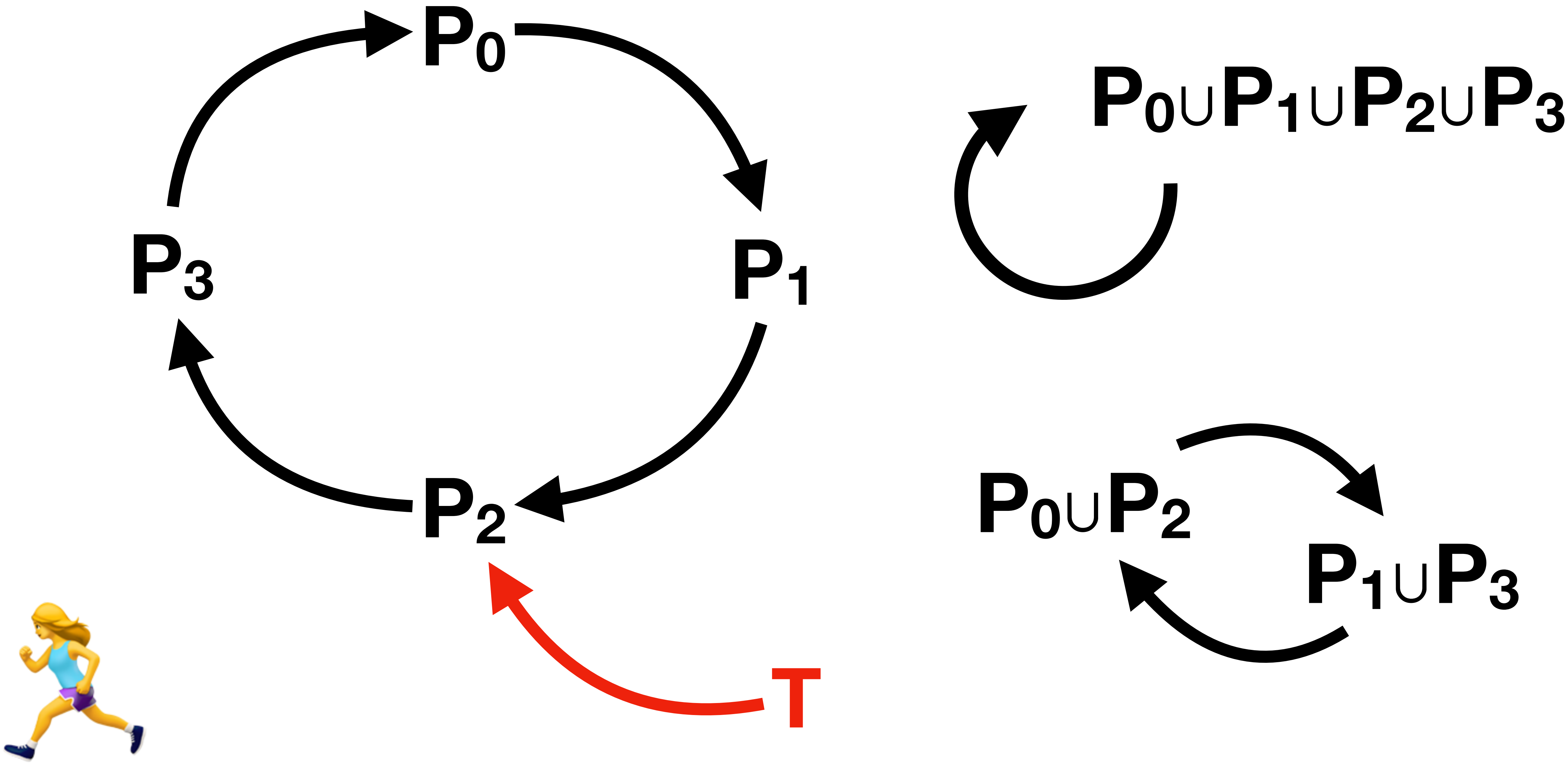
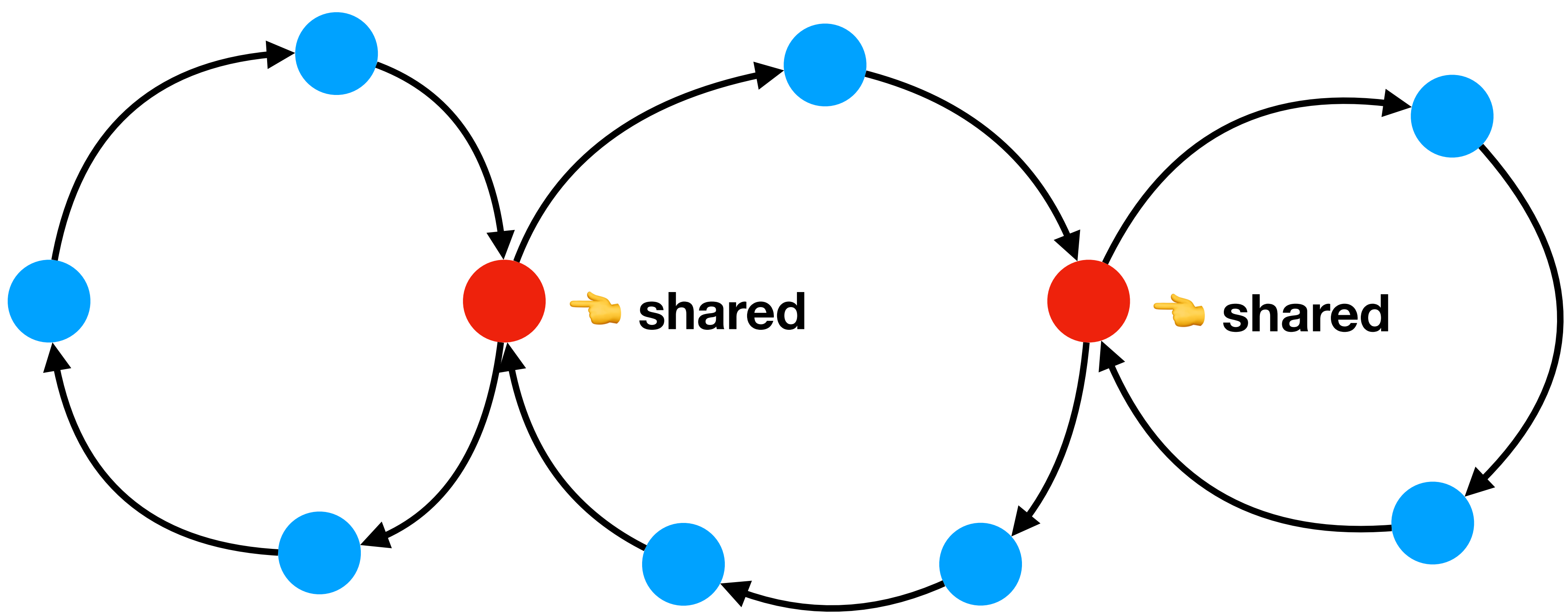


Chains of dependency ⛓️

Chains ⛓️



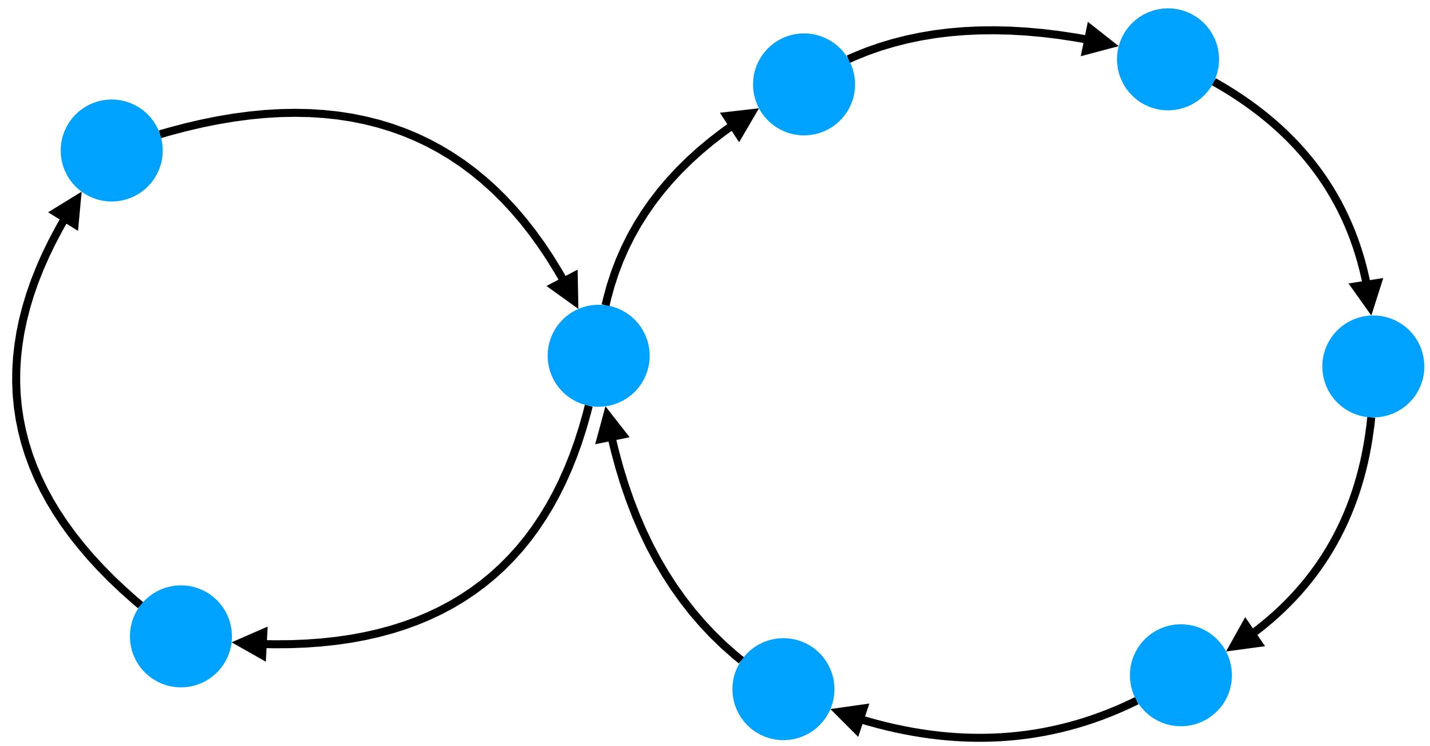
A set of one or more cycles pairwise sharing a point

🗝️ Lemma

🧬 **IF** the dependency graph of a RS contains a chain of two self-sustaining, non self-inhibiting cycles of length m and n

🏃‍♀️ **THEN** when starting from a configuration where at least one reaction involved in the cycles is enabled, eventually all the reactions will be enabled once every gcd(m, n) steps

🗝 Lemma in action



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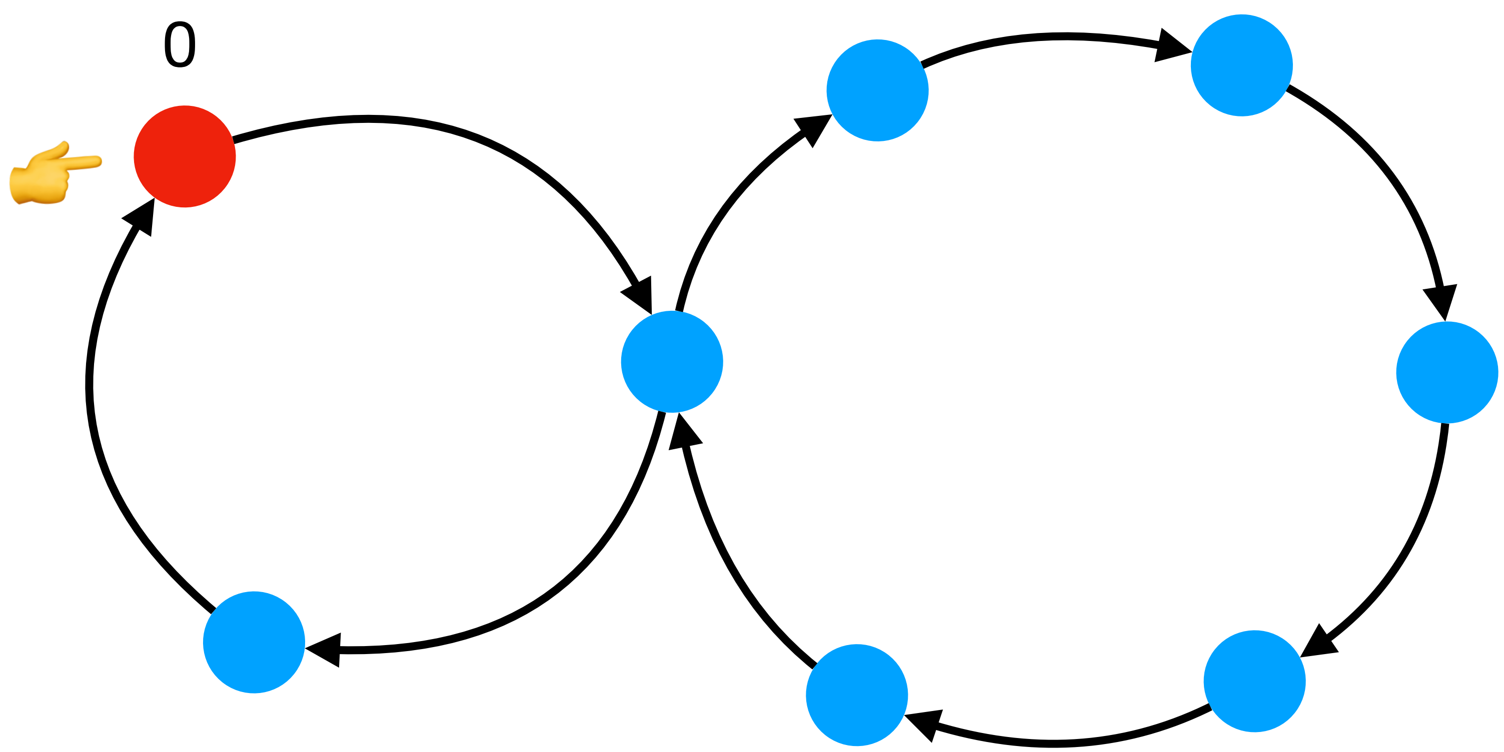
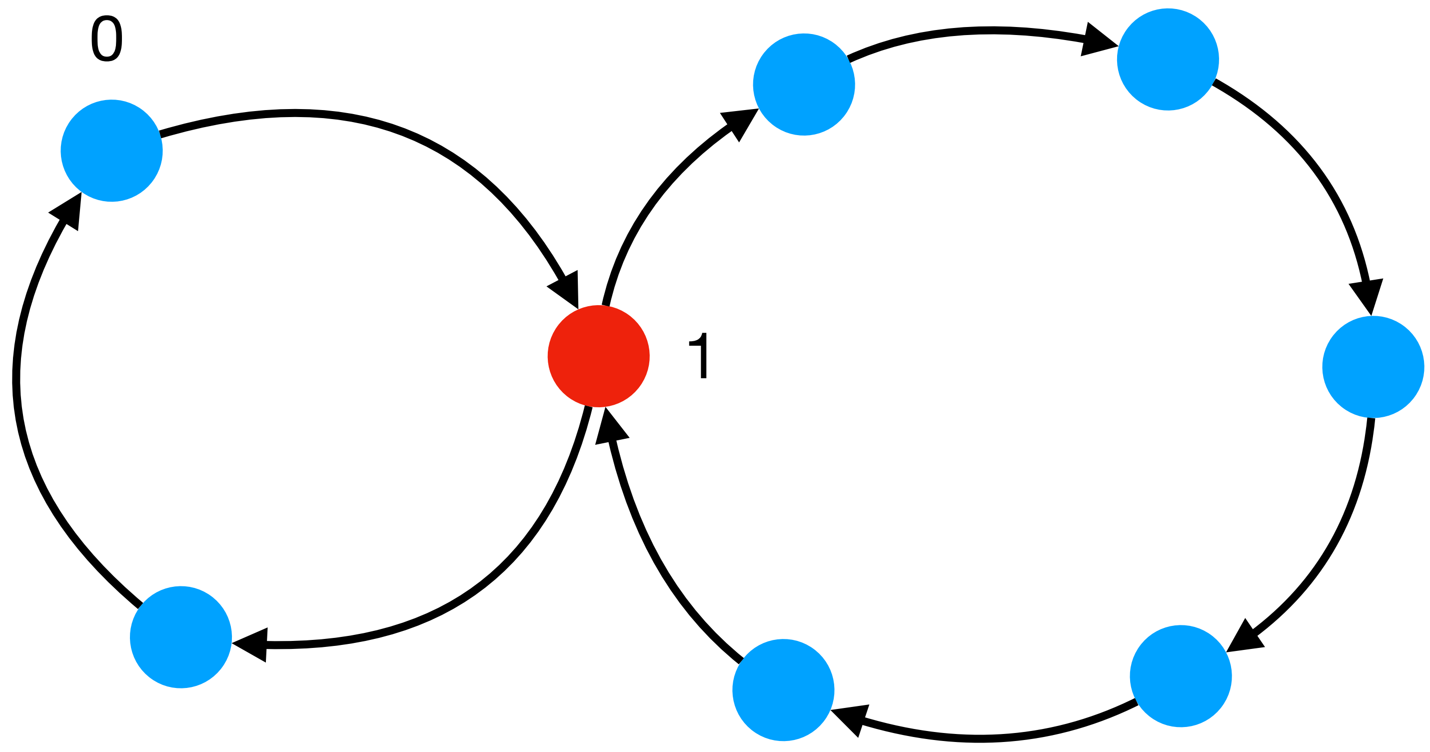


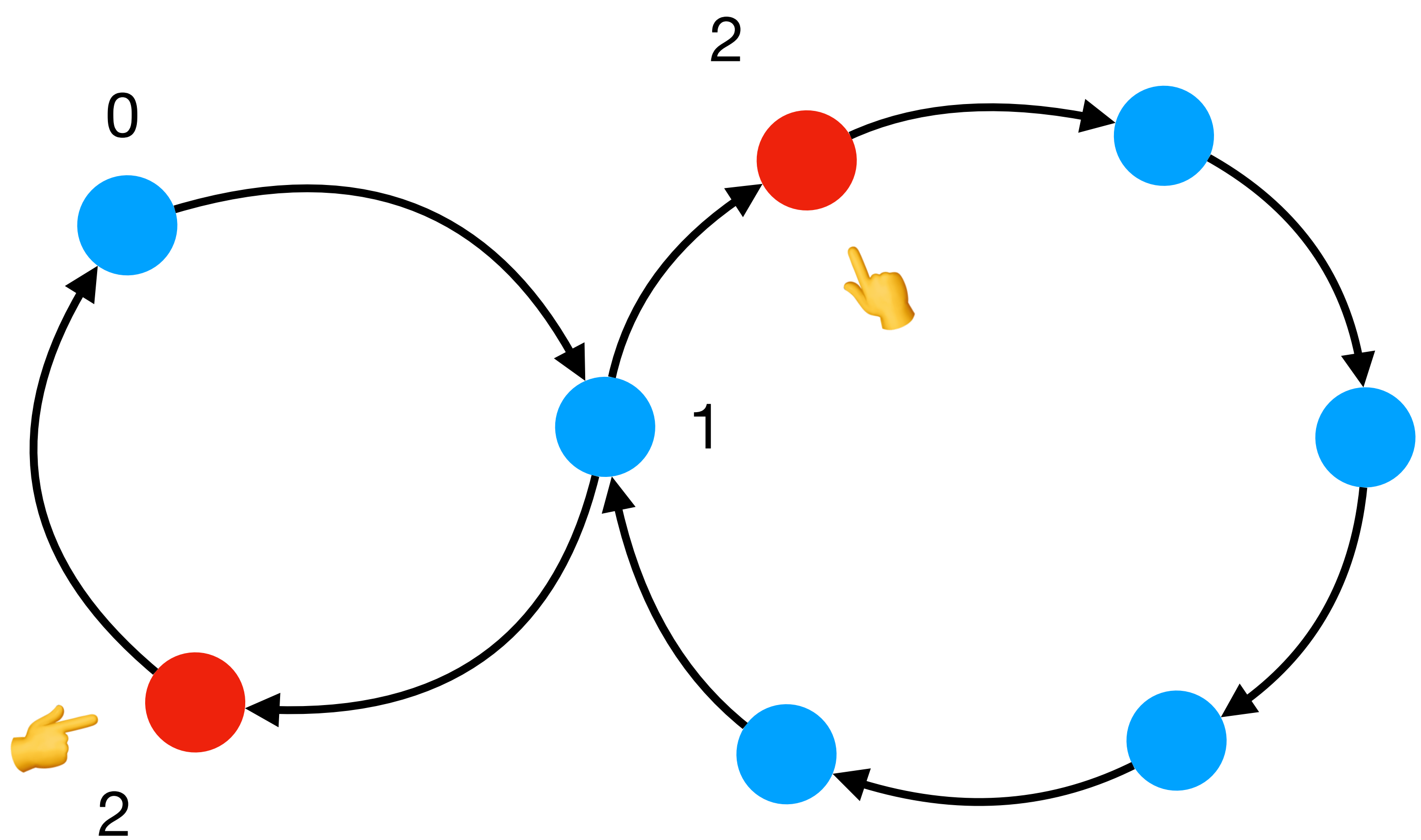
⏰ = 0

🗝️ Lemma in action



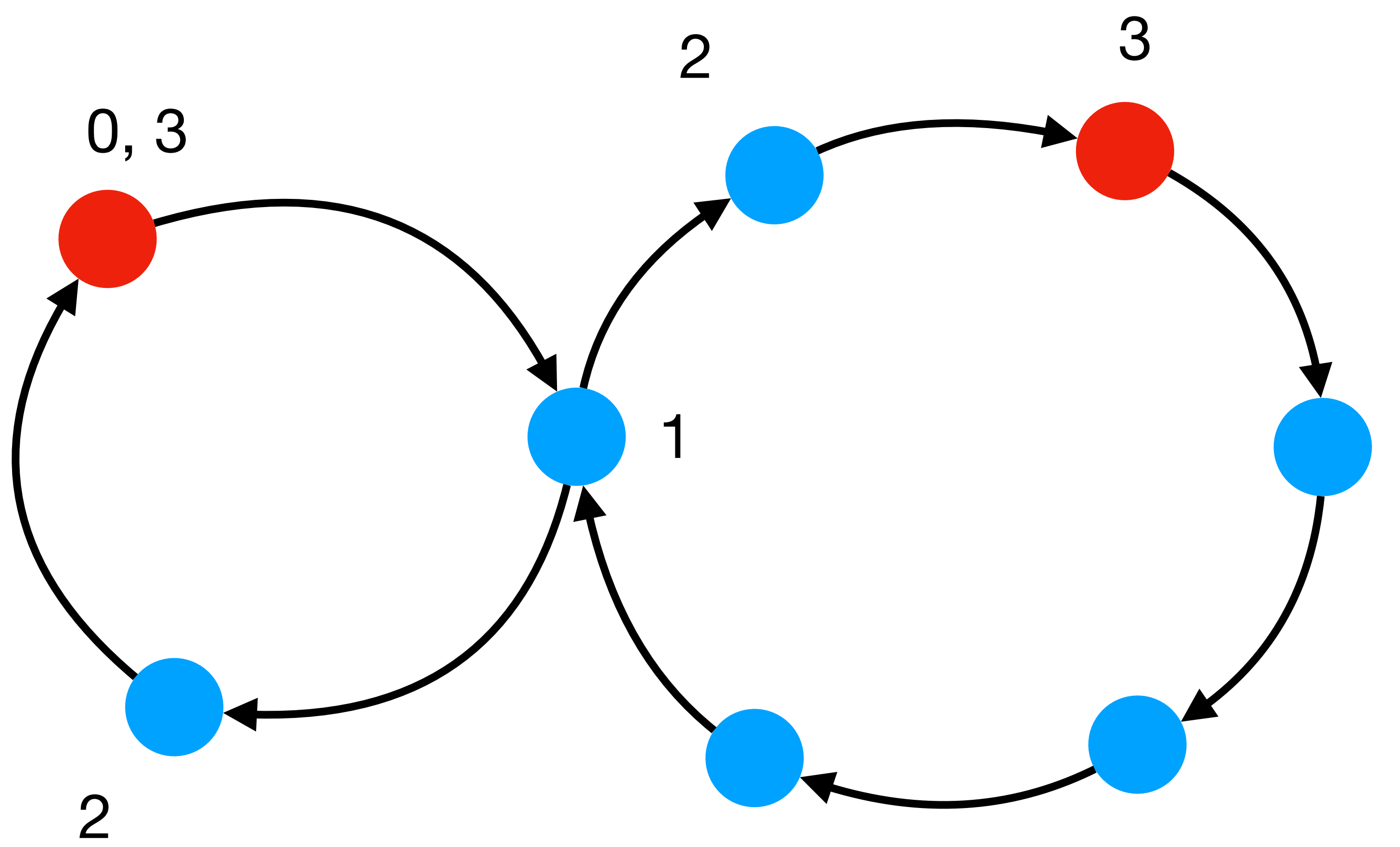
⏰ = 1

🗝 Lemma in action



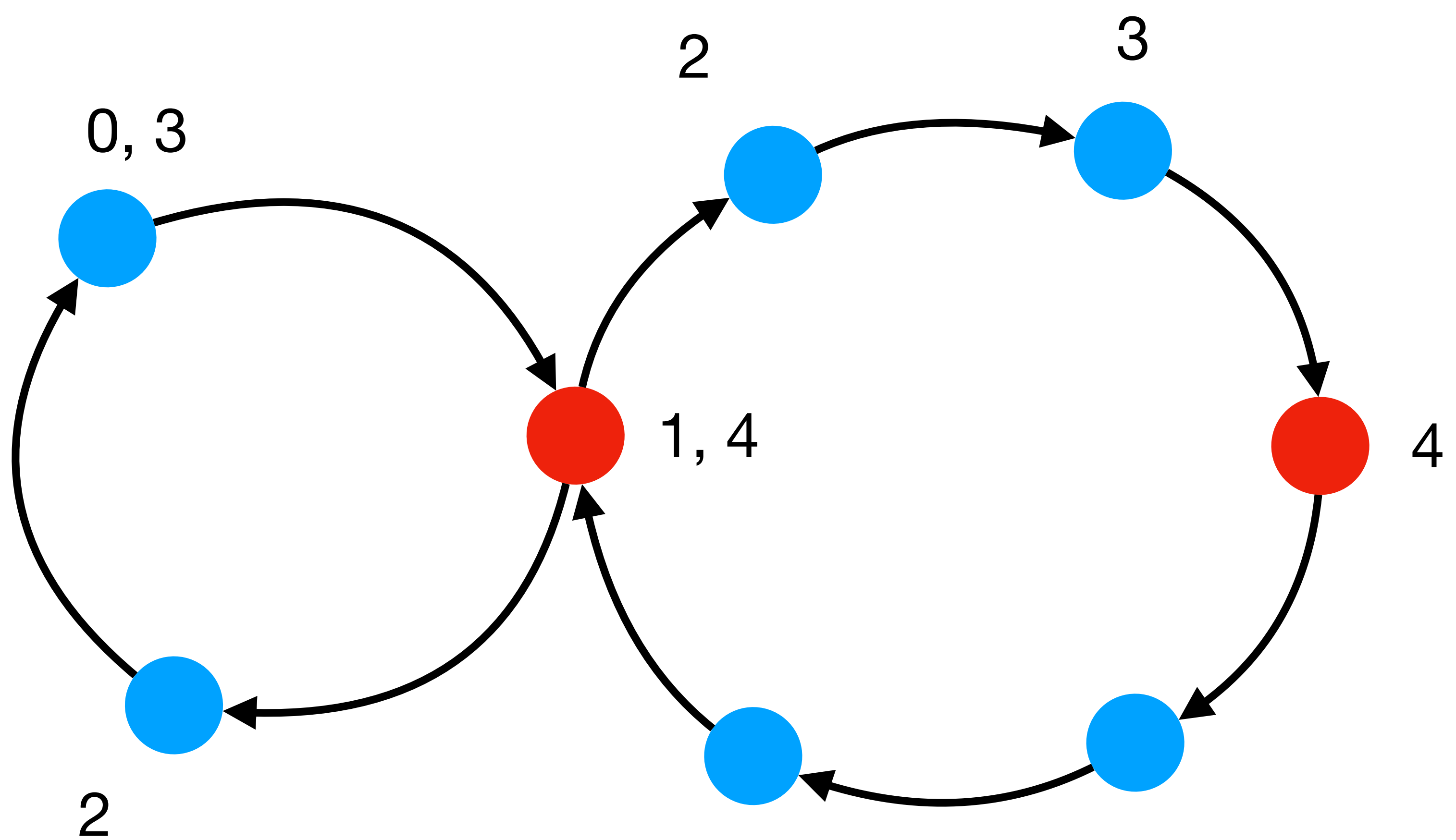
⏰ = 2

🗝 Lemma in action



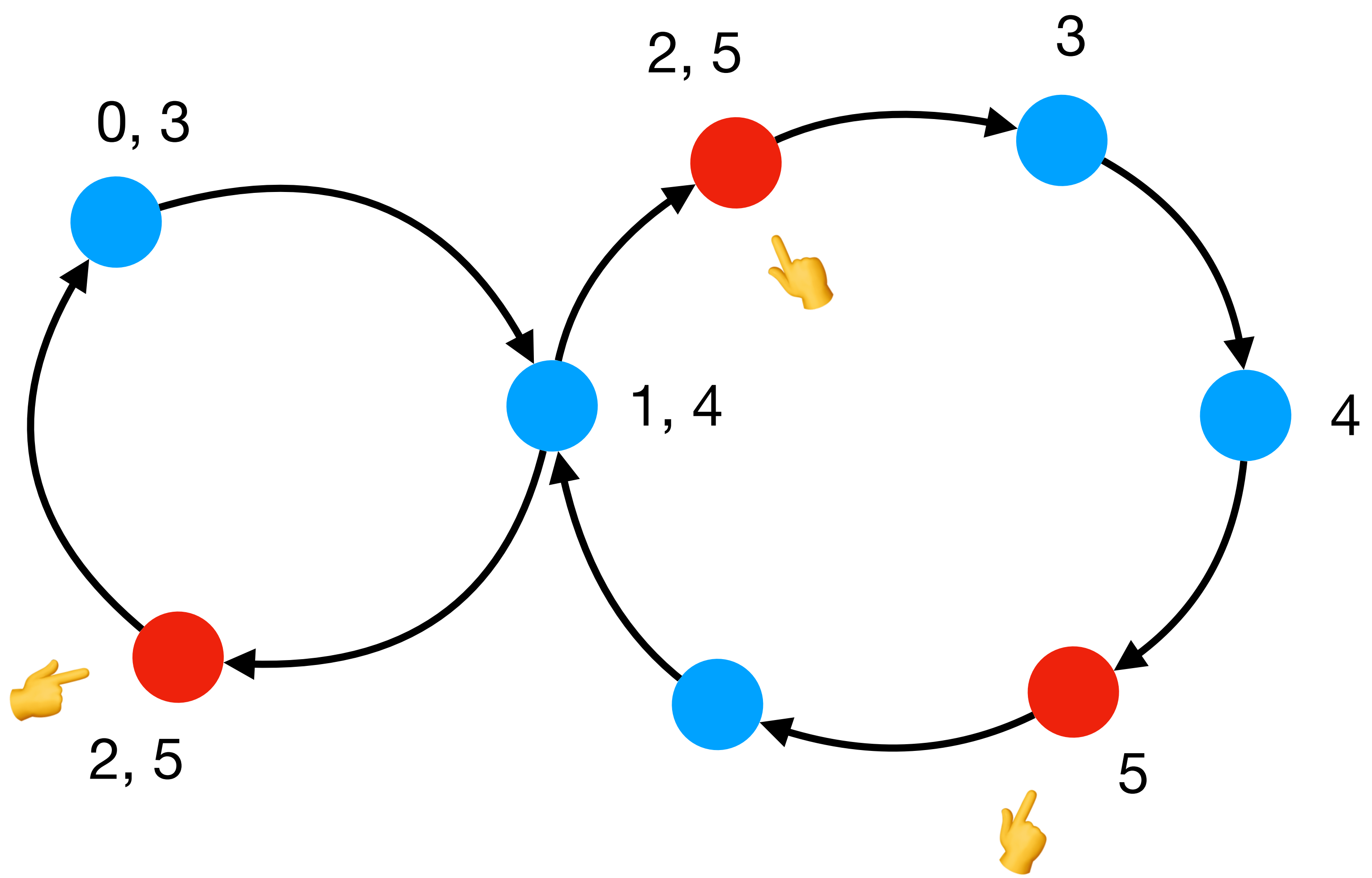
⏰ = 3

🗝 Lemma in action



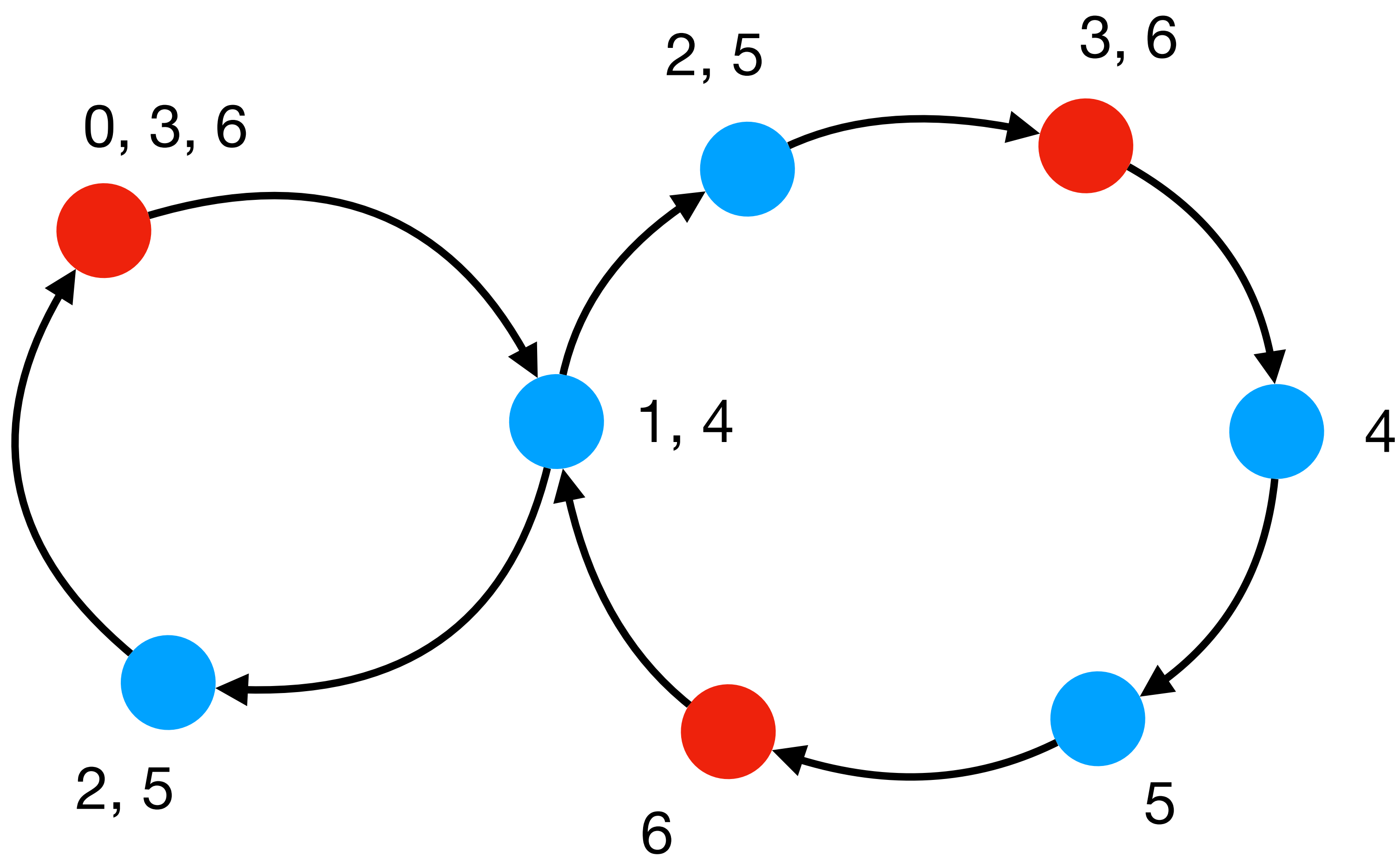
⏰ = 4

🗝 Lemma in action



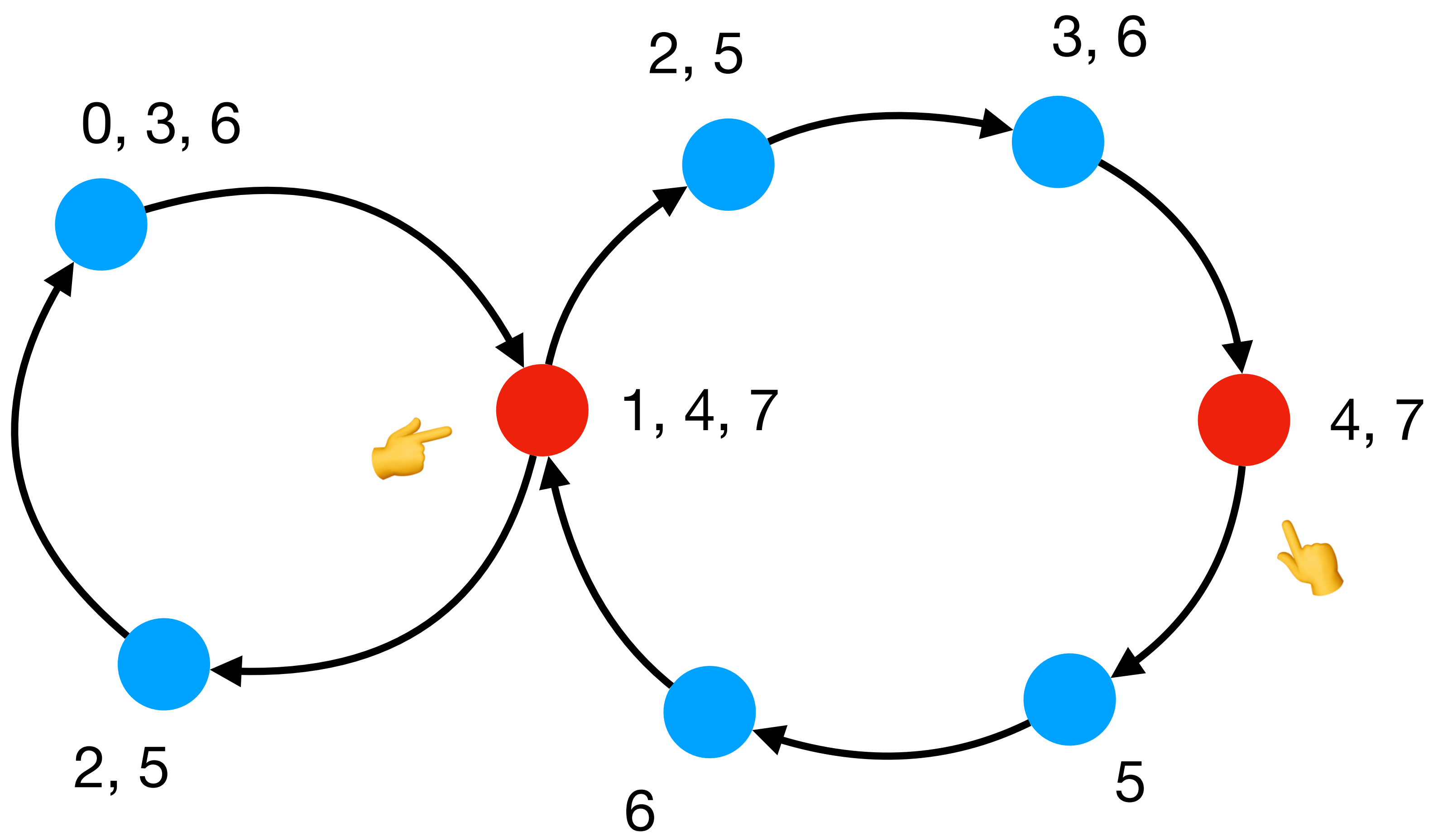
⏰ = 5

🗝 Lemma in action



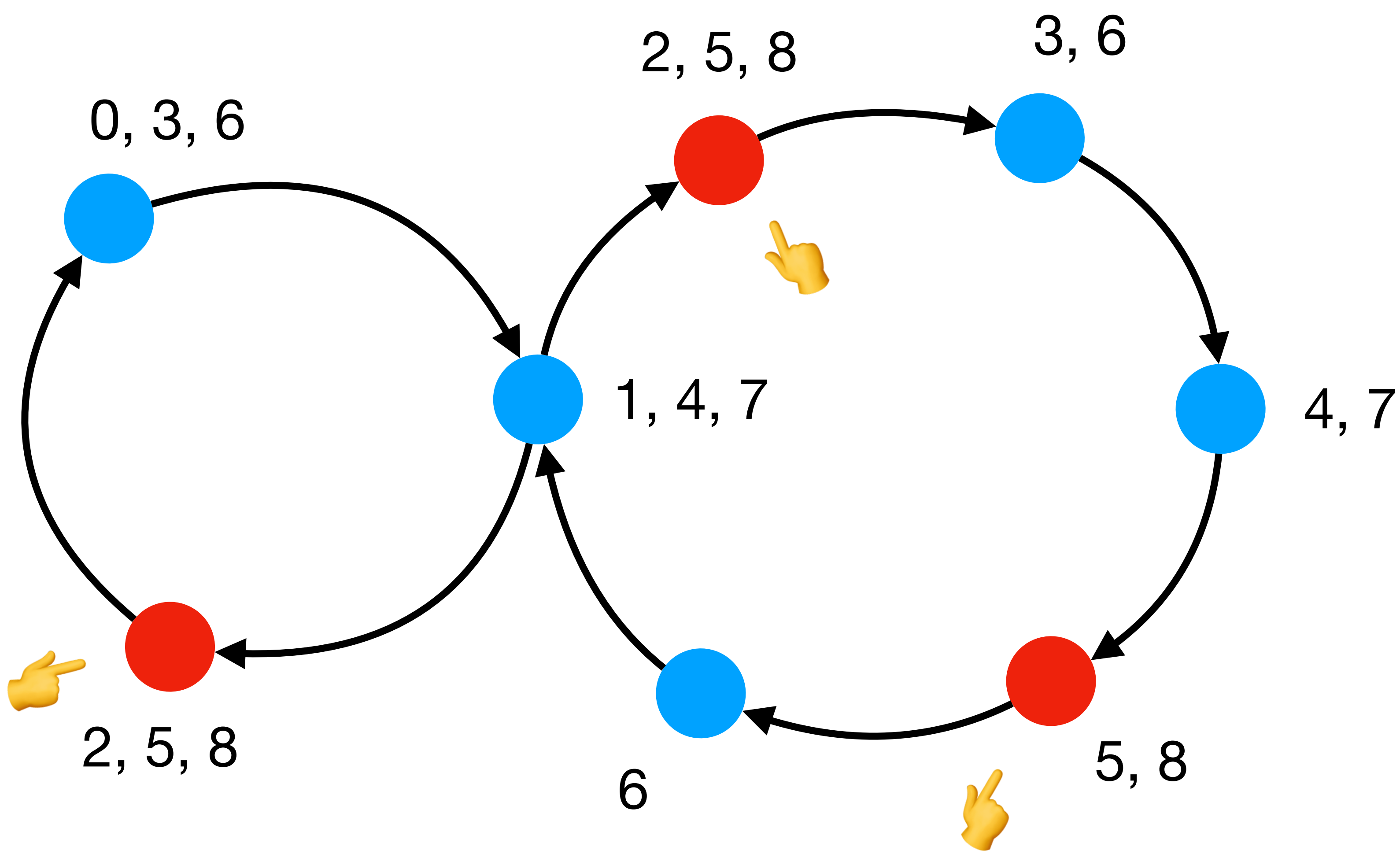
⏰ = 6

🗝 Lemma in action



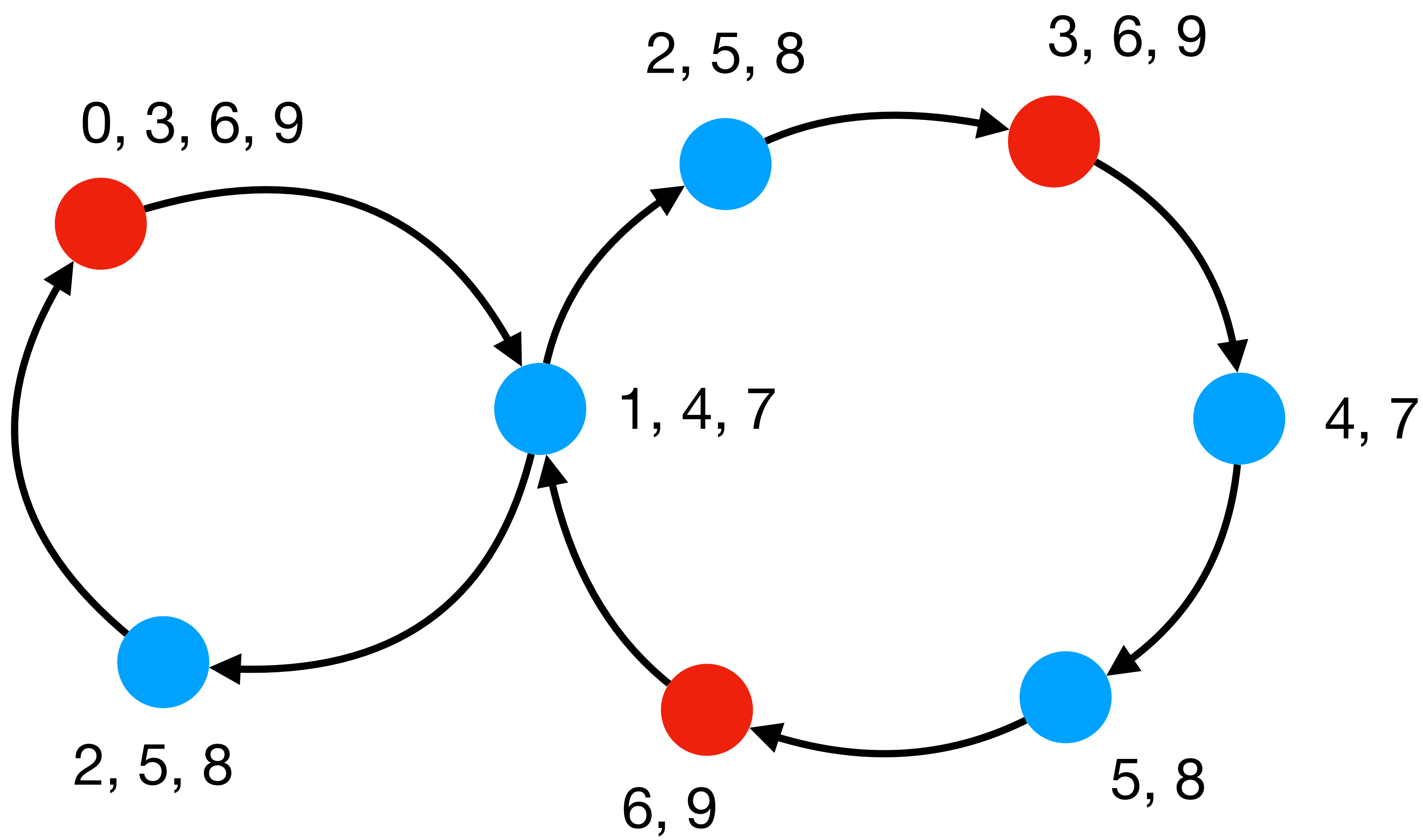
⏰ = 7

🗝 Lemma in action



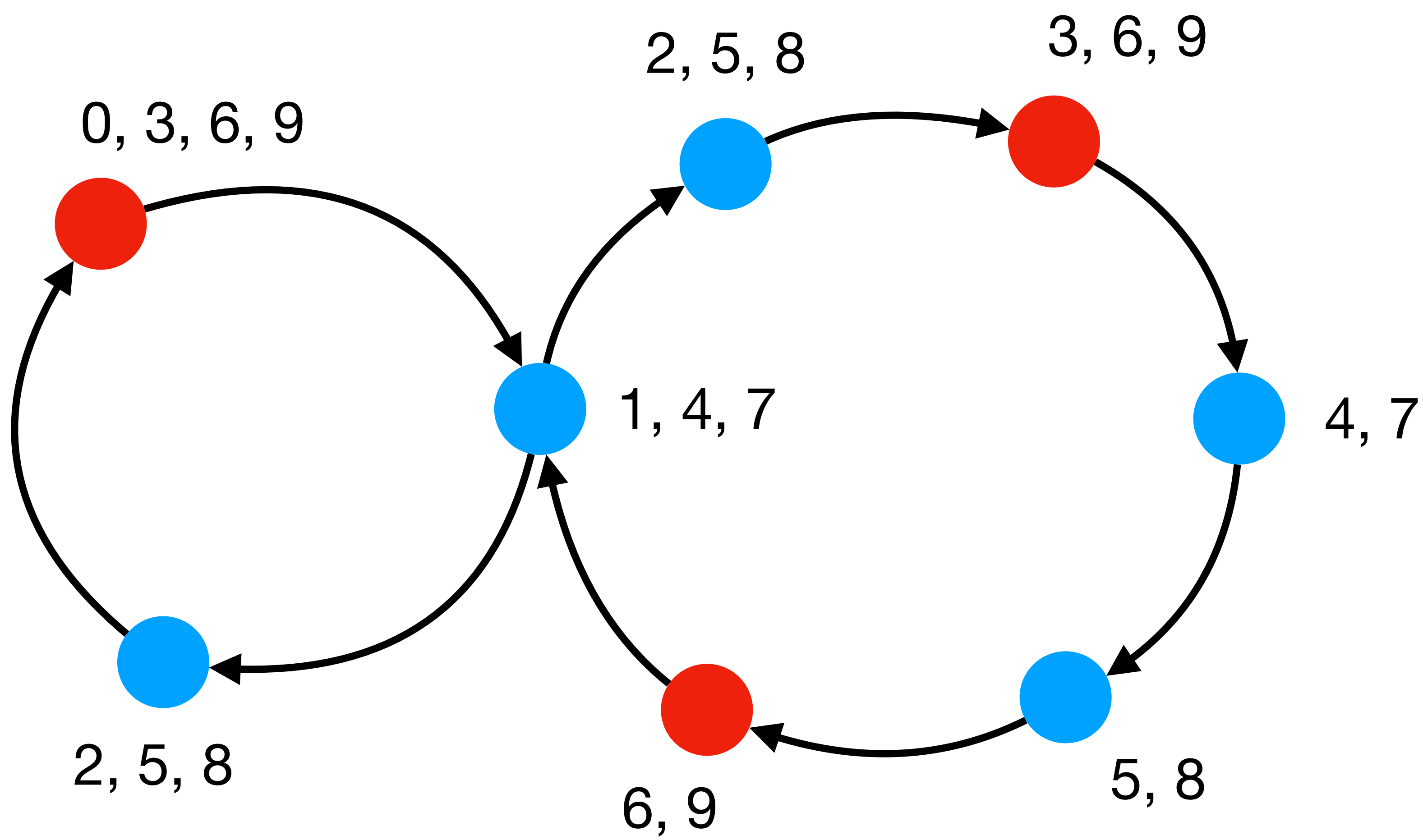
⏰ = 8

🗝️ Lemma in action



⏰ = 9

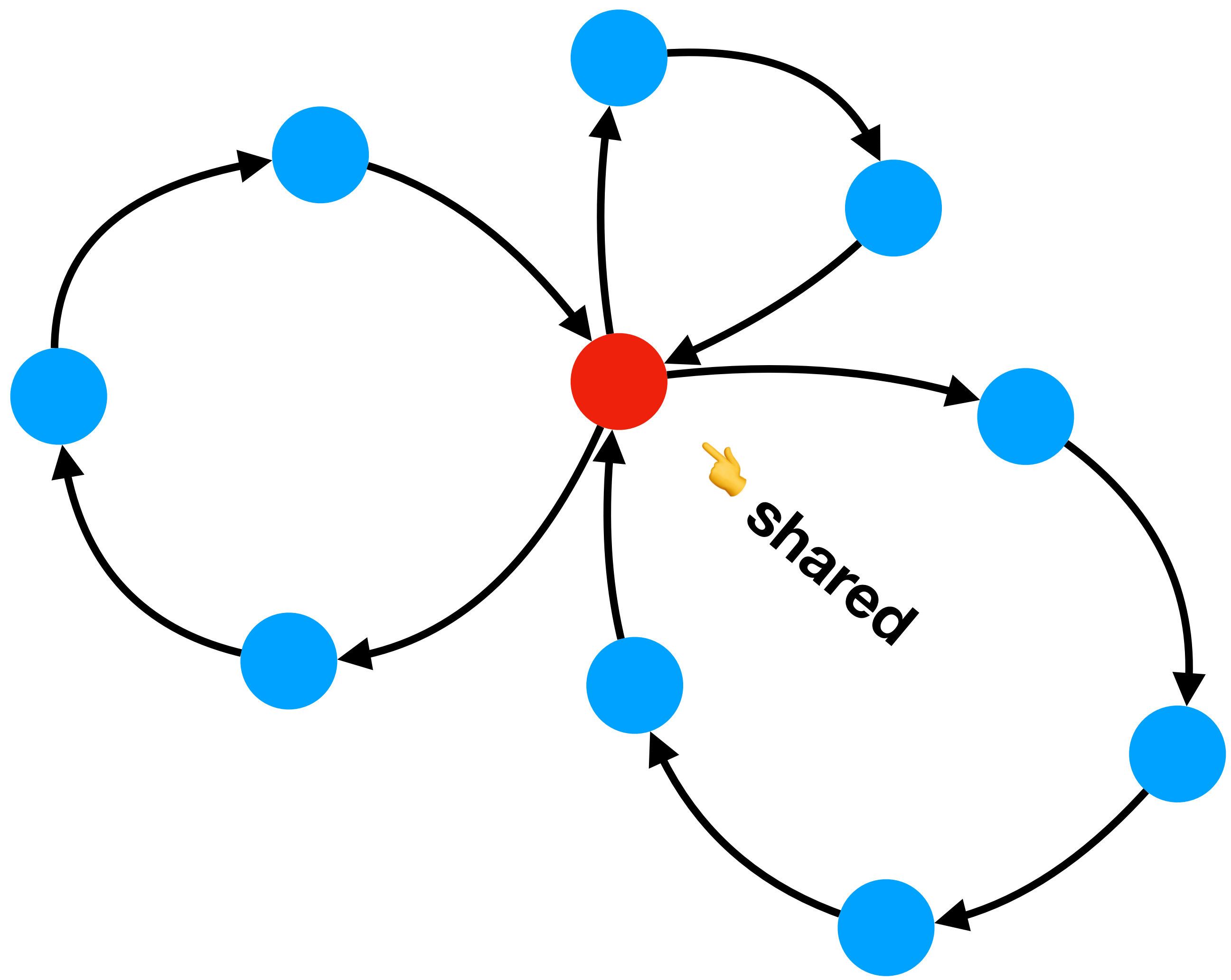
🗝 Lemma in action



All reactions are enabled every 3 = gcd(3, 6) steps

Flower-shaped dependencies 🌼

Flowers 🌼

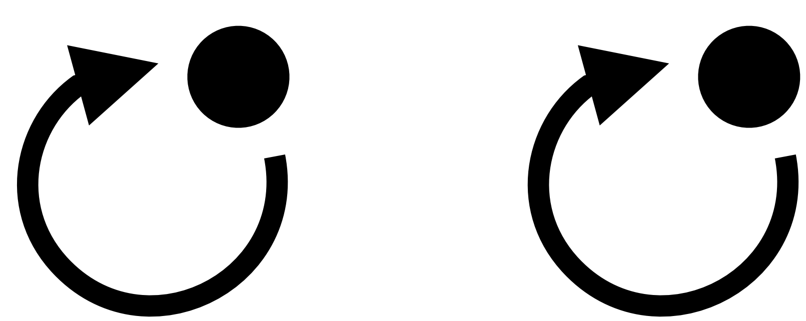


A set of one or more cycles all sharing a single point

🌼 Theorem

IF the dependency graph of a RS consists only of a flower of self-sustaining, non-self-inhibiting cycles (petals) with at lest of them of coprime lengths (STRUCTURE)

THEN the RS has exactly two fixed points (BEHAVIOUR).



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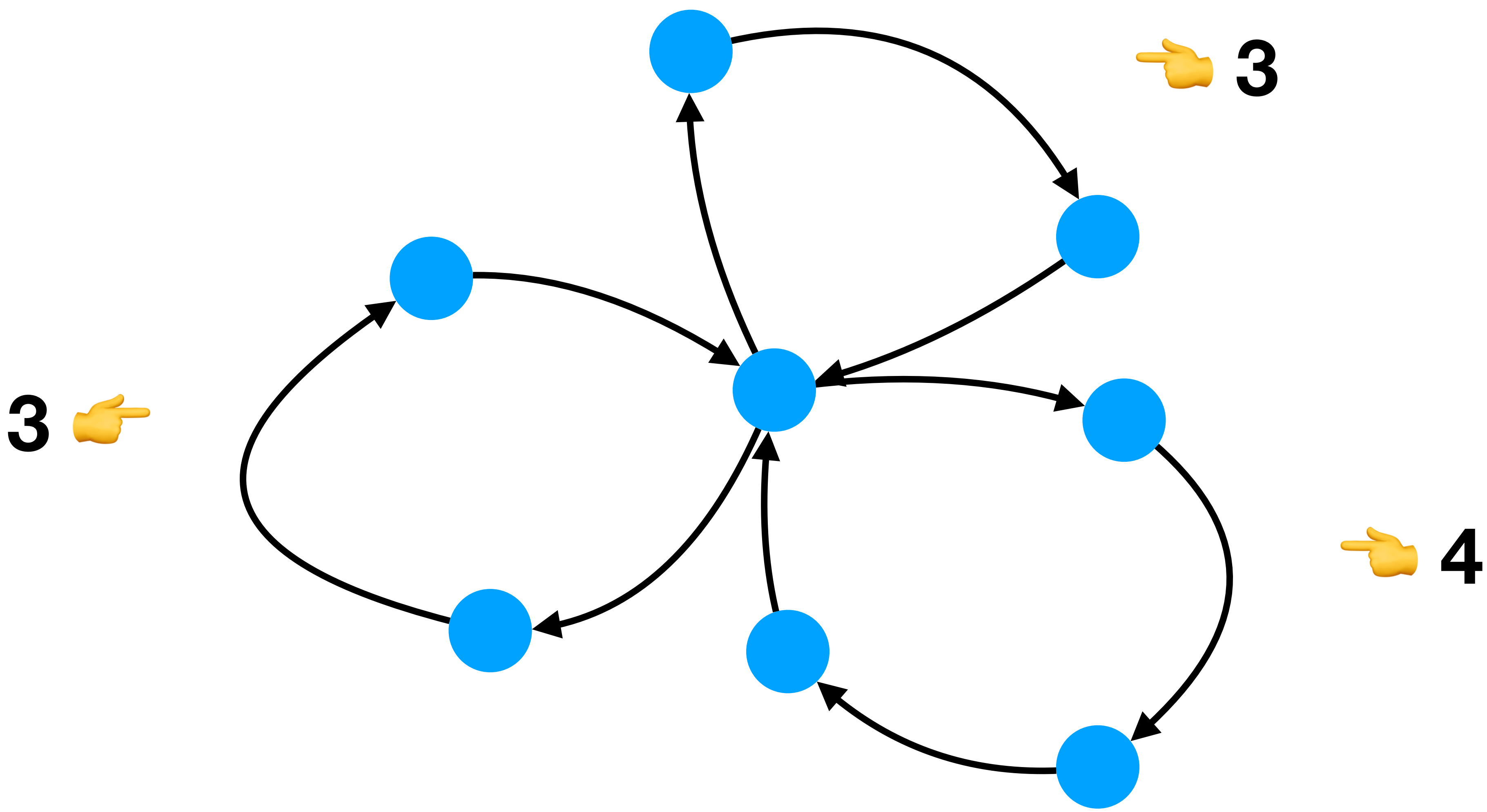

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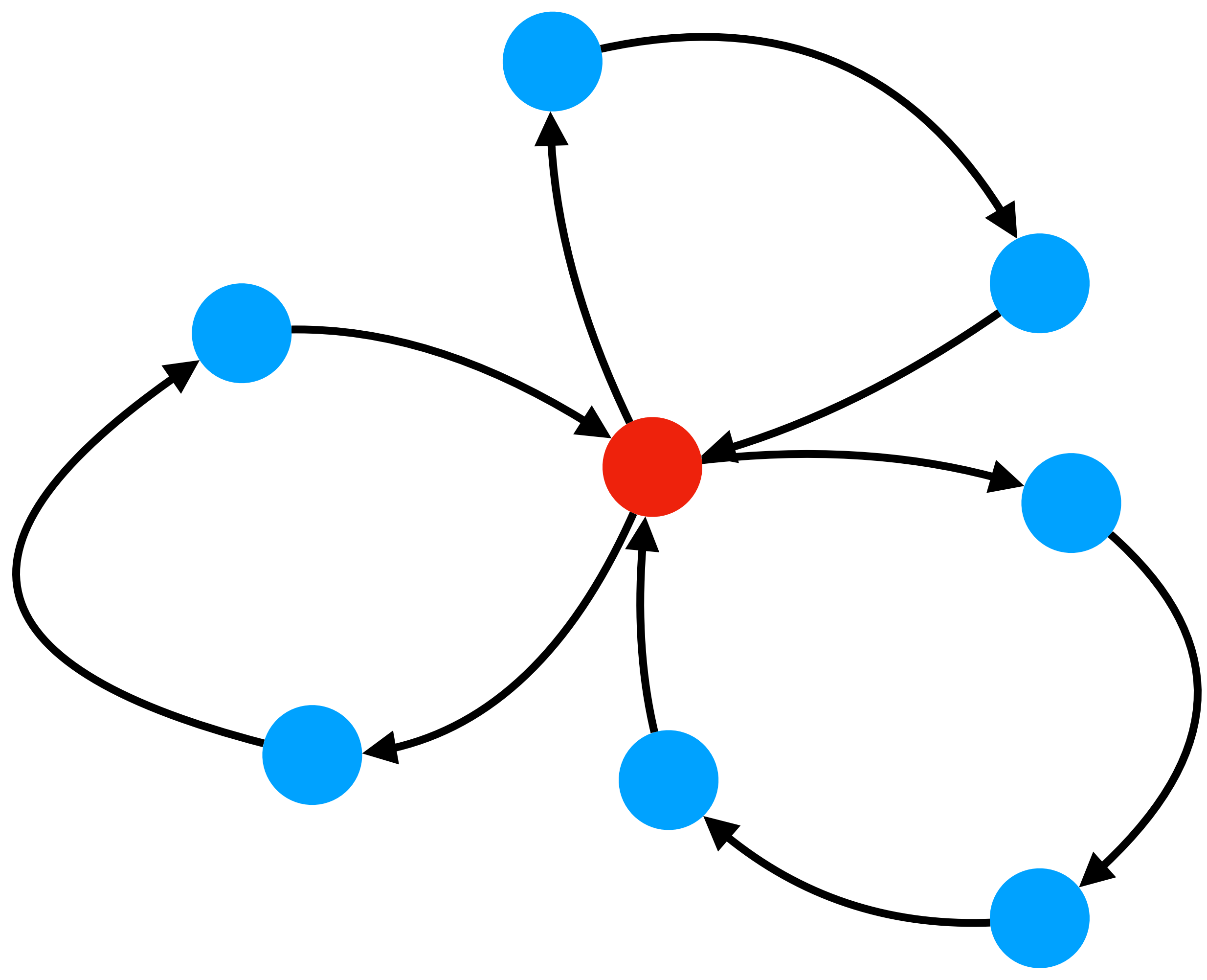

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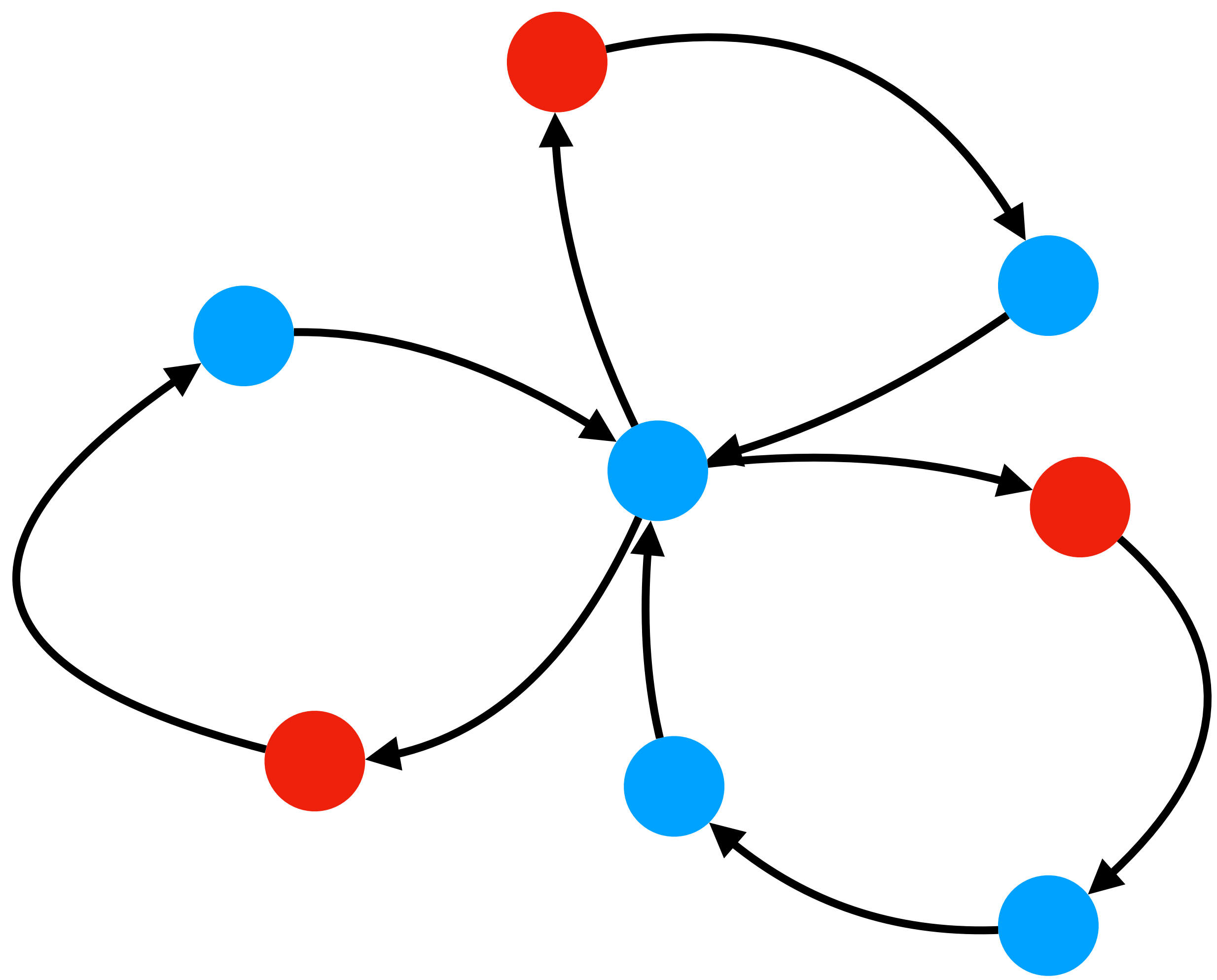

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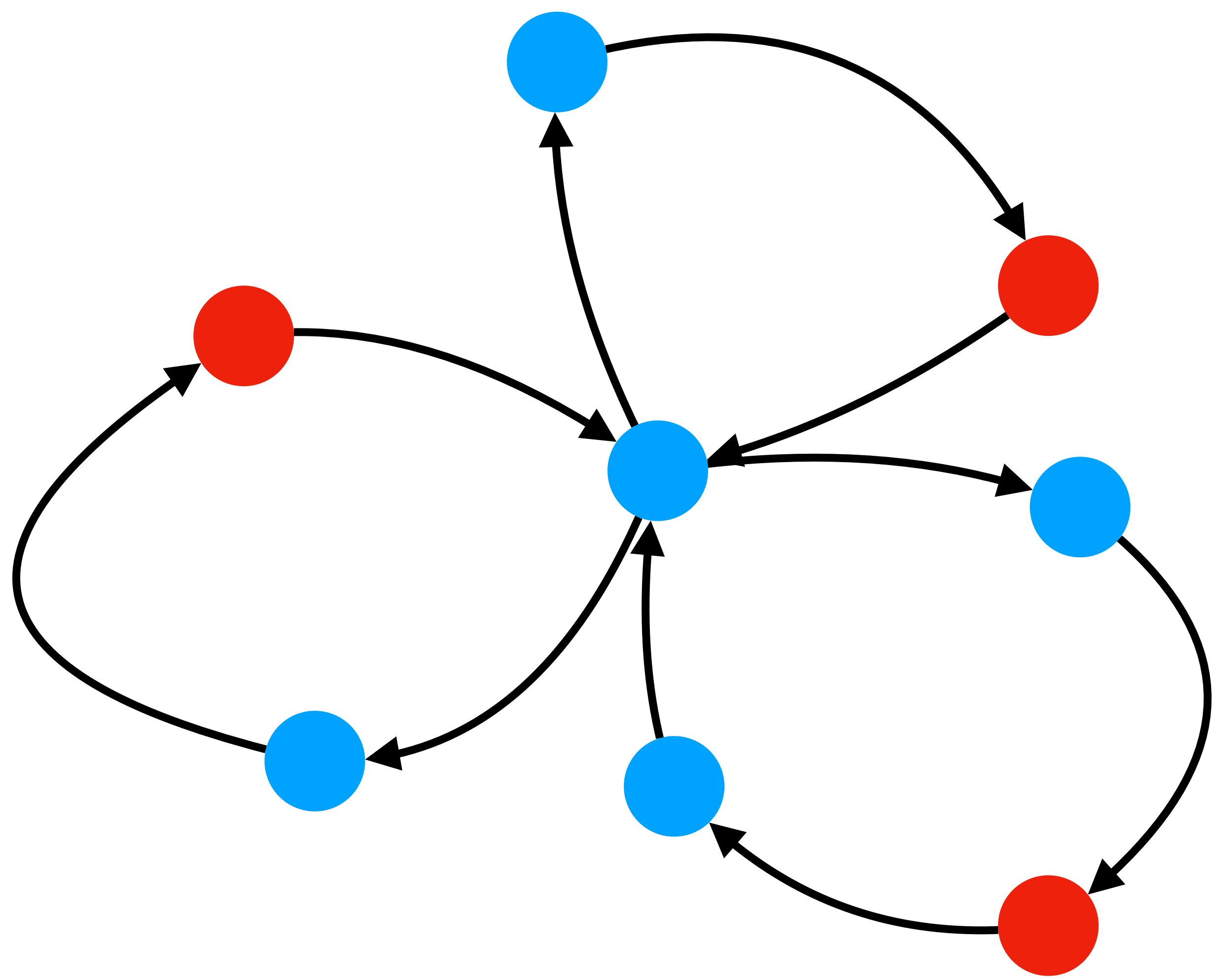

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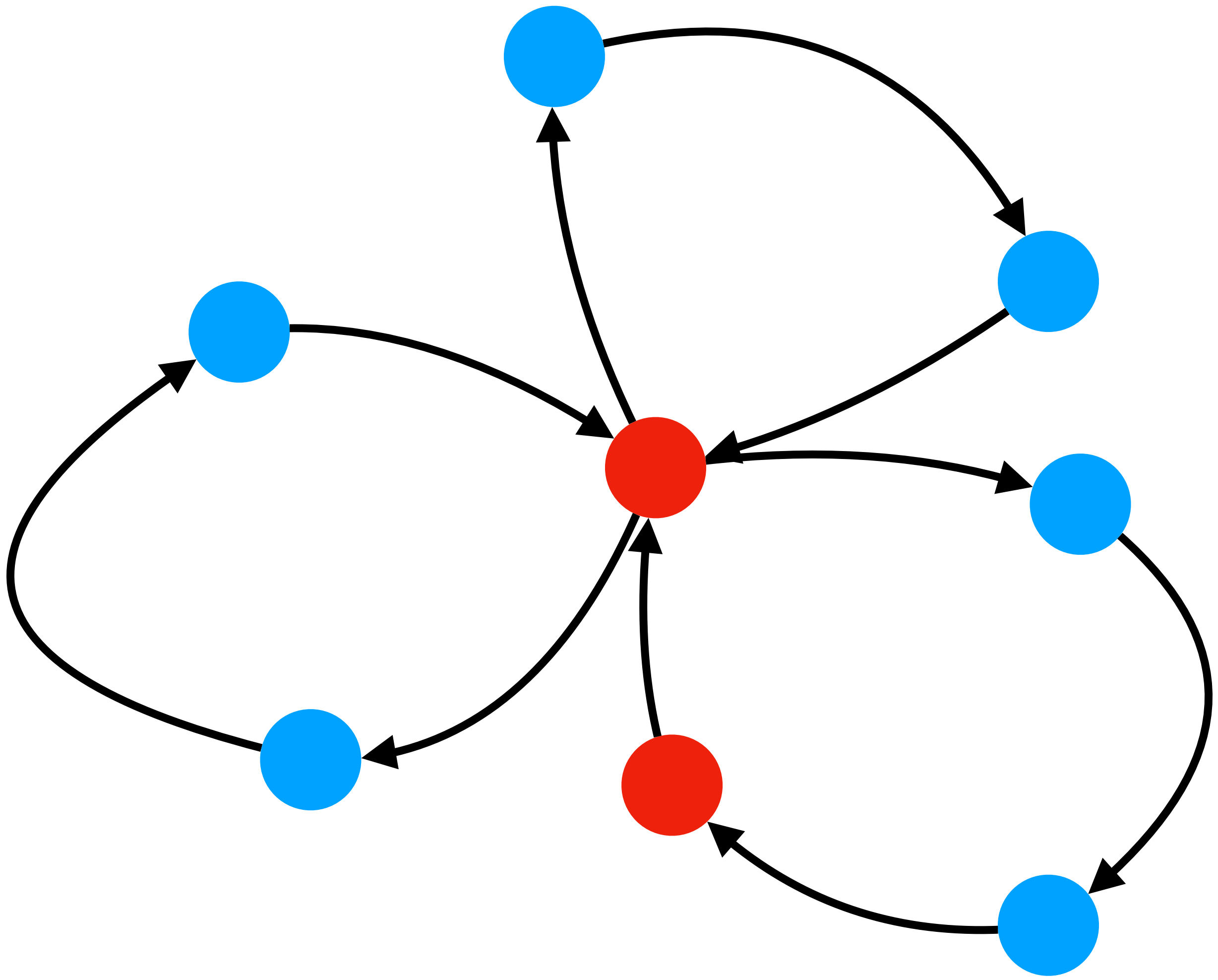

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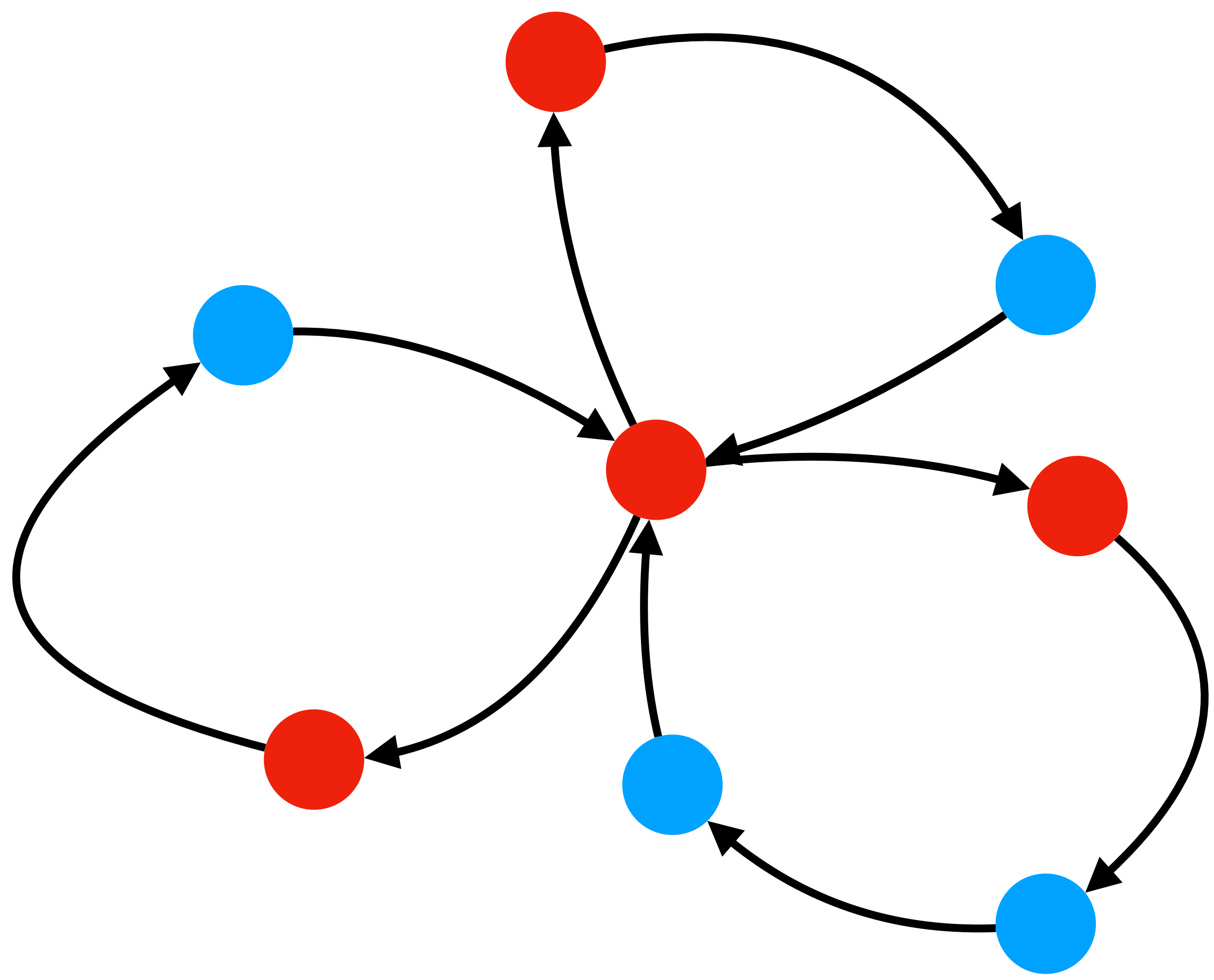

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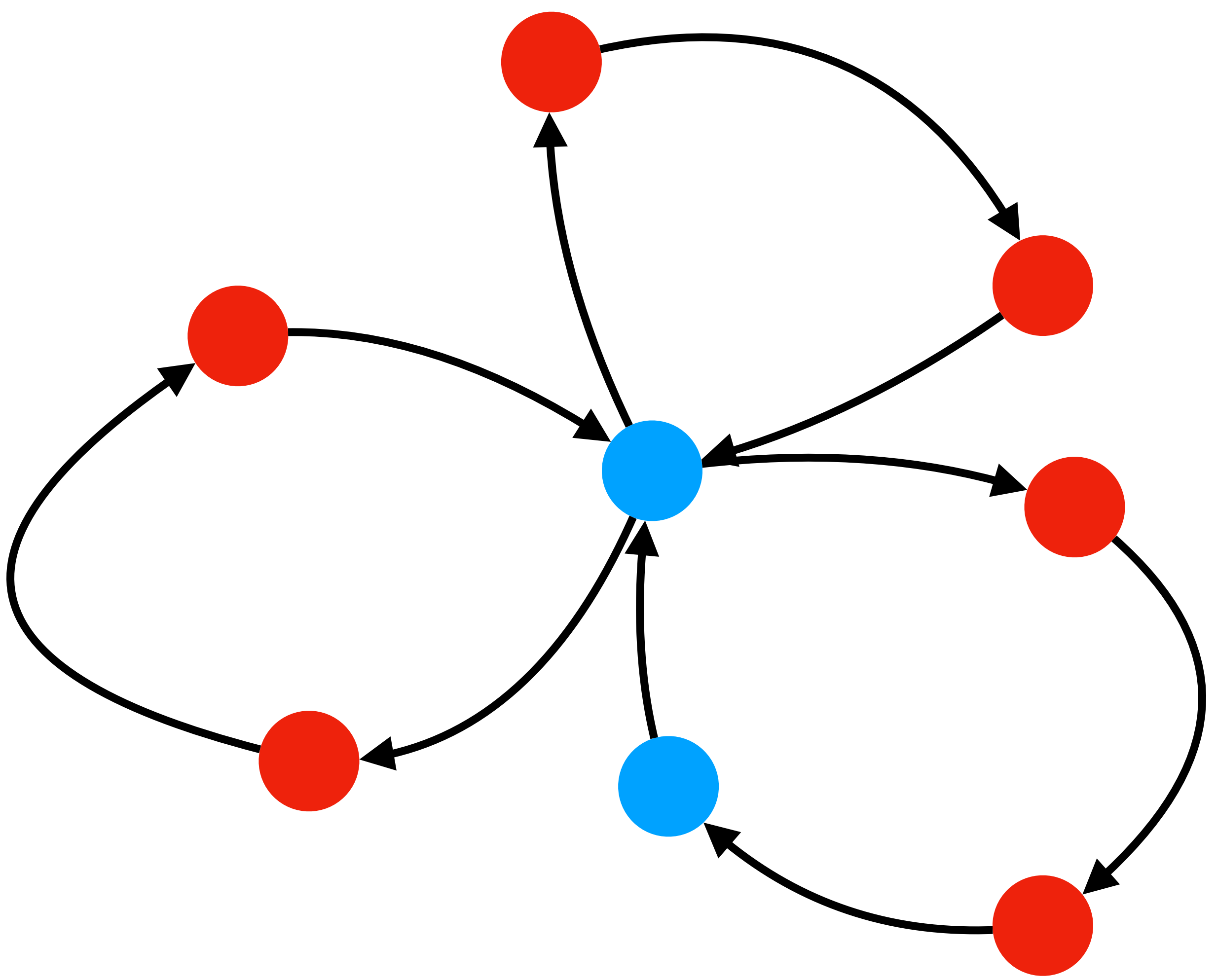

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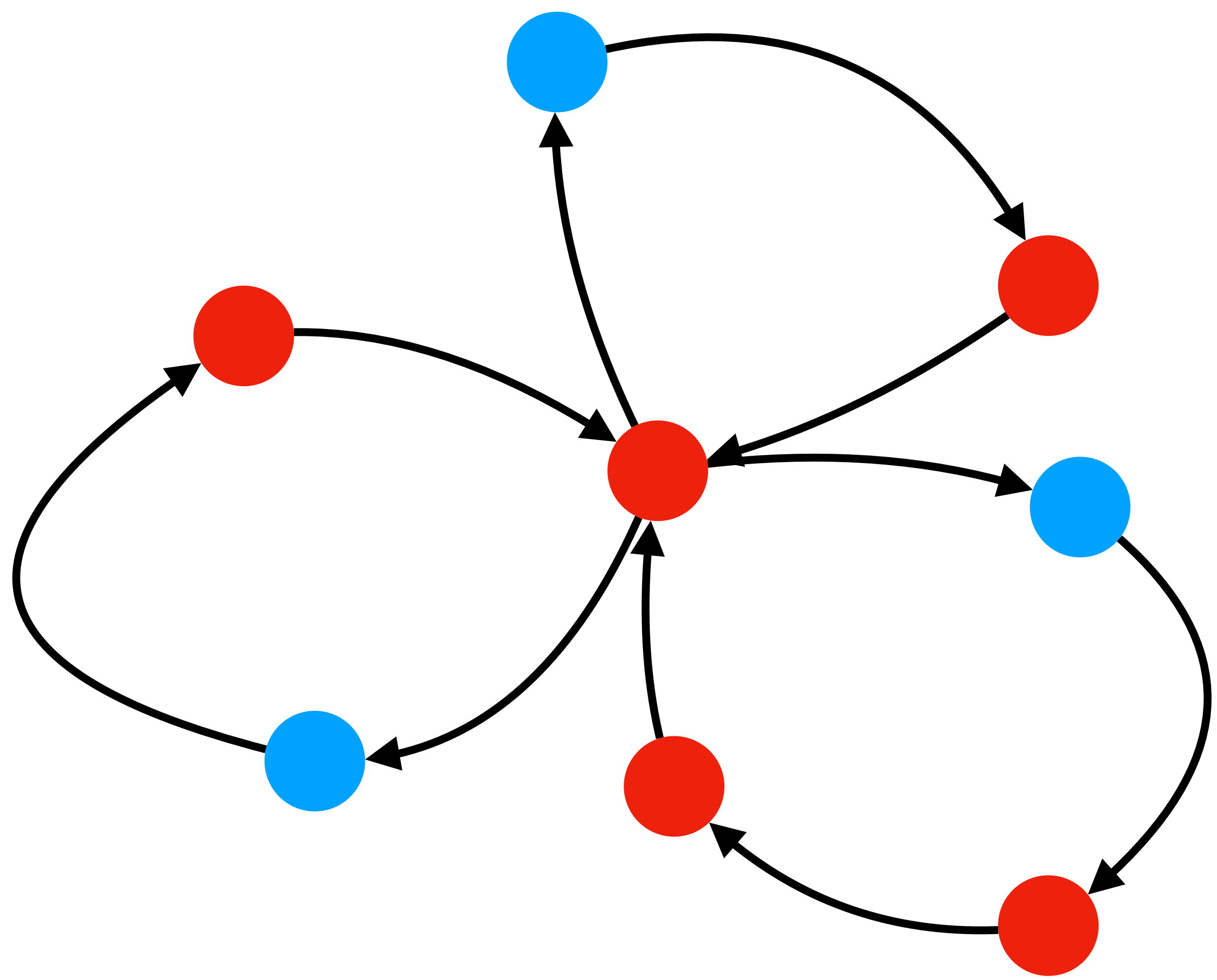

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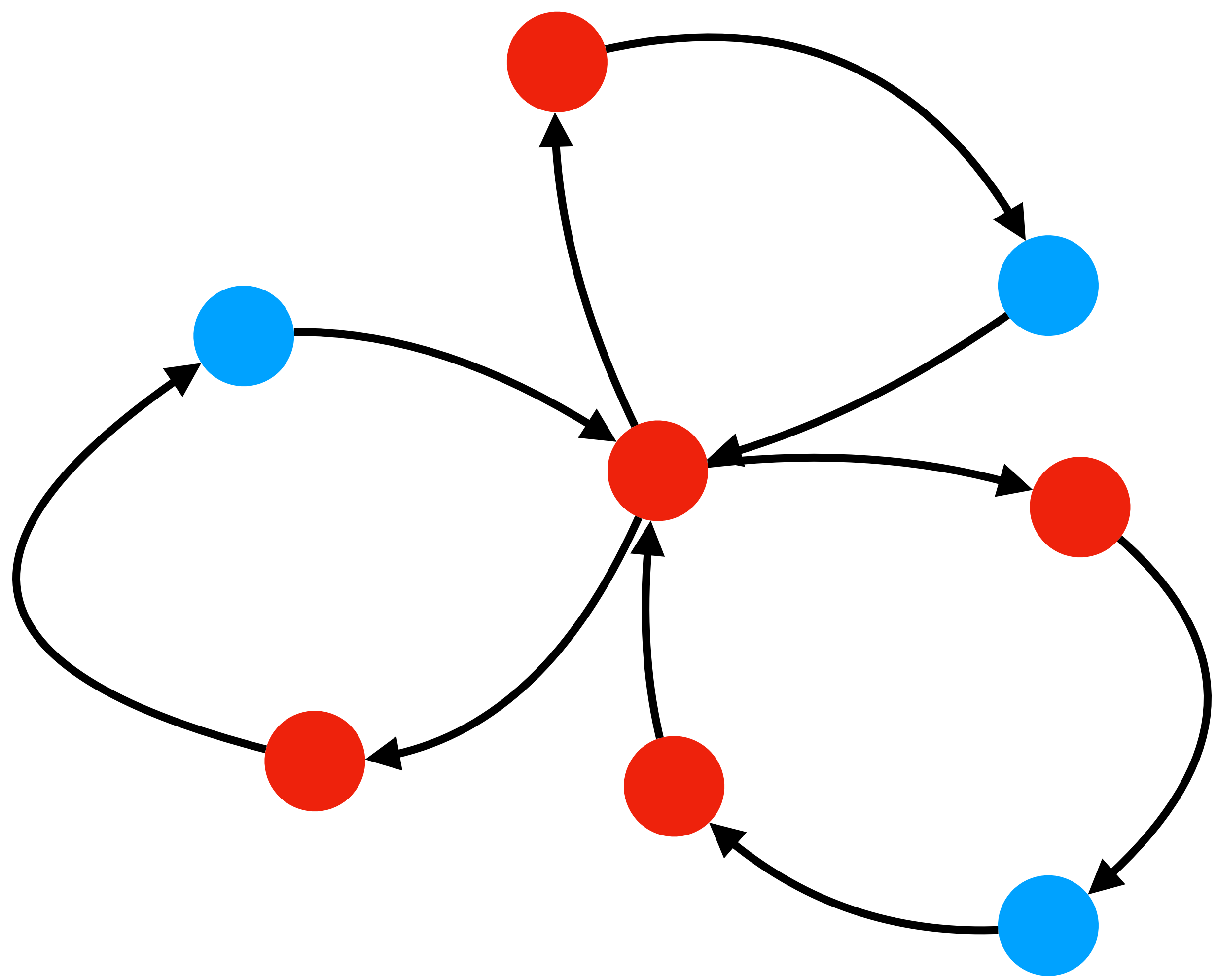

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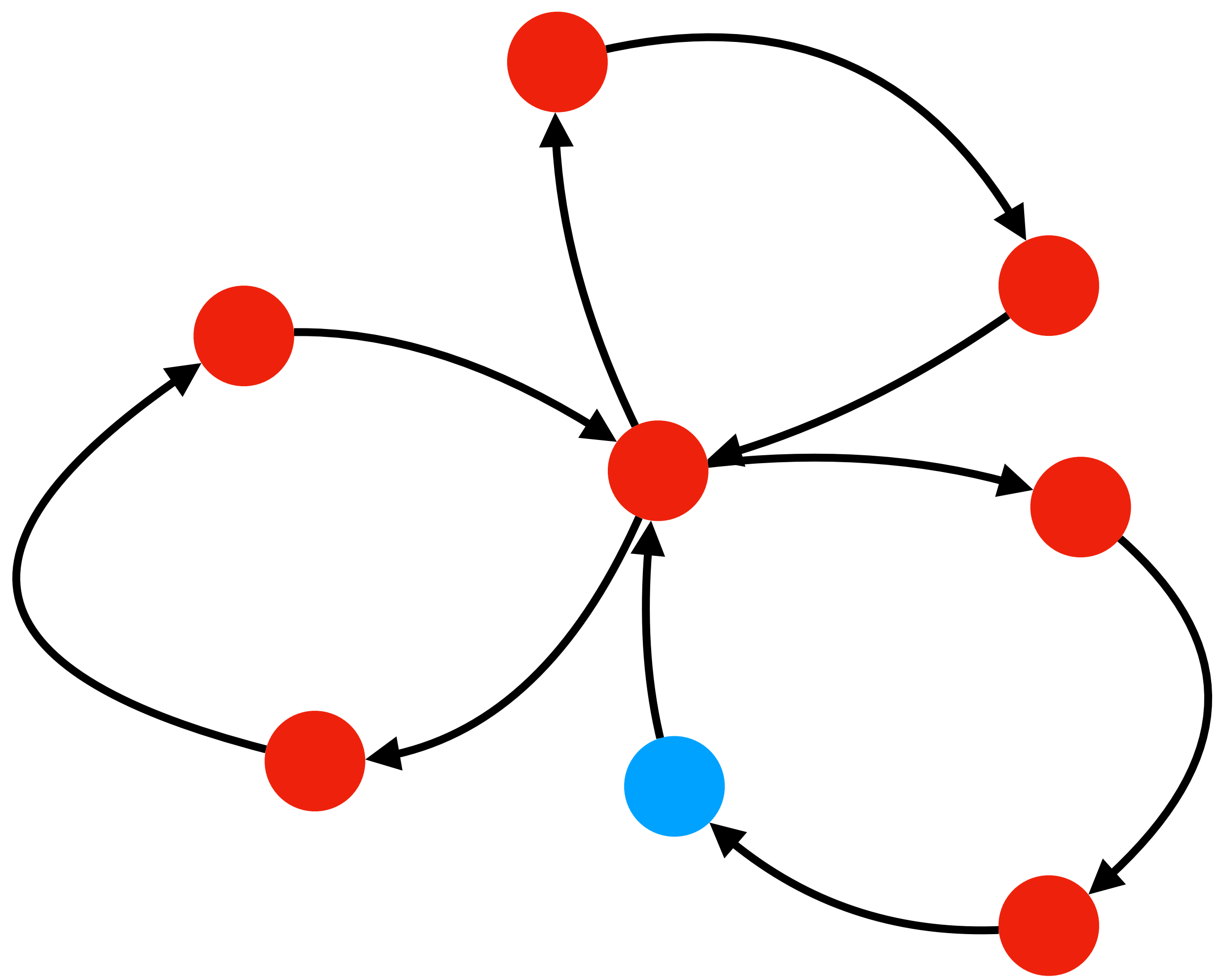

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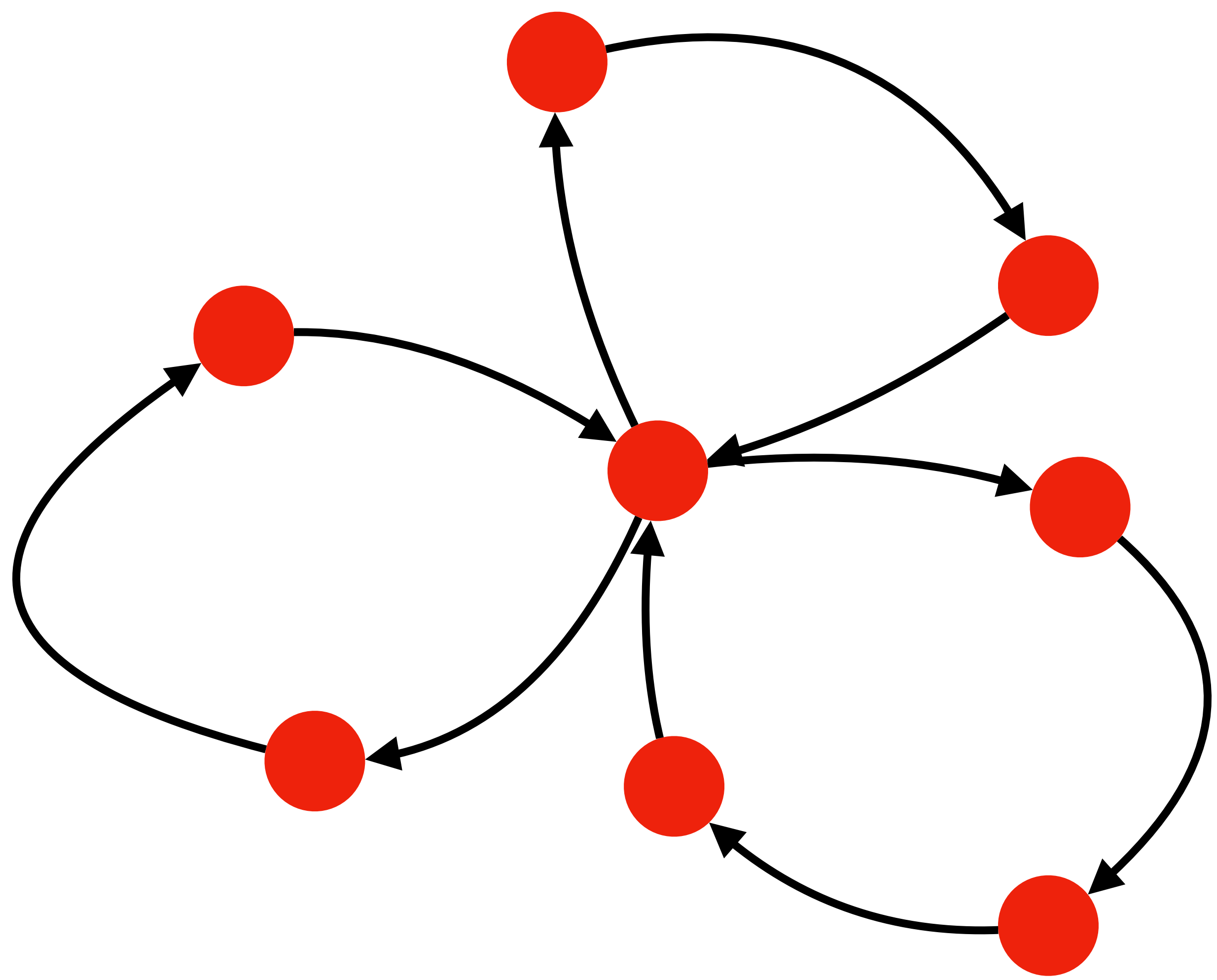

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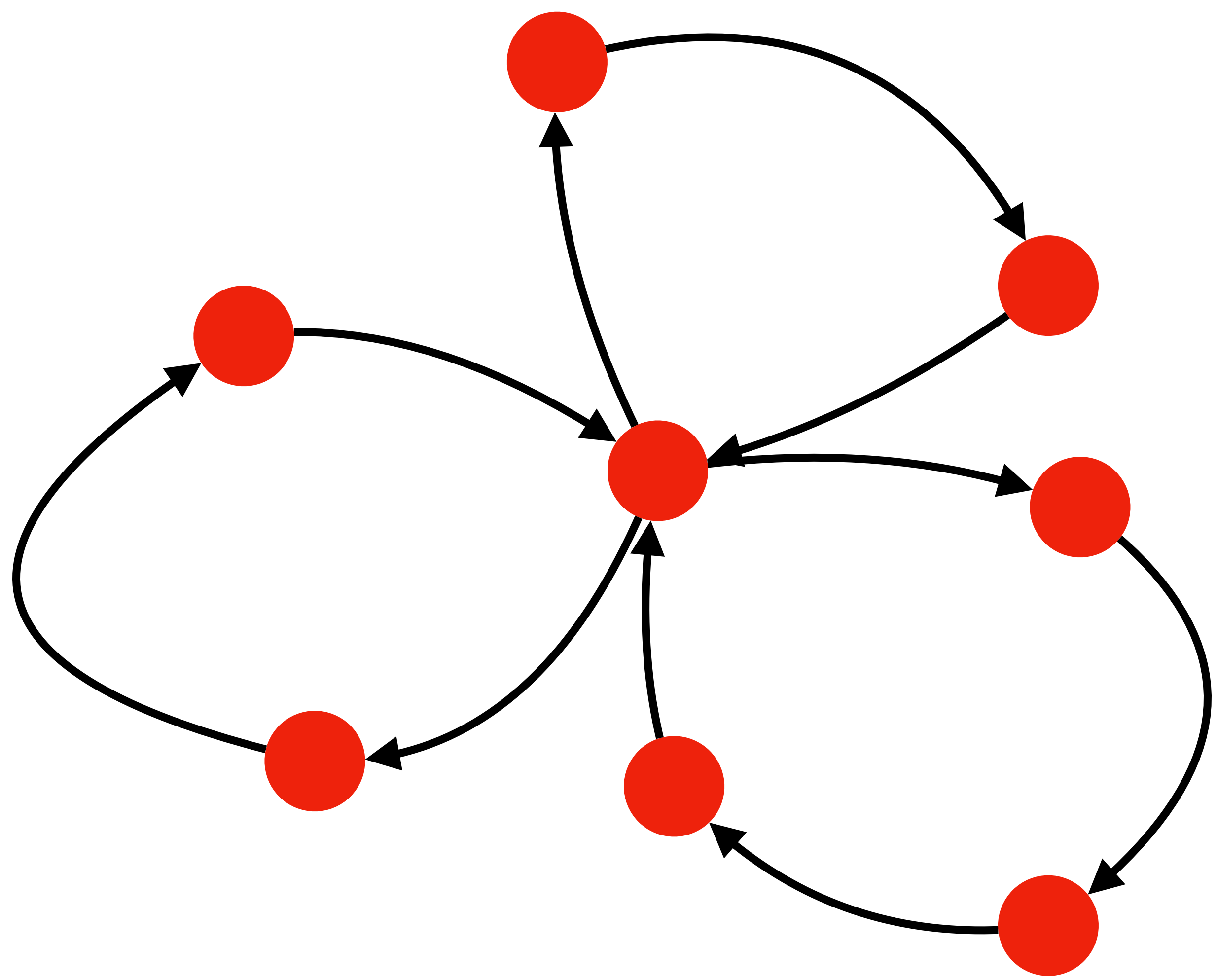


All reactions enabled every 1 = gcd(3, 4) step! Saturation!

🌼 Theorem in action

- When all reactions are always enabled
  the products are always the same: $T = \bigcup\{P_a : a \in A\}$

- Thus the RS enters a nonempty fixed point: $res_{\mathcal{A}}(T) = T$

- The second fixed point is by definition the empty state $\varnothing$

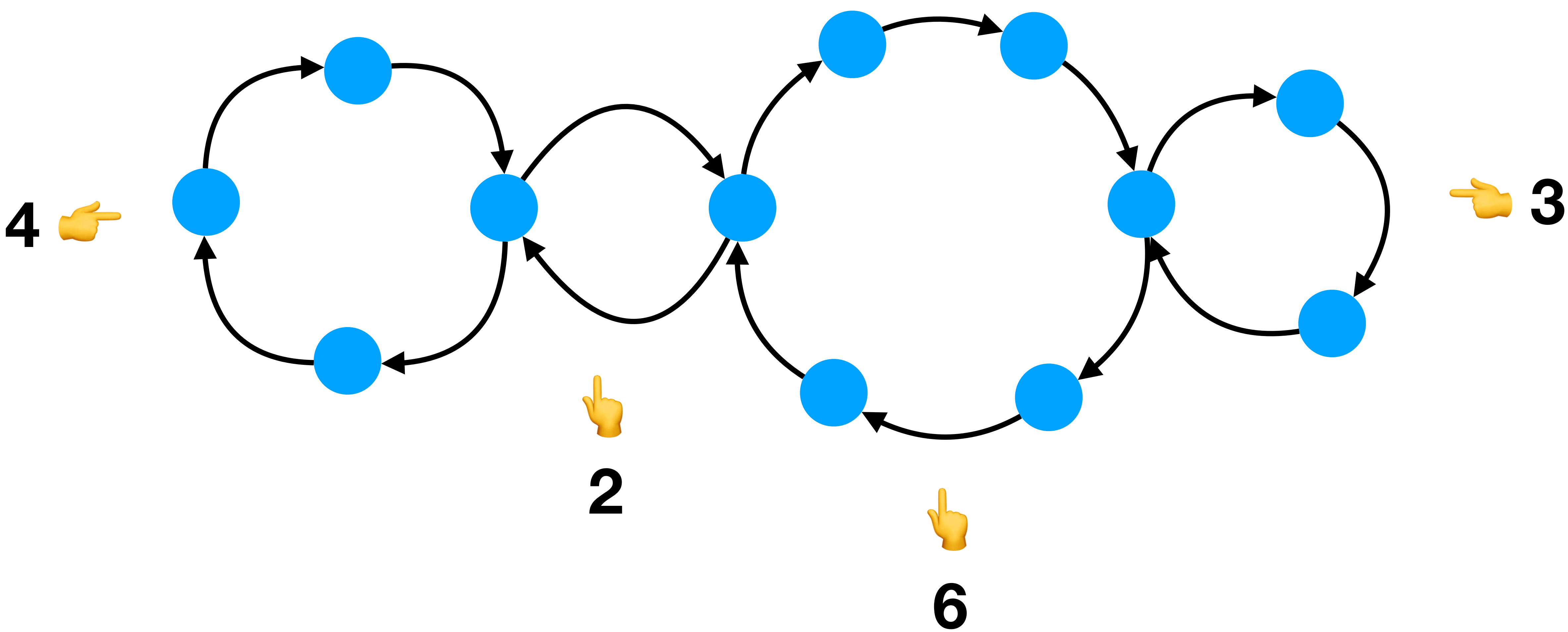
Chain-shaped dependencies ⛓️

⛓️ Theorem

🧬 **IF** the dependency graph of a RS consists only of a chain of self-sustaining, non-self-inhibiting cycles containing two cycles of coprime lengths,

🏃‍♀️ **THEN** the RS has exactly two fixed points

⛓️ Theorem in action



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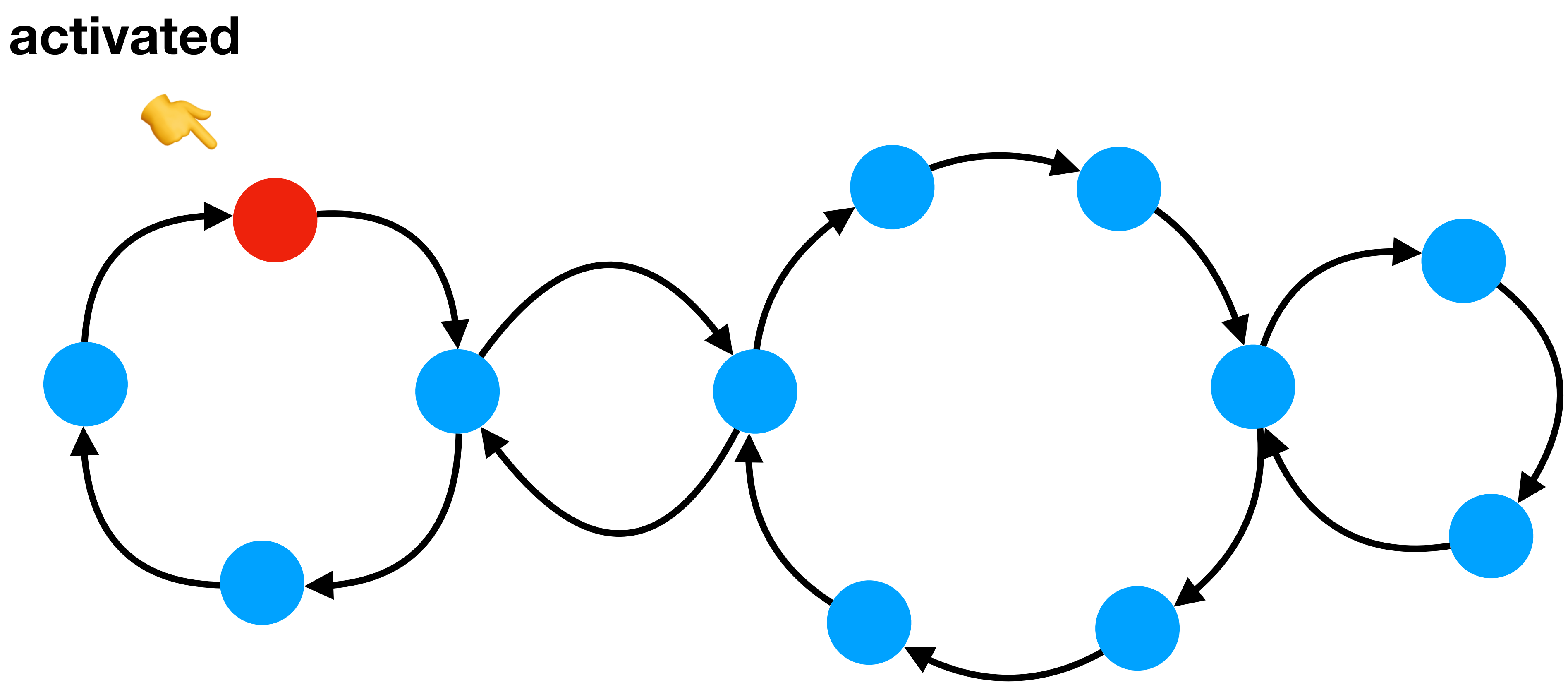

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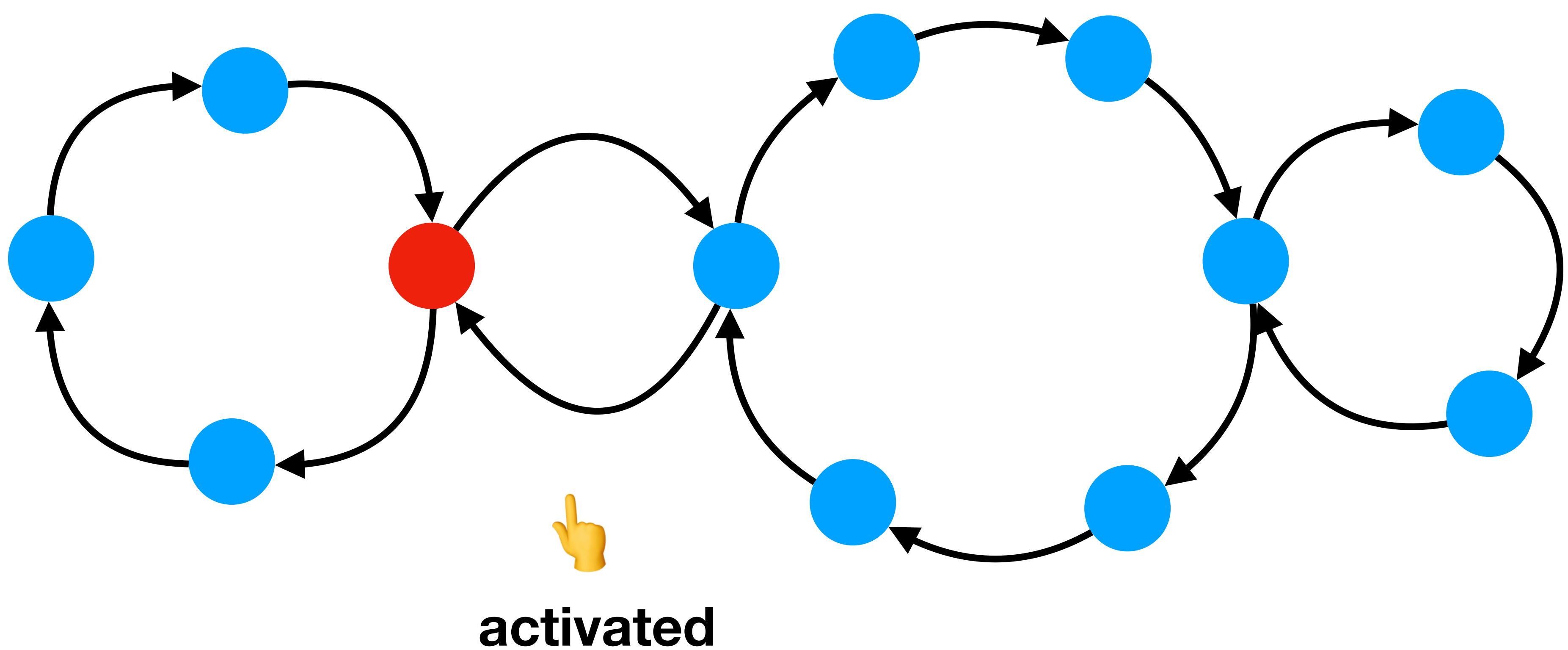

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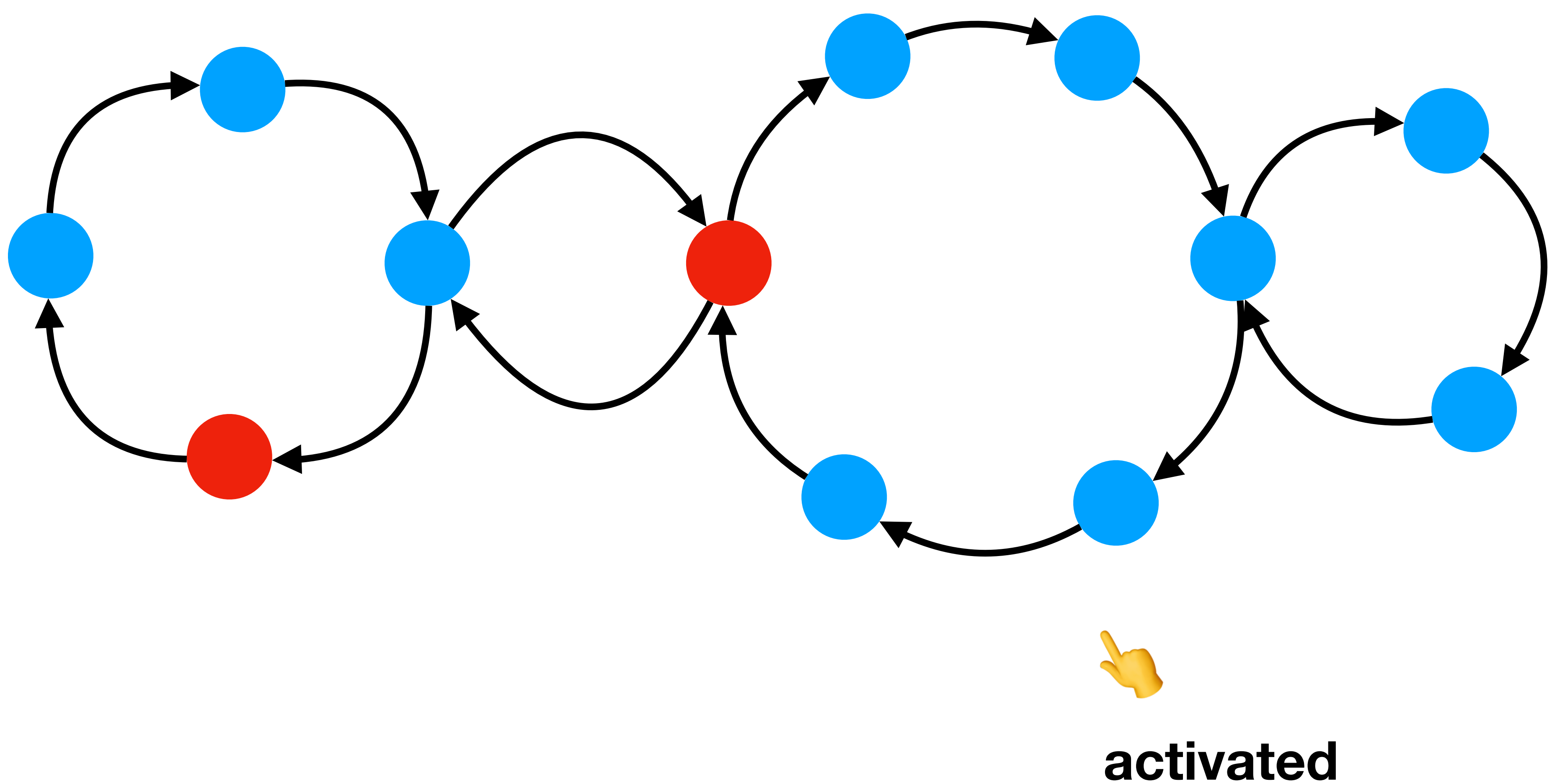

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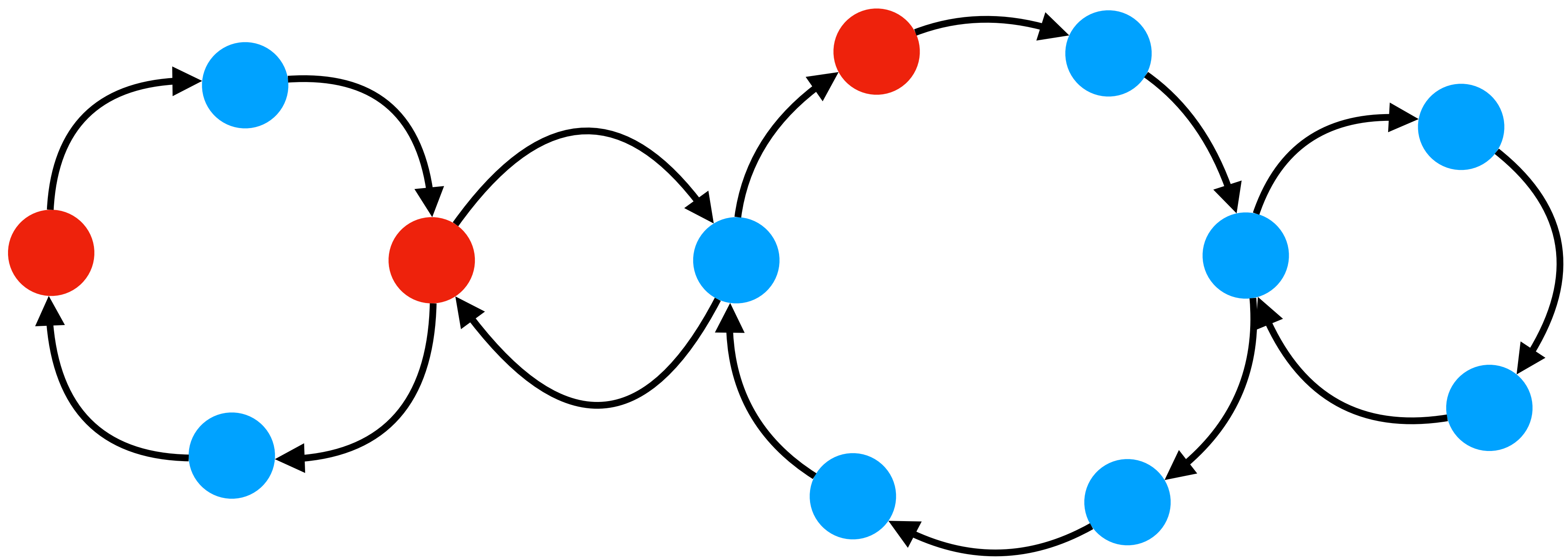

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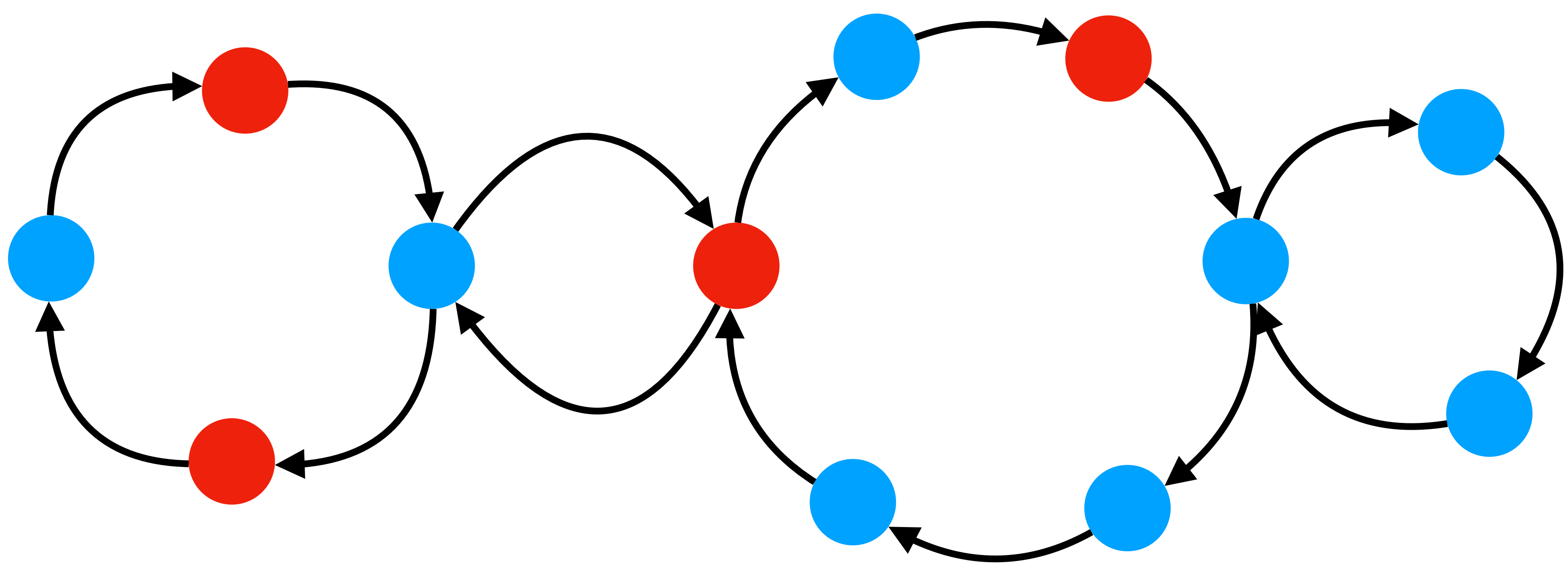

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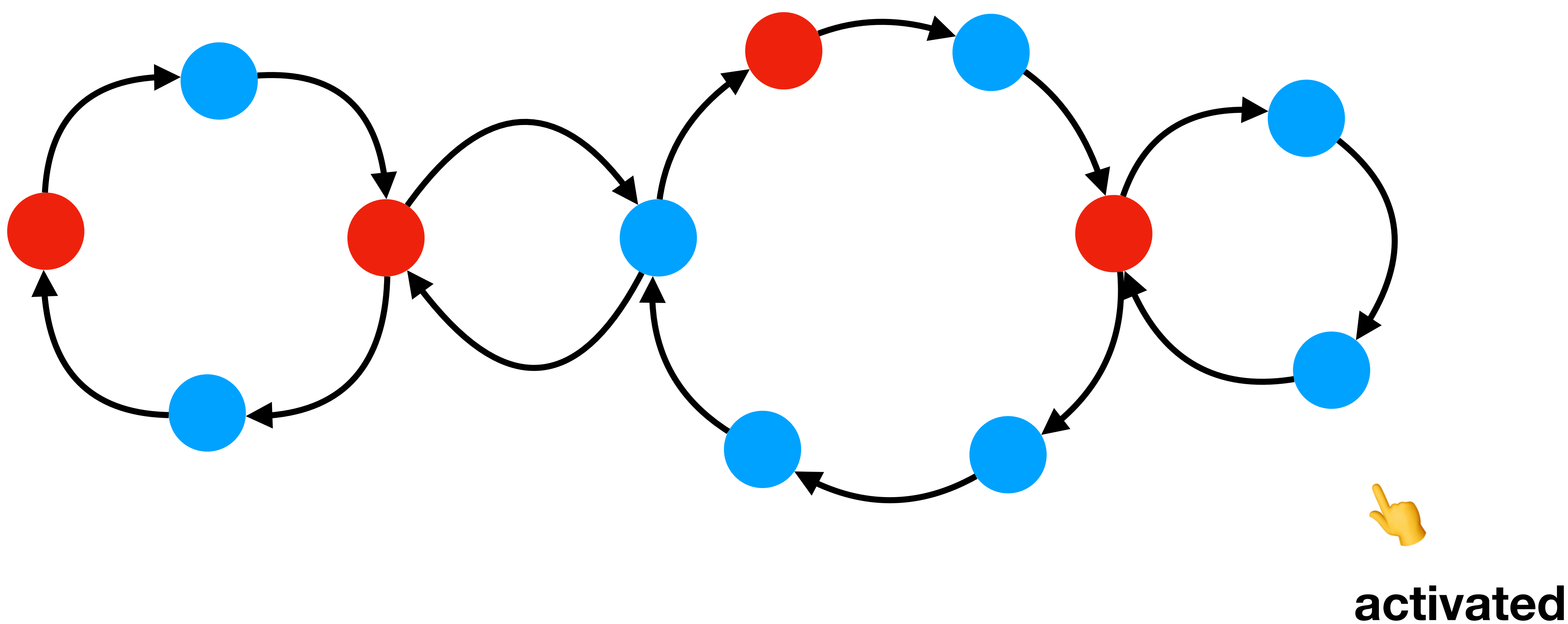
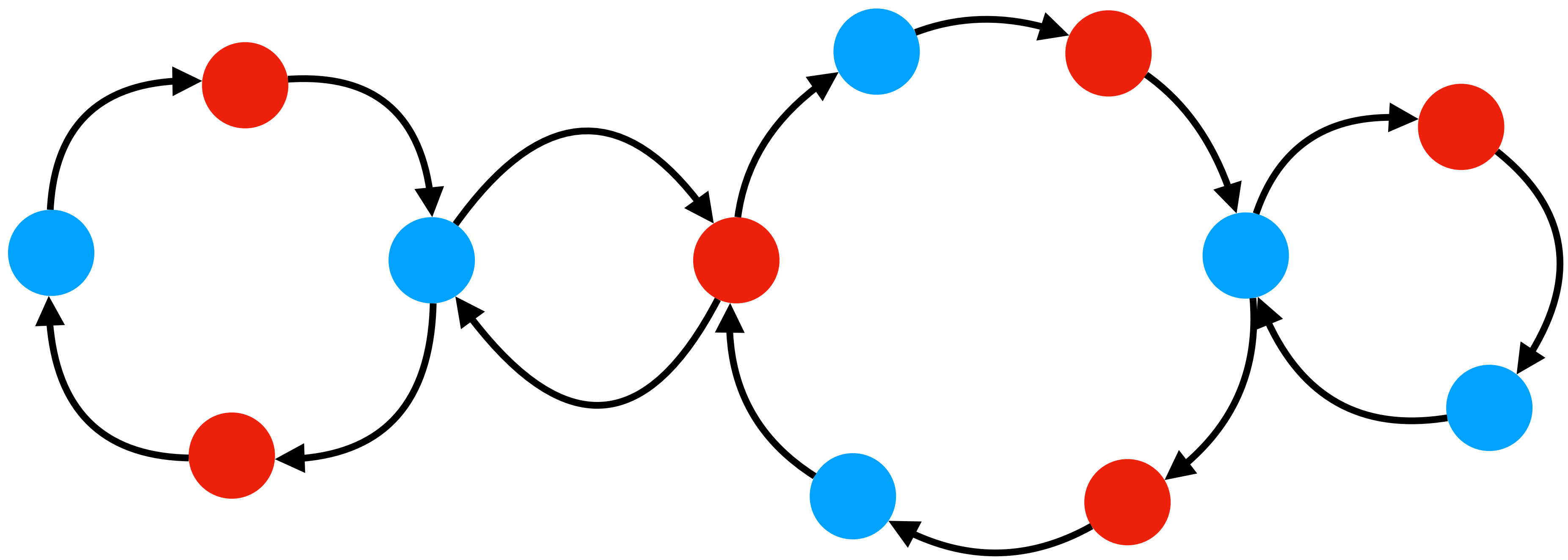


Theorem in action



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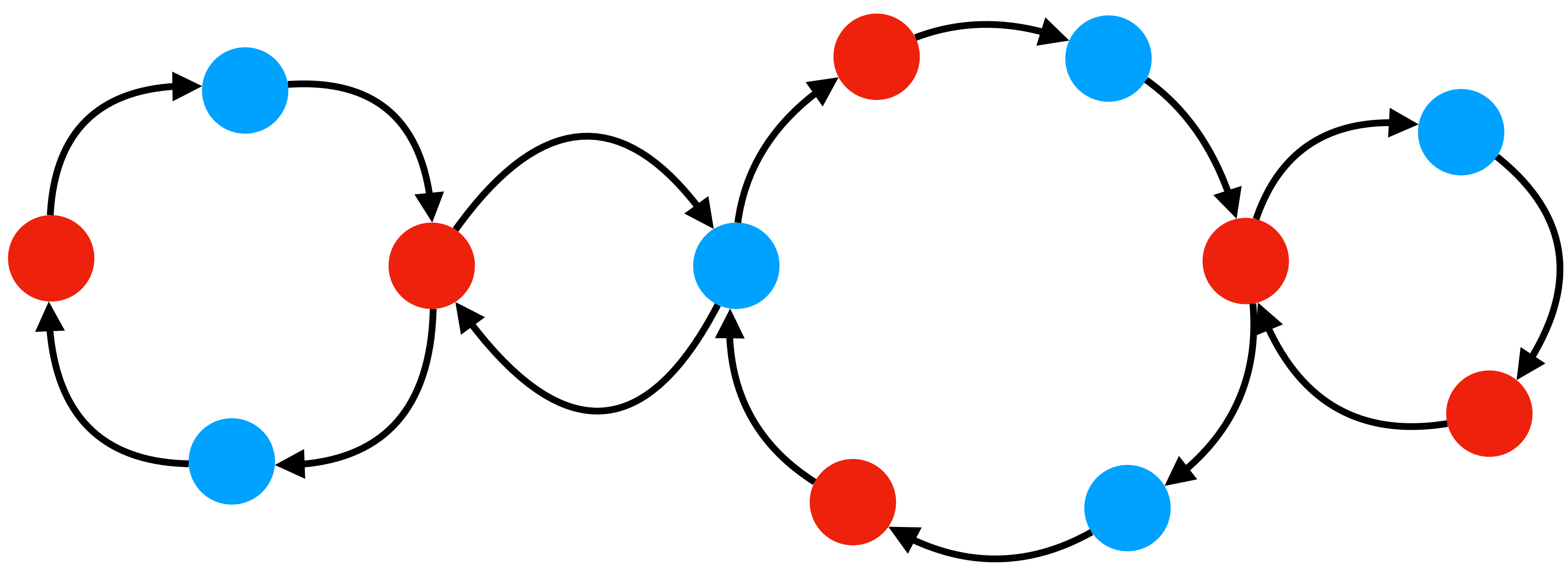

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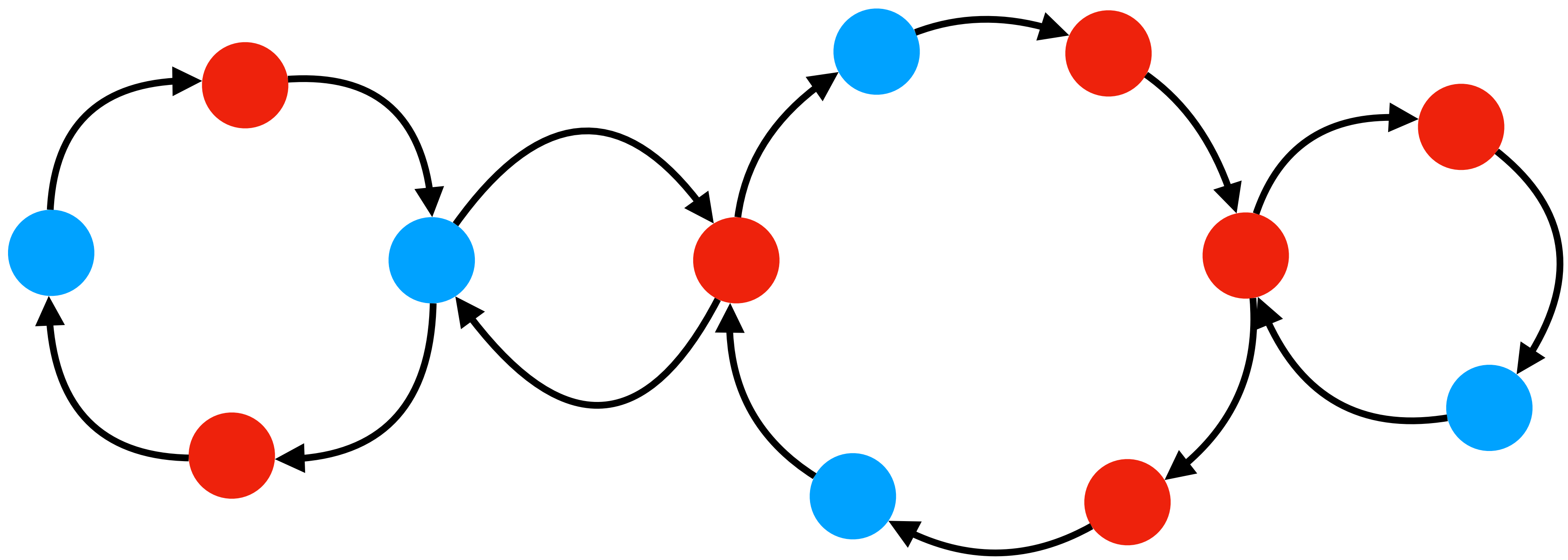

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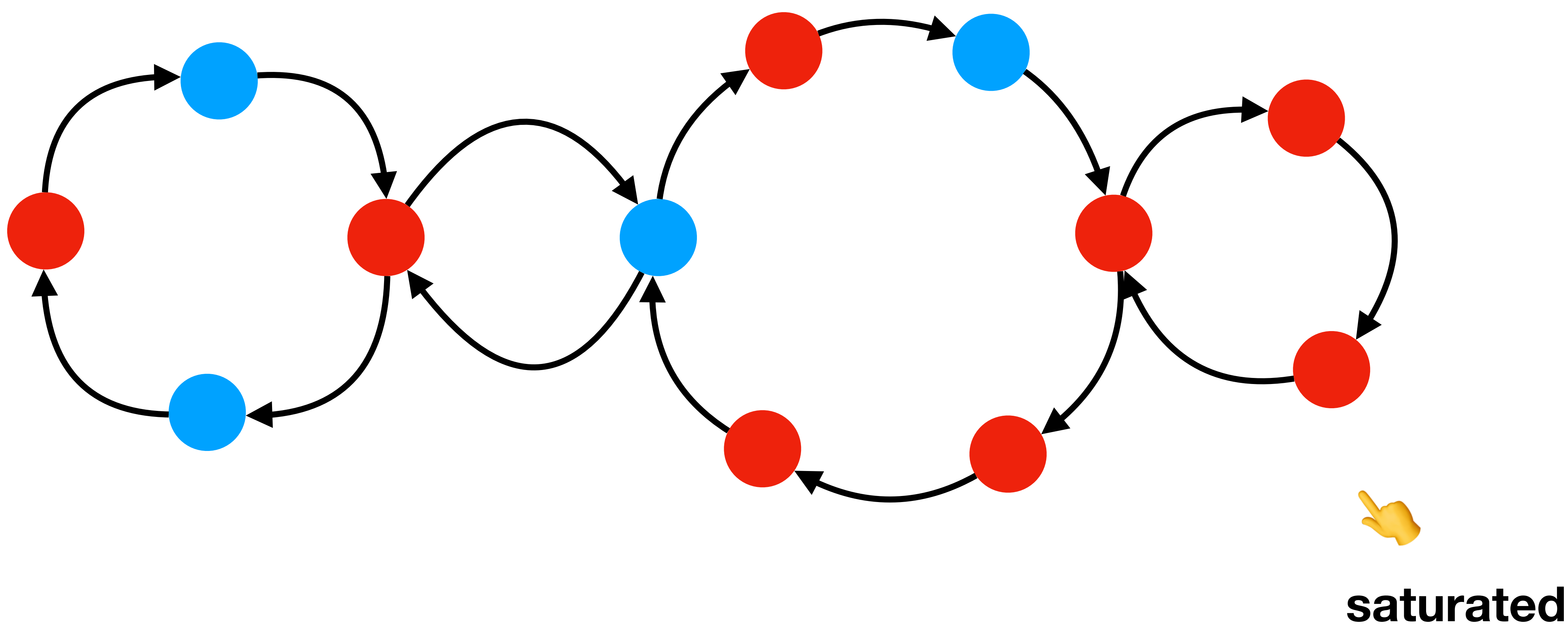

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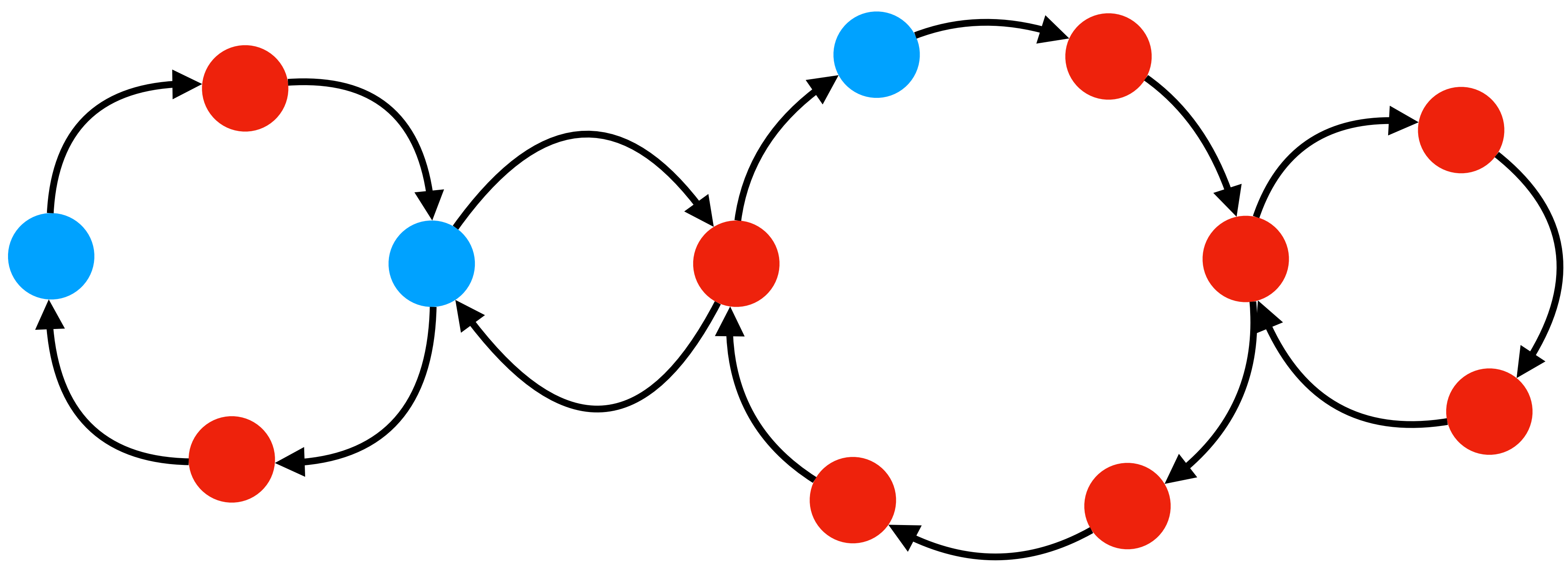

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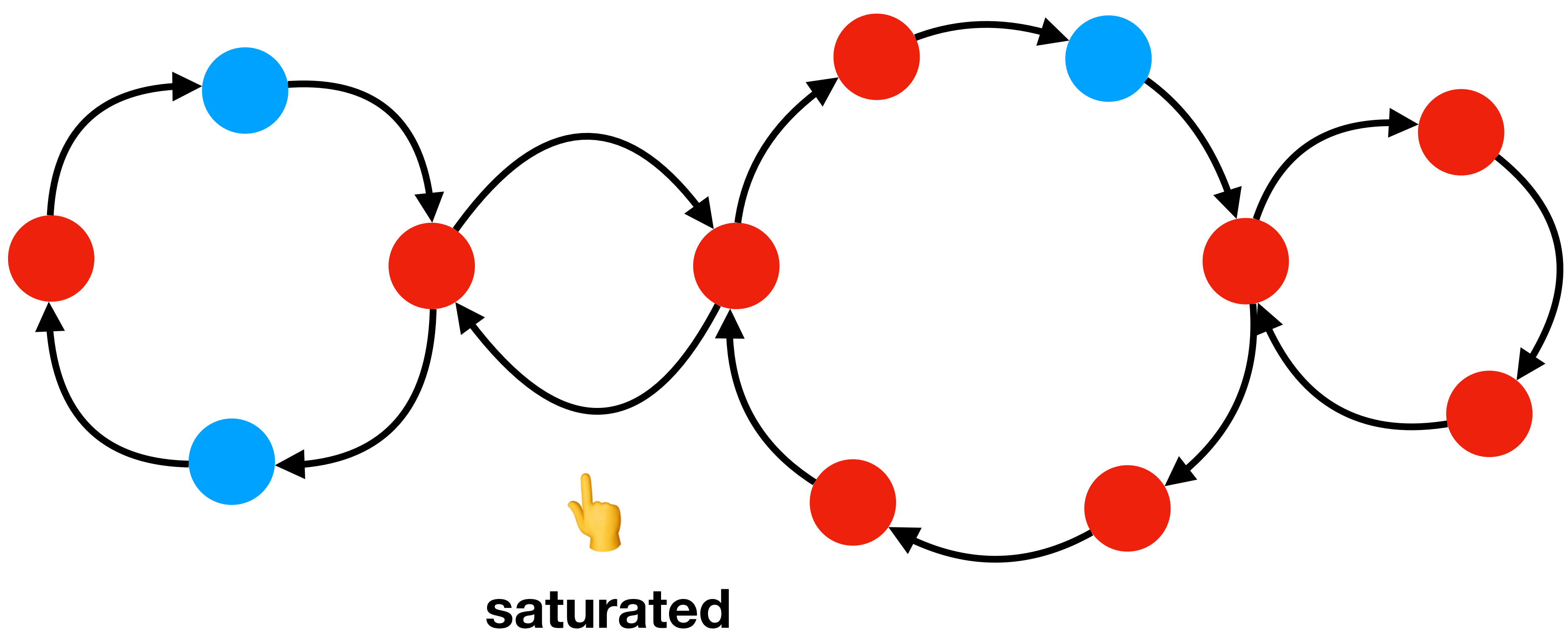

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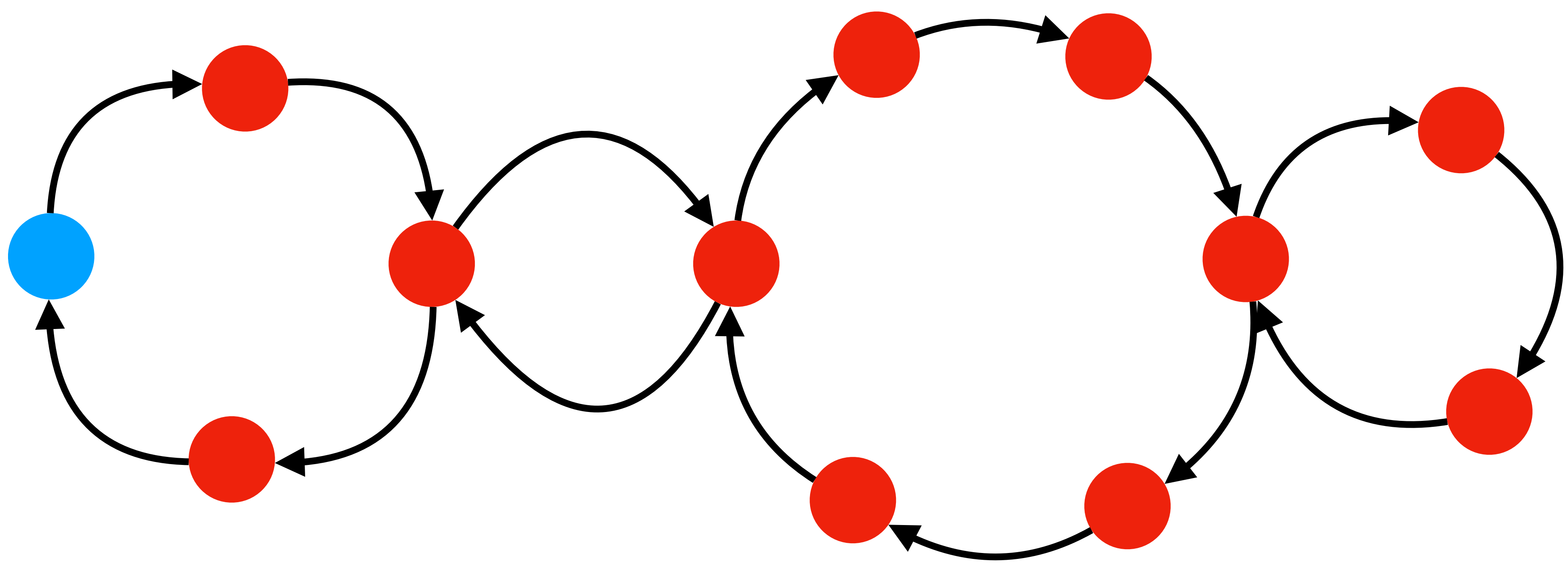
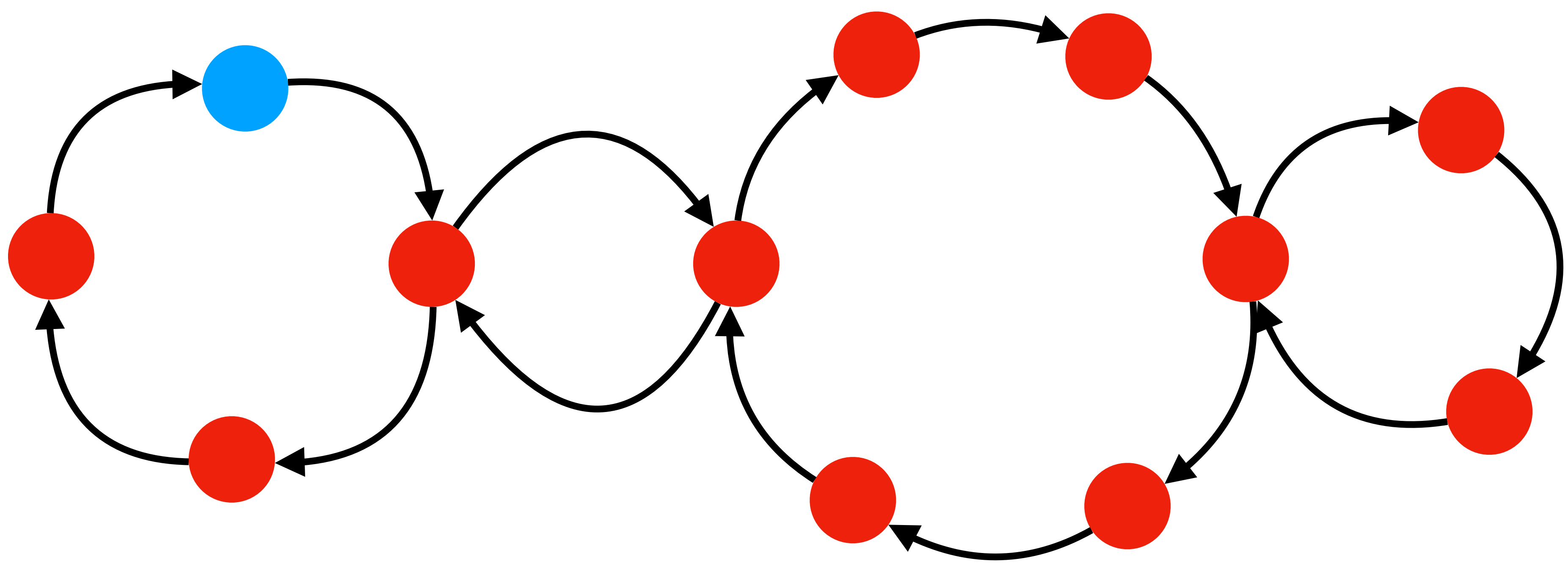


👆

saturated

⛓ Theorem in action



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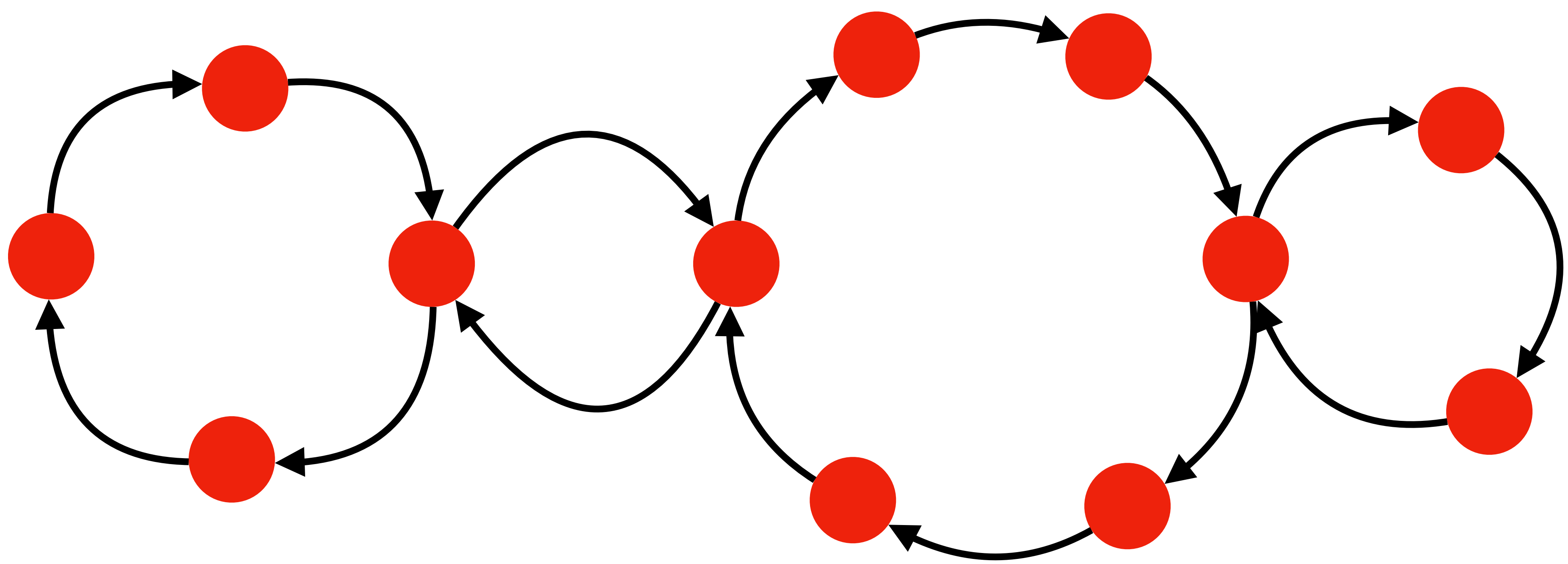

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Conclusions

Summary

Behaviour 🏃‍♀️ of RS having a dependency graph 🧬 consisting of self-sustaining, non-self-inhibiting cycles:

- with a single cycle of length n 🧬, the dynamics of the RS contains only cycles of length dividing n 🏃‍♀️
- with a chain or flower with two cycles of coprime length 🧬, the RS has exactly two fixed points 🏃‍♀️

Future work

- Does restricting the dependency graphs to cycles, chains and flowers 🧬 reduce the complexity of decision problems related to the dynamics? 🏃‍♀️ (e.g., fixed points, reachability)

- Investigate the relationship with Boolean automata networks and their interaction graphs 🧬

- Investigate more sophisticated dependency graphs 🧬 (e.g., pre-periods, multiple intersections between cycles)

Dziękuje za uwagę!

Thanks for your attention!