

On the power of oritatami cotranscriptional folding with unary bead sequence⁰

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科学技術振興機構
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What is oritatami system?

Oritatami system is a mathematical model for co-transcriptional folding(CF). (Geary, Meunier, Schabanel and Seki. MFCS 2016.)

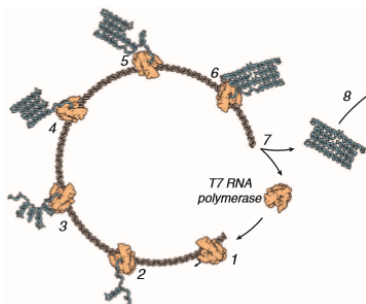


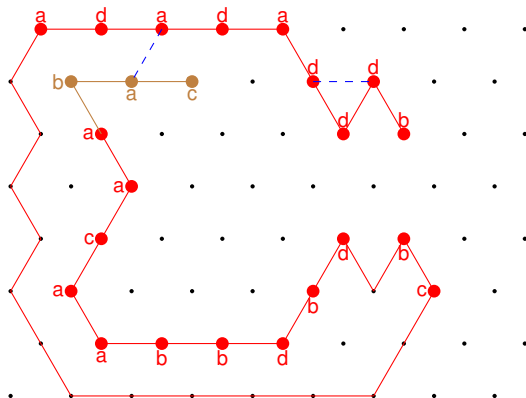
Figure: RNA tile is self-assembled (RNA Origami)

(Geary, Rothmund and Andersen. Science 345(6198), 2014)

How oritatami system works?

An example

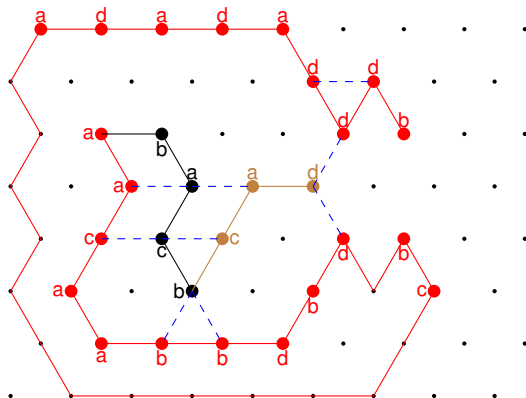
$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, delay $\delta = 3$, $w = \underline{bac}bcadbcbab$



How oritatami system works?

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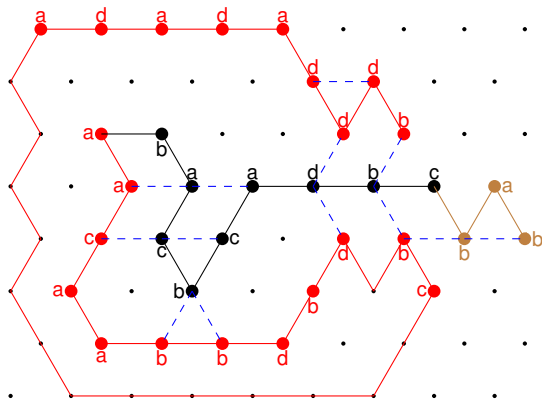
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Oritatami system and determinism

An example

$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, delay $\delta = 3$, $w = \text{bacbcadbcbab}$



Turing universality

Theorem (Geary, Meunier, Schabanel and Seki. ISAAC 2018.)

Deterministic oritatami system at *delay* $\delta = 3$ are Turing complete. (the simulation needs 542 bead types)

- A smaller Turing universal system
- The characterization of non-Turing-universal systems

Theorem

Polynomial upper bounds on the size of structures

→ Not Turing universal

The system at *delay* $\delta = 1$ and *arity* $\alpha = 1$ is not Turing universal. (Demaine et al. DNA24, 2018.)

Problem

Problem

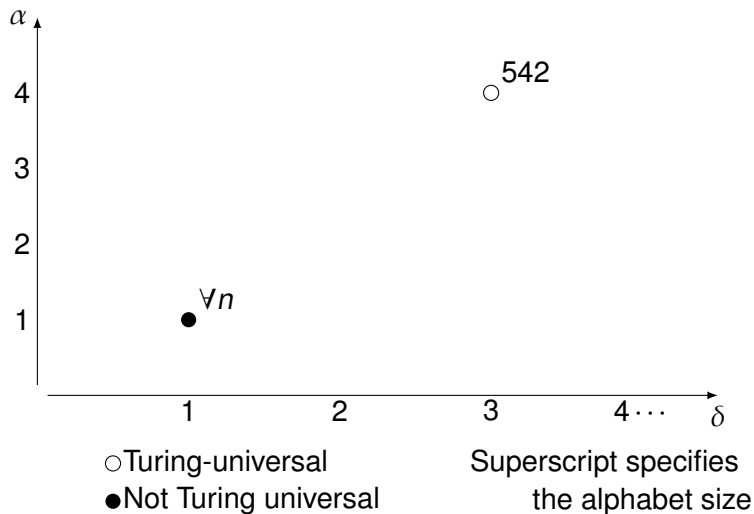
Give an upper bound on the length of a transcript of a *delay* δ , *arity* α deterministic oritatami system by a function in δ , α , and seed length n .

- input : *delay* δ , *arity* α and seed of length n
- output : an upper bound

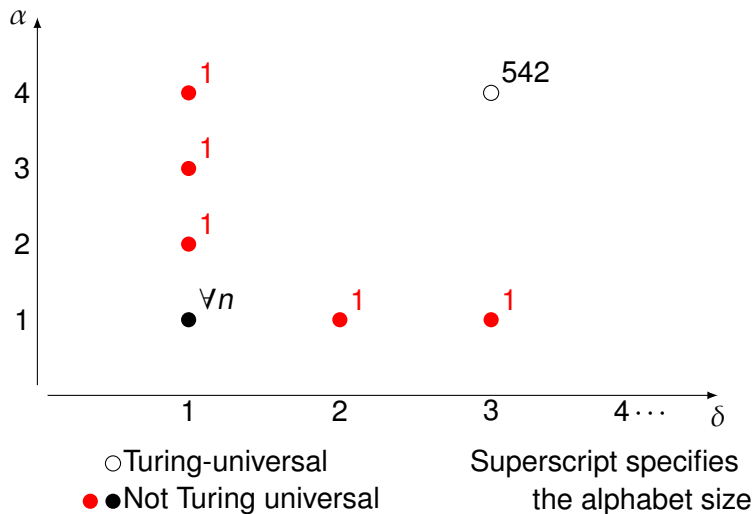
Unary variant

Let's focus on **unary**.

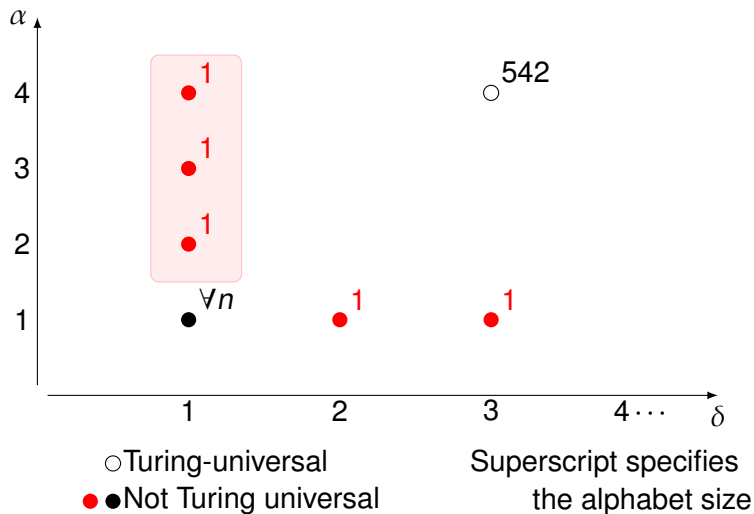
Turing universality and oritatami systems



Turing universality and oritatami systems



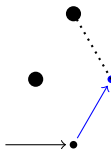
Turing universality and oritatami systems



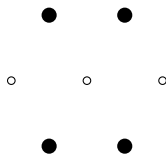
Oritatami systems at delay 1

The two ways to stabilize a bead at delay 1

- To be bound to another bead.
- Through a 1-in-1-out structure called the tunnel section.



Bond

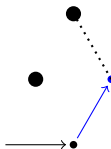


Tunnel section

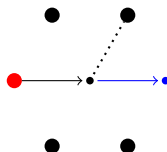
Oritatami systems at delay 1

The two ways to stabilize a bead at delay 1

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Tunnel section

Deterministic unary oritatami systems at delay 1

Results ($\delta = 1$)

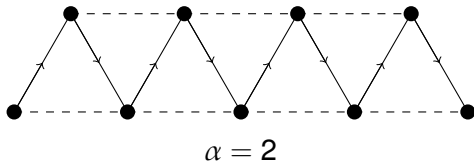
$$\alpha = 4 \quad 3n^2 + 3n + 1$$

$$\alpha = 3 \quad 4n + 14$$

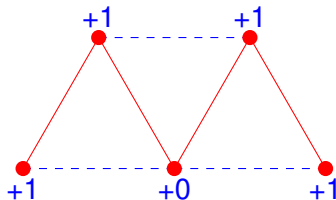
$$\alpha = 2 \quad \infty \text{ but zigzag after } (27n^2 + 9n + 1)$$

^a a

^ac.f. $\alpha = 1$: $10n$ (Demaine et al. 2018 DNA24)

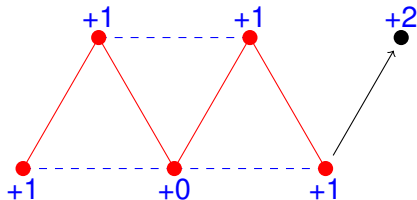


Deterministic **unary** oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag but cannot at larger arity



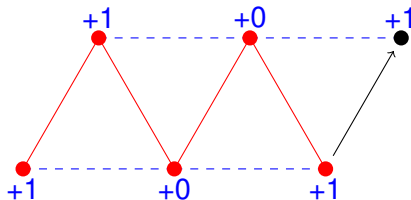
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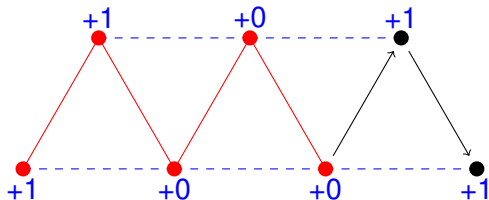
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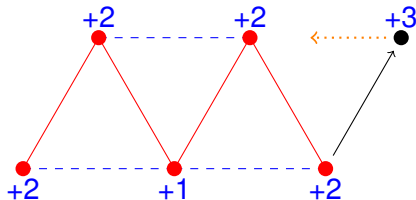
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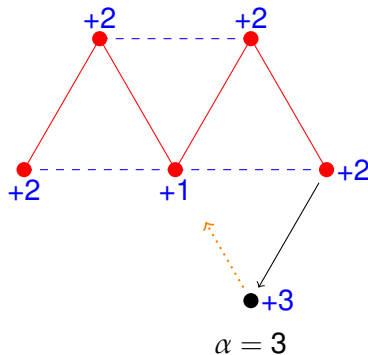
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Deterministic **unary** oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag but cannot at larger arity



$$\alpha = 3$$

Deterministic **unary** oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag but cannot at larger arity



Deterministic unary oritatami systems at delay 1

Results ($\delta = 1$)

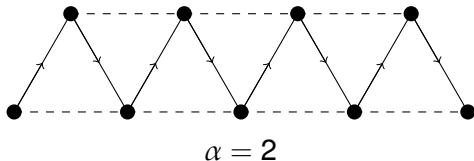
$$\alpha = 4 \quad 3n^2 + 3n + 1$$

$$\alpha = 3 \quad 4n + 14$$

$$\alpha = 2 \quad \infty \text{ but zigzag after } (27n^2 + 9n + 1)$$

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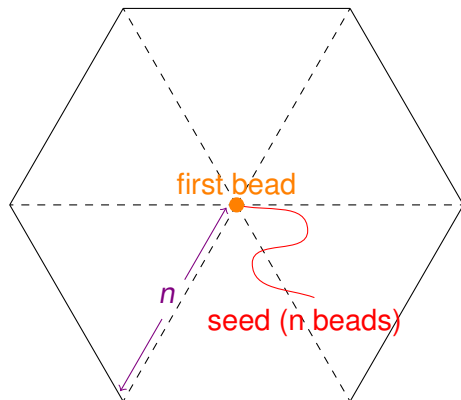
^ac.f. $\alpha = 1$: $10n$ (Demaine et al. 2018 DNA24)



Deterministic unary oritatami systems at delay 1

$$\alpha = 4$$

The terminal conformation at $\alpha = 4$ is of length at most $3n^2 + 3n + 1(\odot_O^n)$.

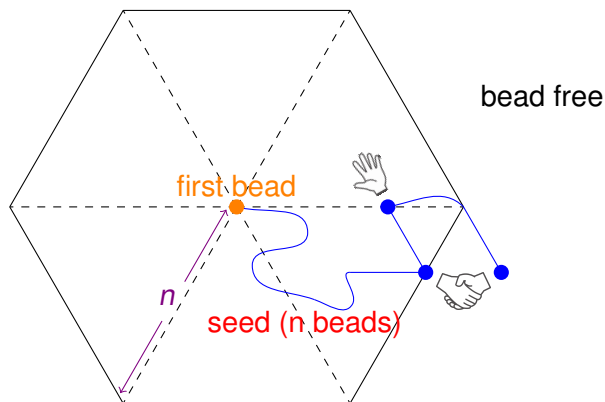


bead free

Deterministic unary oritatami systems at delay 1

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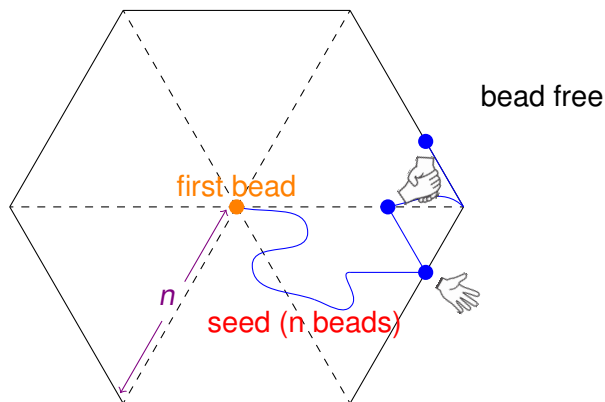
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Deterministic unary oritatami systems at delay 1

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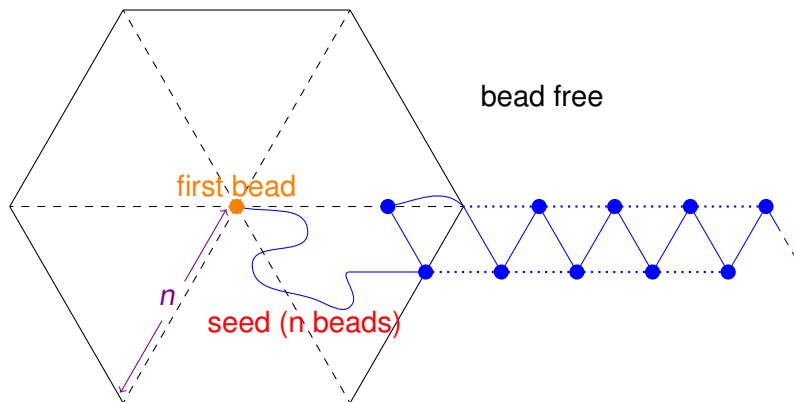
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Deterministic unary oritatami systems at delay 1

$$\alpha = 2 \ (\delta = 1)$$

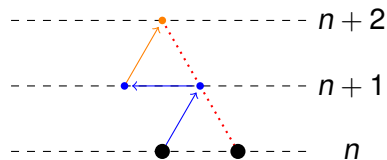
A transcript folds into the zig-zag conformation after its $(27n^2 + 9n + 1)$ -th bead ($\odot_{\mathcal{O}}^{3n}$).



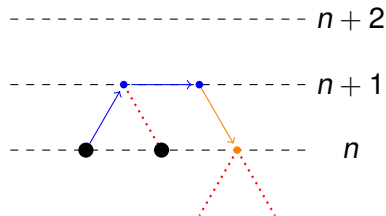
Deterministic unary oritatami systems at delay 1

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zig-zag

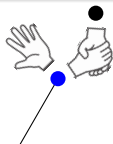


free hands: -2

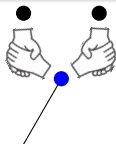
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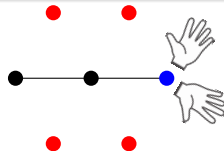
A transcript folds into the zig-zag conformation after its $(27n^2 + 9n + 1)$ -th bead (\hexagon_O^{3n}).



free hands: ± 0



free hands: -2

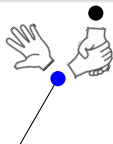


free hands: $\leq +2$

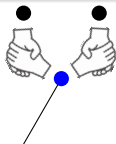
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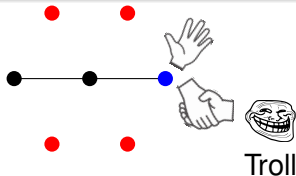
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Tunnel Troll Theorem



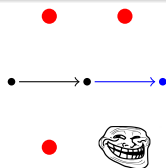
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Tunnel Troll Theorem

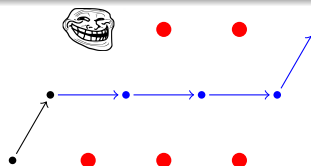
$\alpha \geq 4$ # of free hands does not increase / tunnel section.

$\alpha = 3$ Troll consumes bonds / tunnel section.

$\alpha = 2$ Troll consumes bonds / tunnel.



Tunnel section

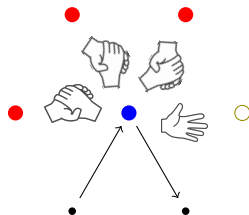
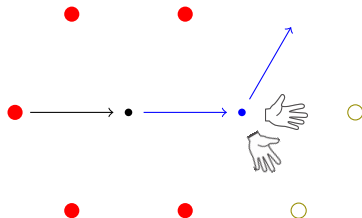


Tunnel

Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

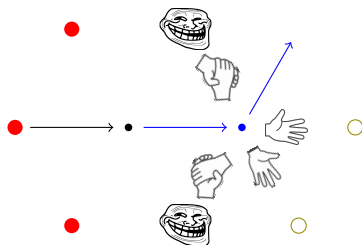
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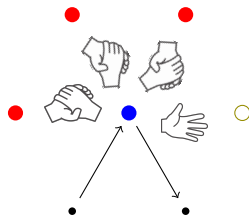
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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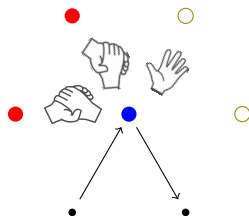
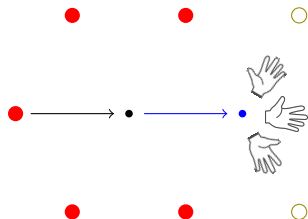
free hands ≤ 0



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

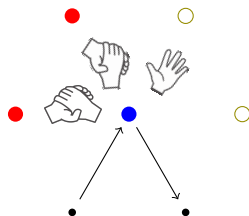
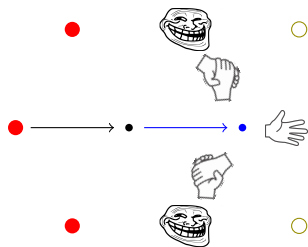
$\alpha = 3$ At least one free hand is consumed / tunnel section.



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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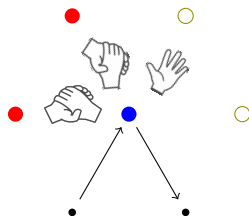
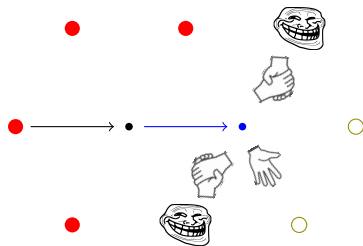


free hands ≤ -1

Deterministic unary oritatami systems at delay 1

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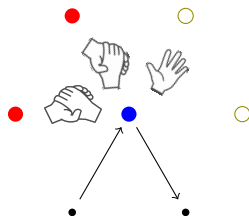
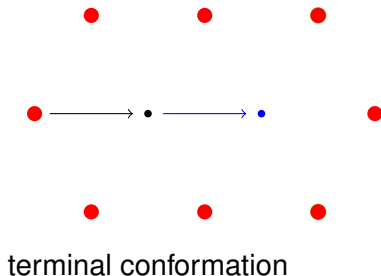


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Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

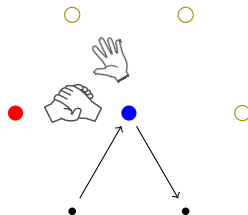
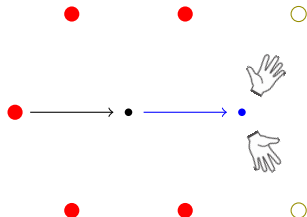
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Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

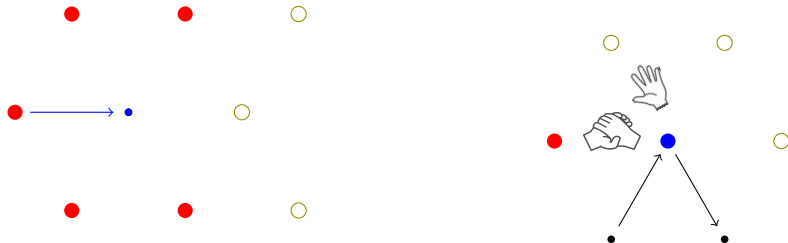
$\alpha = 2$ At least one free hand is consumed / tunnel.



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

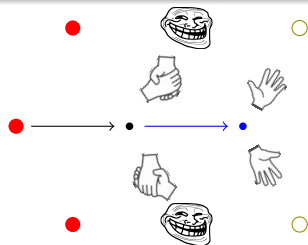
$\alpha = 2$ At least one free hand is consumed / tunnel.



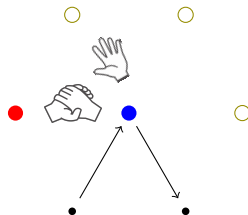
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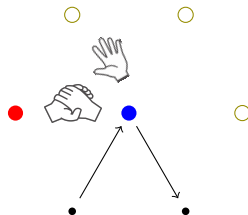
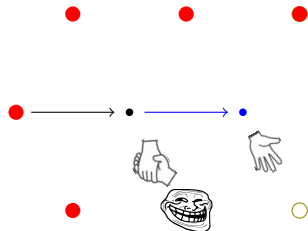
free hands ≤ 0



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

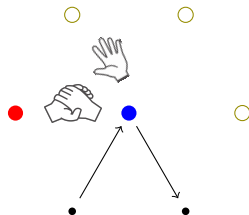
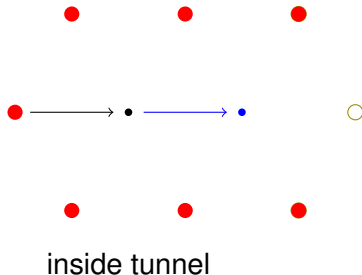
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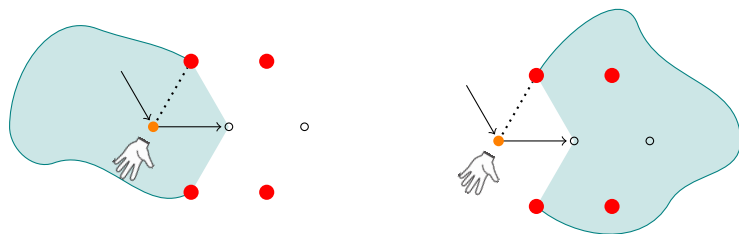
$\alpha = 2$ At least one free hand is consumed / tunnel.



Deterministic unary oritatami systems at delay 1

Jordan curve theorem

A closed curve which is non-self-intersecting, divides the plane into inside and outside.



At $\alpha = 2$, Troll consumes free hands at an entrance of tunnel, too.

ご清聴ありがとうございました。



Szilárd Zsolt Fazekas



Shinnosuke Seki

Collaborators

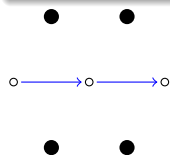
Future works

- Case of $\delta \geq 4$
- Non unary case
- Other ways of simulating Turing machine

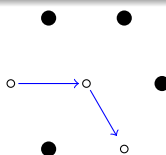
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

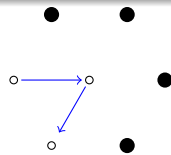
Type of tunnel sections



Straight



Obtuse

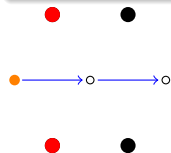


Accute

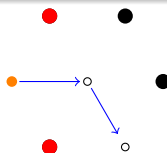
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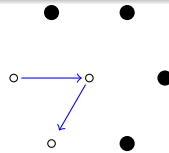
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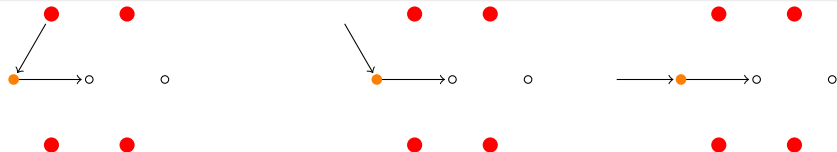


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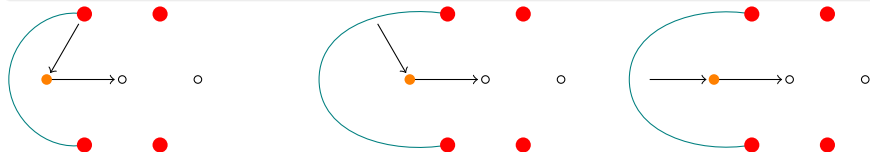
Directions to enter a tunnel



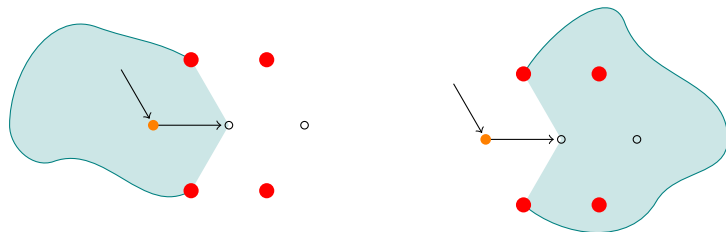
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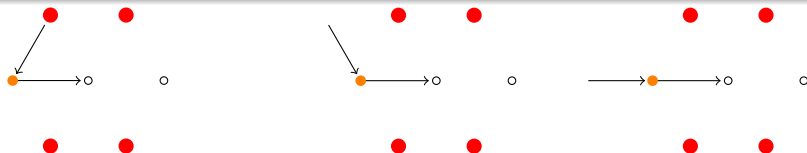
freehands $\leq \pm 0$



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

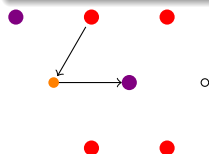
If this orange bead is stabilized by bonds, total bonds decrease.



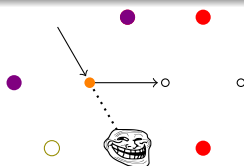
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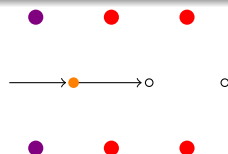
If this orange bead is stabilized by bonds, total bonds decrease.



cannot follow



Troll...



inside tunnel

freehands ≤ -1

