

# On the power of oritatami cotranscriptional folding with unary bead sequence<sup>0</sup>

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科学技術振興機構  
Japan Science and Technology Agency

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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.)

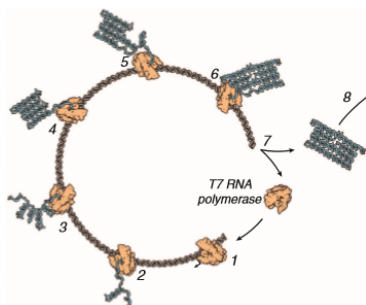


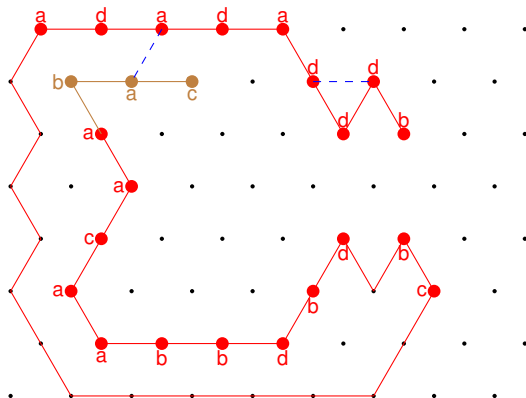
Figure: RNA tile is self-assembled (RNA Origami)

(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  $\delta = 3$ ,  $w = \underline{bac}bcadbcbab$

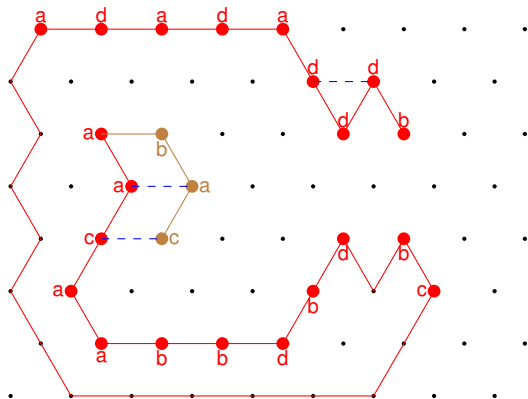




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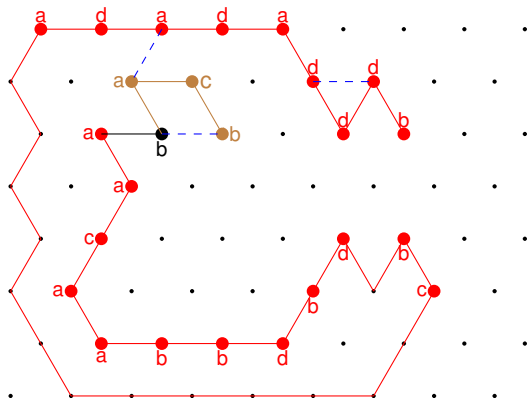


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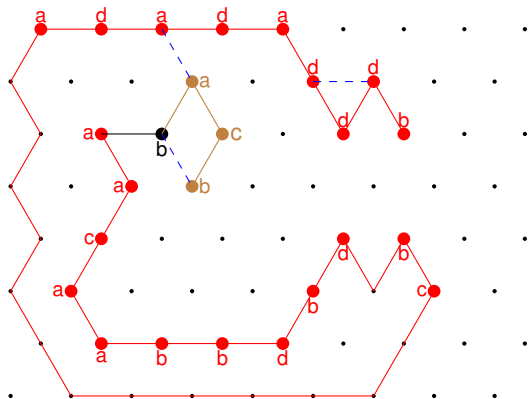
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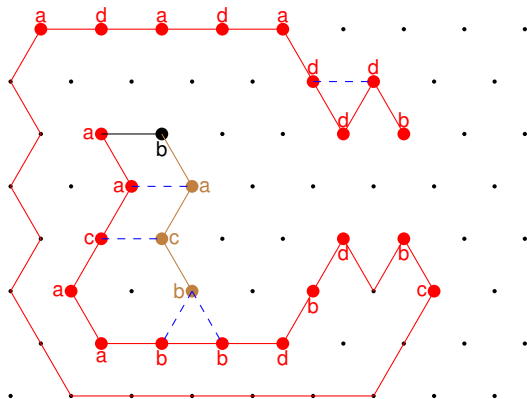
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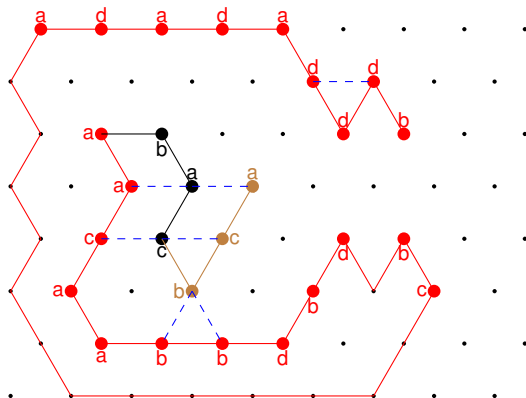




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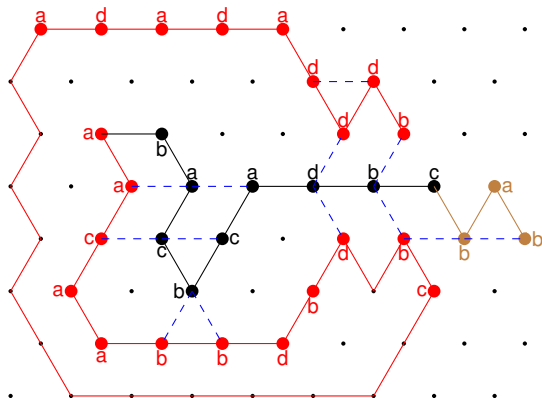


# Oritatami system and determinism

## An example

$$\Sigma = \{a, b, c, d\}, R = \{(a, a), (b, b), (c, c), (d, d)\},$$

arity  $\alpha = 2$ , delay  $\delta = 3$ ,  $w = bacbcadbcbab$



# 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

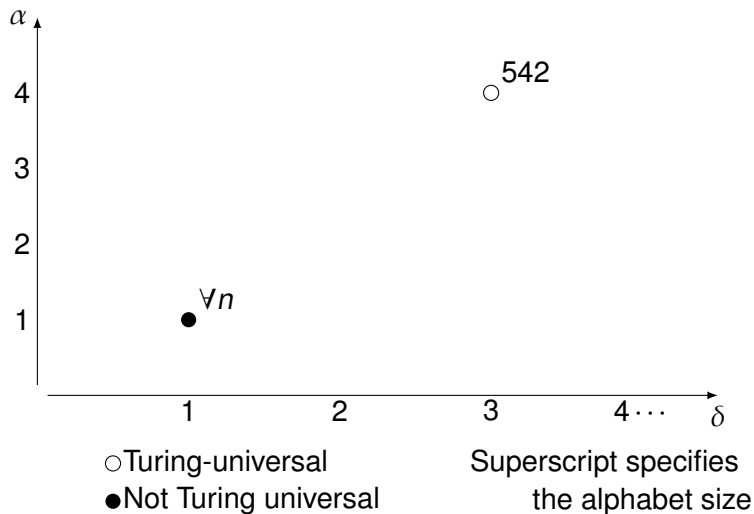
Give an upper bound on the length of a transcript of a *delay*  $\delta$ , *arity*  $\alpha$  deterministic oritatami system by a function in  $\delta$ ,  $\alpha$ , and seed length  $n$ .

- input : *delay*  $\delta$ , *arity*  $\alpha$  and seed of length  $n$
- output : an upper bound

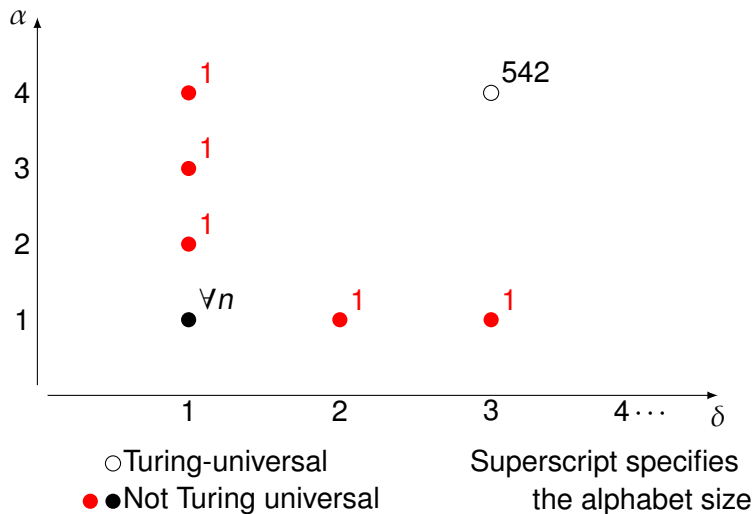
## Unary variant

Let's focus on **unary**.

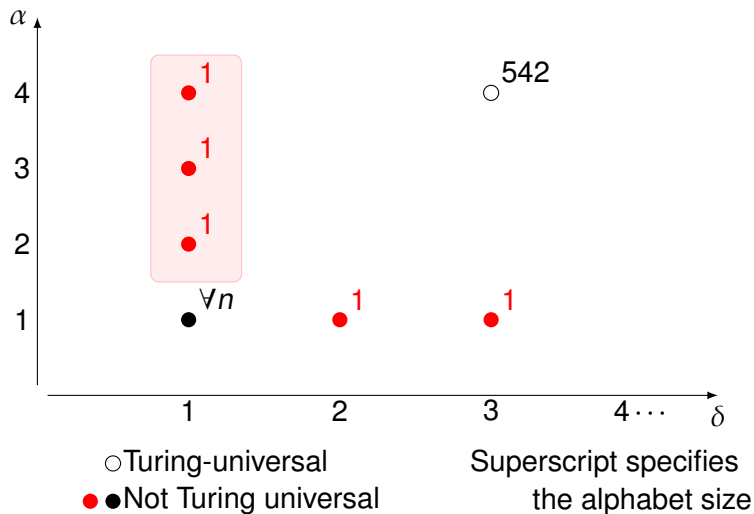
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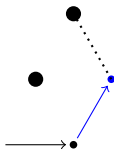
# Turing universality and oritatami systems



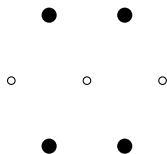
# Oritatami systems at delay 1

## 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

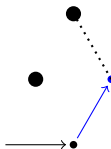


Tunnel section

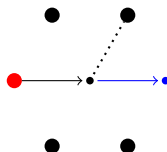
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Tunnel section

# Deterministic unary oritatami systems at delay 1

## Results ( $\delta = 1$ )

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

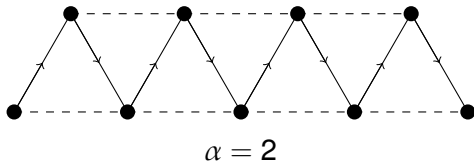
$$\alpha = 3 \quad 4n + 14$$

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

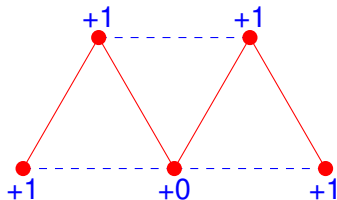
<sup>a</sup> $a$

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<sup>a</sup>c.f.  $\alpha = 1$ :  $10n$  (Demaine et al. 2018 DNA24)



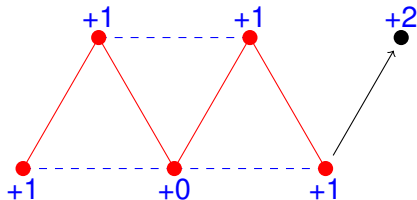
Deterministic **unary** oritatami system at  $\delta = 1$  and at  $\alpha = 2$  can make zig-zag but cannot at larger arity



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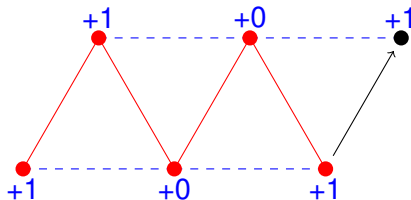


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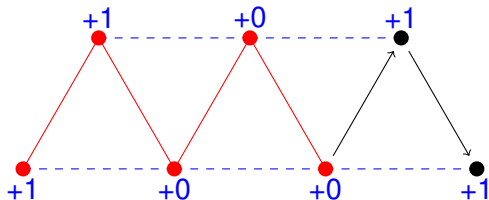
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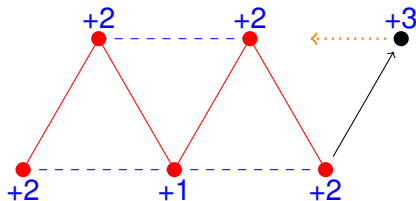
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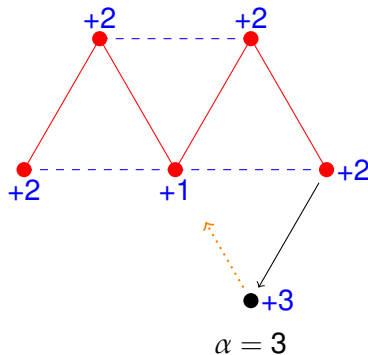
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Deterministic **unary** oritatami system at  $\delta = 1$  and at  $\alpha = 2$  can make zig-zag but cannot at larger arity



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# Deterministic unary oritatami systems at delay 1

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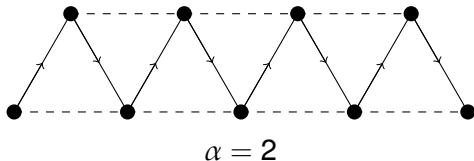
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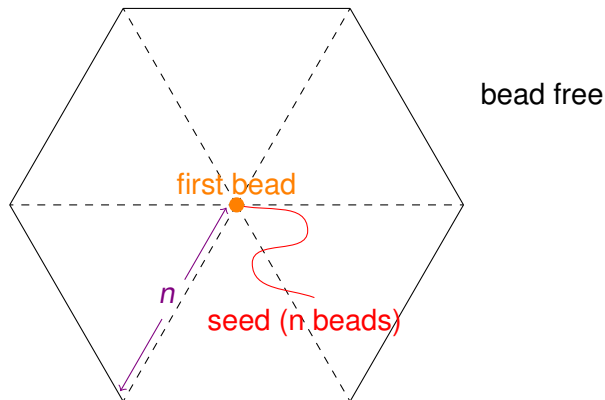
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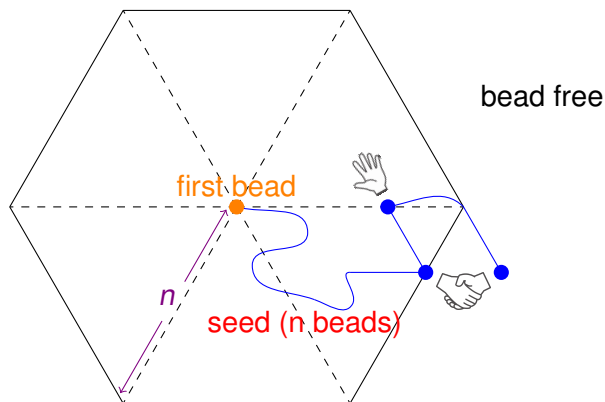
The terminal conformation at  $\alpha = 4$  is of length at most  $3n^2 + 3n + 1(\odot_O^n)$ .



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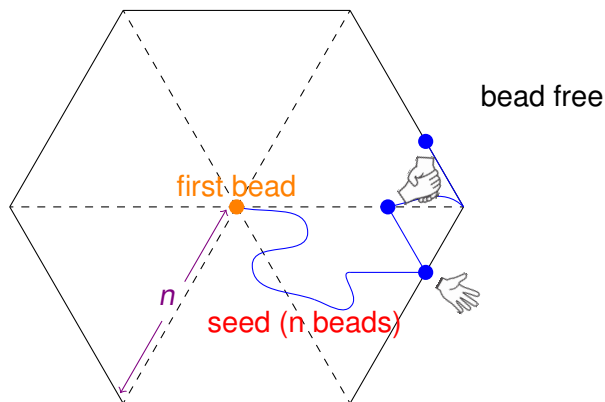




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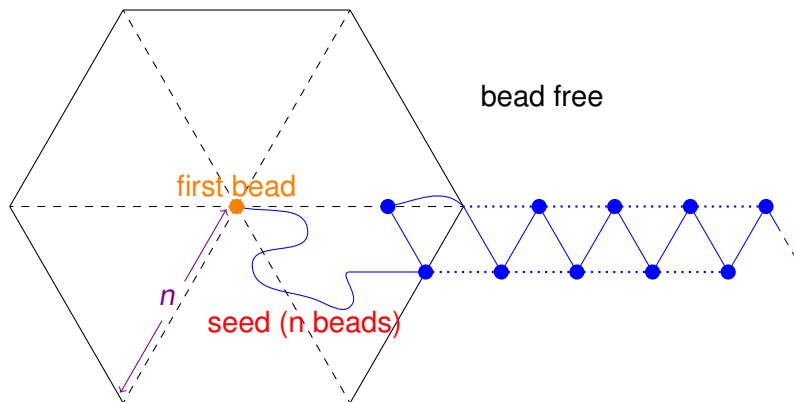
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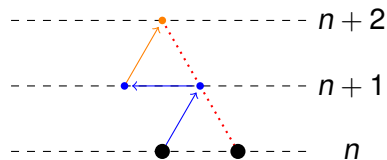
A transcript folds into the zig-zag conformation after its  $(27n^2 + 9n + 1)$ -th bead ( $\odot_{\mathcal{O}}^{3n}$ ).



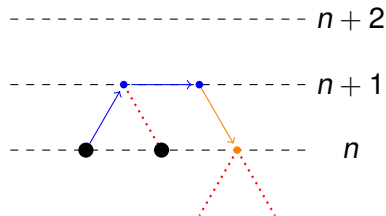
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zig-zag

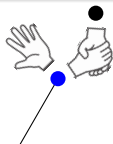


free hands:  $-2$

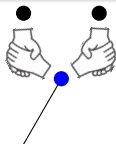
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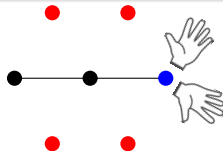
A transcript folds into the zig-zag conformation after its  $(27n^2 + 9n + 1)$ -th bead ( $\hexagon_O^{3n}$ ).



free hands:  $\pm 0$



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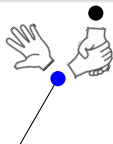


free hands:  $\leq +2$

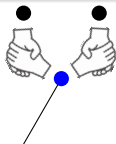
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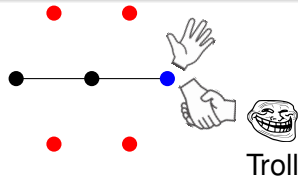
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## Tunnel Troll Theorem



Illustrated by Gido

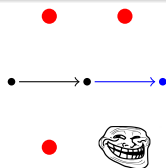
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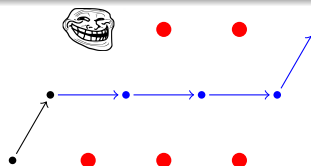
$\alpha \geq 4$  # of free hands does not increase / tunnel section.

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

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Tunnel section

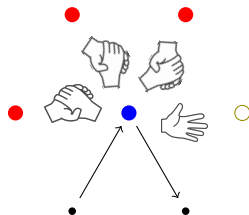
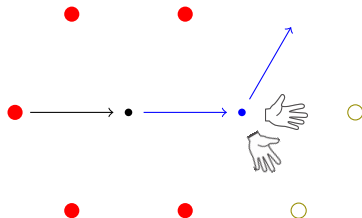


Tunnel

# Deterministic unary oritatami systems at delay 1

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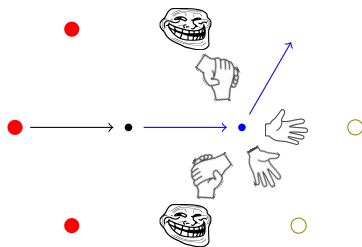




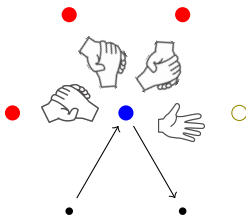
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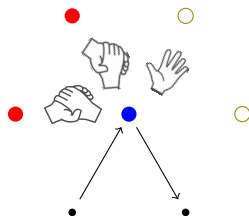
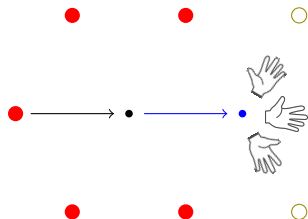
free hands  $\leq 0$



# Deterministic unary oritatami systems at delay 1

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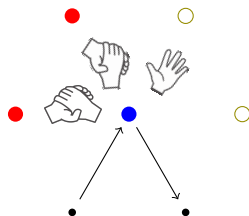
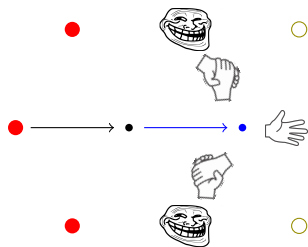
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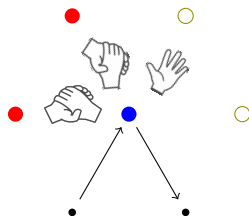
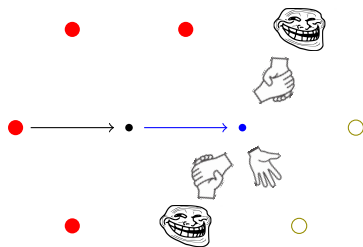


free hands  $\leq -1$

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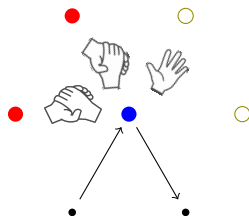
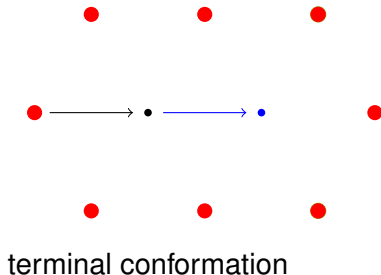


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## Tunnel Troll Theorem

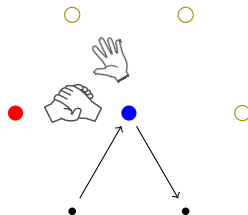
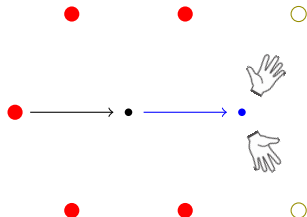
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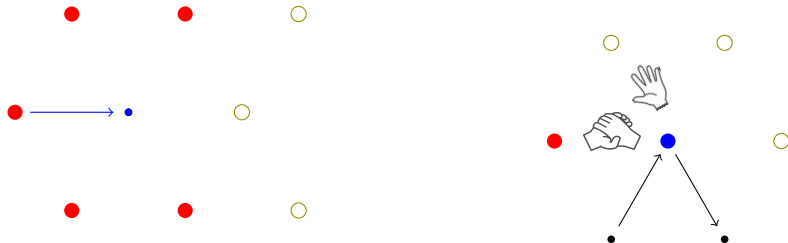
$\alpha = 2$  At least one free hand is consumed / tunnel.



# Deterministic unary oritatami systems at delay 1

## Tunnel Troll Theorem

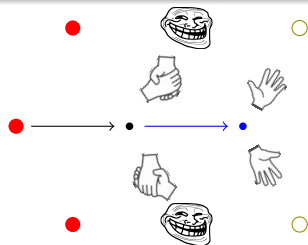
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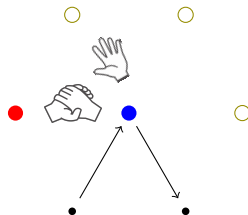
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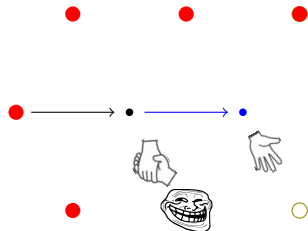




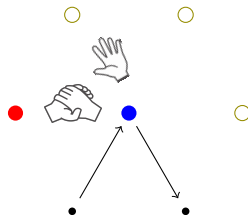
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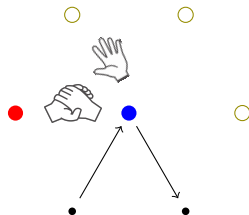
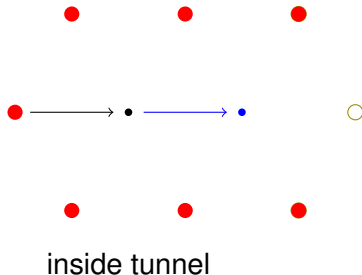
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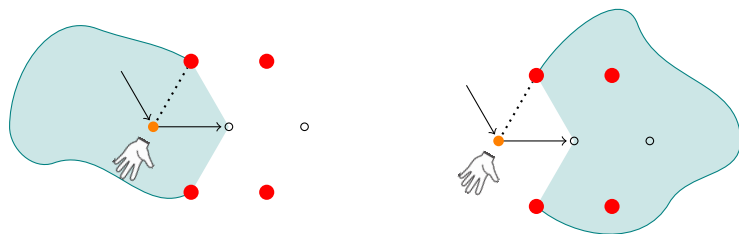
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# Deterministic unary oritatami systems at delay 1

## 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

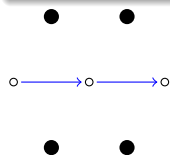
## Future works

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

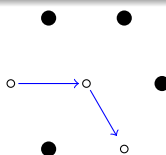
# Deterministic unary oritatami systems at delay 1

## Tunnel Troll Theorem ( $\alpha = 2$ )

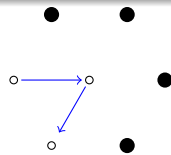
Type of tunnel sections



Straight



Obtuse

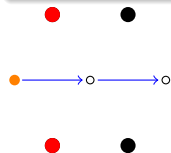


Accute

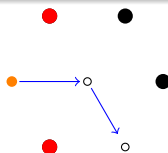
# Deterministic unary oritatami systems at delay 1

## Tunnel Troll Theorem ( $\alpha = 2$ )

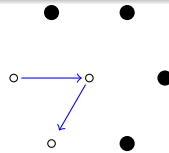
Type of tunnel sections



Straight



Obtuse

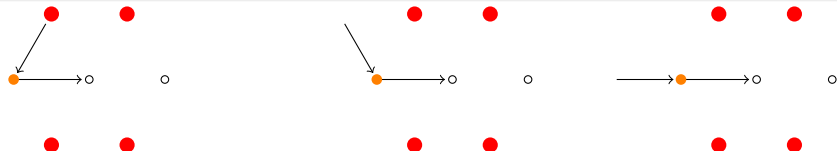


Accute

# Deterministic unary oritatami systems at delay 1

## Tunnel Troll Theorem ( $\alpha = 2$ )

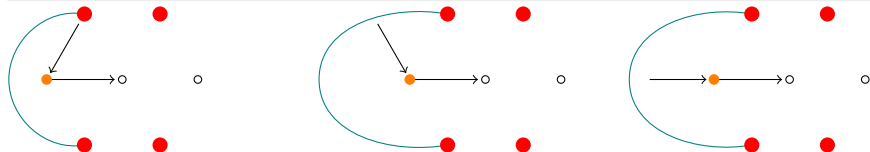
Directions to enter a tunnel



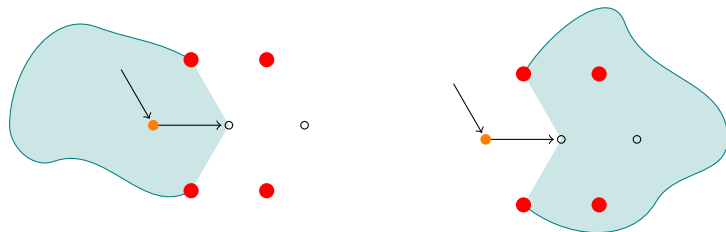
# Deterministic unary oritatami systems at delay 1

## Tunnel Troll Theorem ( $\alpha = 2$ )

### Directions to enter a tunnel



freehands  $\leq \pm 0$

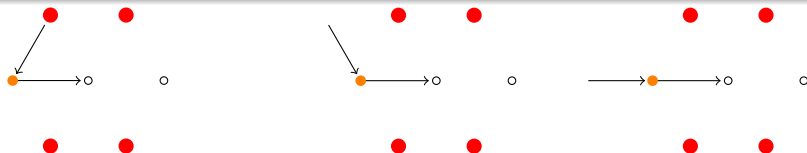




# Deterministic unary oritatami systems at delay 1

## Tunnel Troll Theorem ( $\alpha = 2$ )

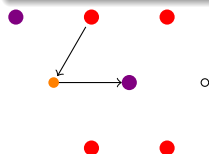
If this orange bead is stabilized by bonds, total bonds decrease.



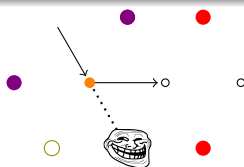
# Deterministic unary oritatami systems at delay 1

## Tunnel Troll Theorem ( $\alpha = 2$ )

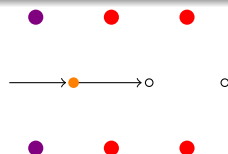
If this orange bead is stabilized by bonds, total bonds decrease.



cannot follow



Troll...



inside tunnel

freehands  $\leq -1$

