

On the power of oritatami cotranscriptional folding with unary bead sequence⁰

Szilárd Zsolt Fazekas¹, Kohei Maruyama², Reoto Morita²,
Shinnosuke Seki²

¹Akita University, ²University of Electro-Communications

TAMC2019



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

⁰ Supported by KAKENHI Grant-in-Aid for Challenging Research (Exploratory) No. 18K19779 and JST Program to Disseminate Tenure Tracking System No. 6F36

What is oritatami system?

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

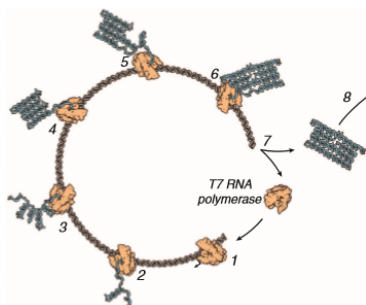


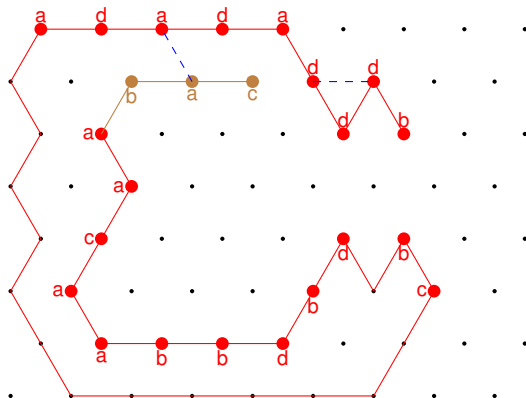
Figure: RNA tile is self-assembled (RNA Origami)

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

How oritatami system works?

An example

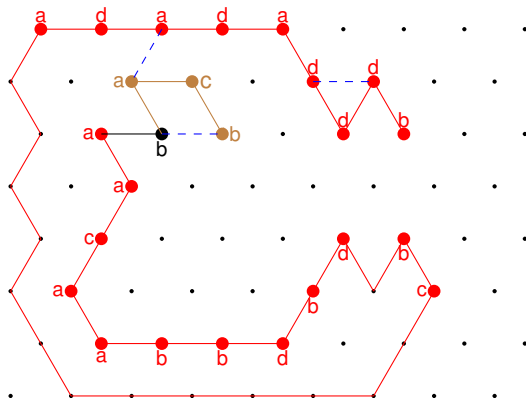
$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, delay $\delta = 3$, $w = \underline{bac}bcadbcbab$



How oritatami system works?

An example

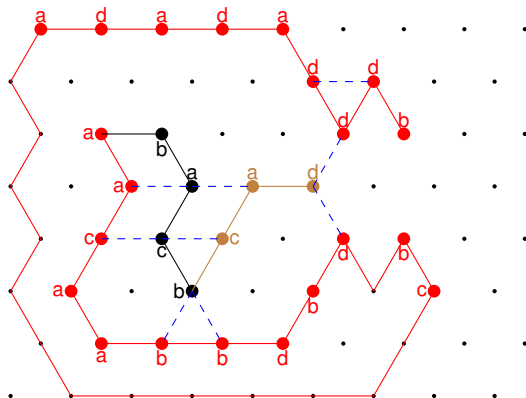
$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, delay $\delta = 3$, $w = \underline{bacb}cadbcbab$



How oritatami system works?

An example

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

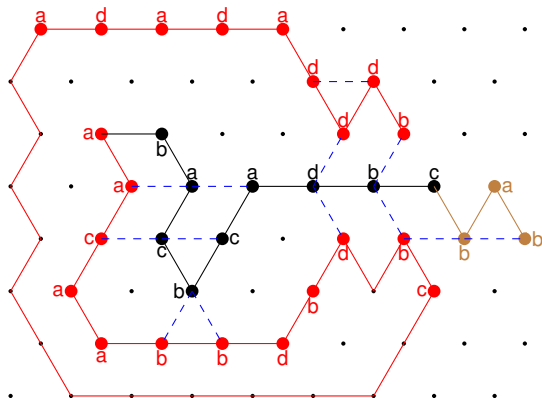


Oritatami system and determinism

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.)

The deterministic oritatami system at *delay* $\delta = 3$ with 542 types of beads is Turing universal.

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

Theorem

Polynomial upper bounds on the size of structures
→ Non-Turing-universality

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

Problem

Problem

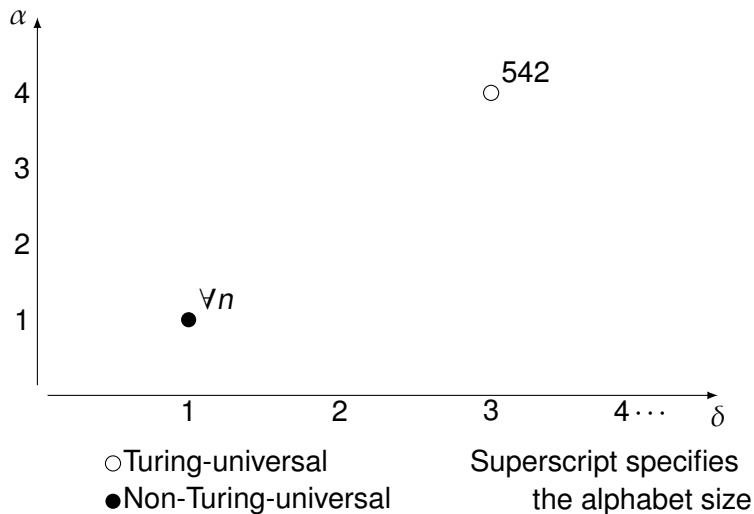
Give an upper bound on the length of a transcript of a *delay* δ , *arity* α deterministic oritatami system by a function in δ , α , and seed n .

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

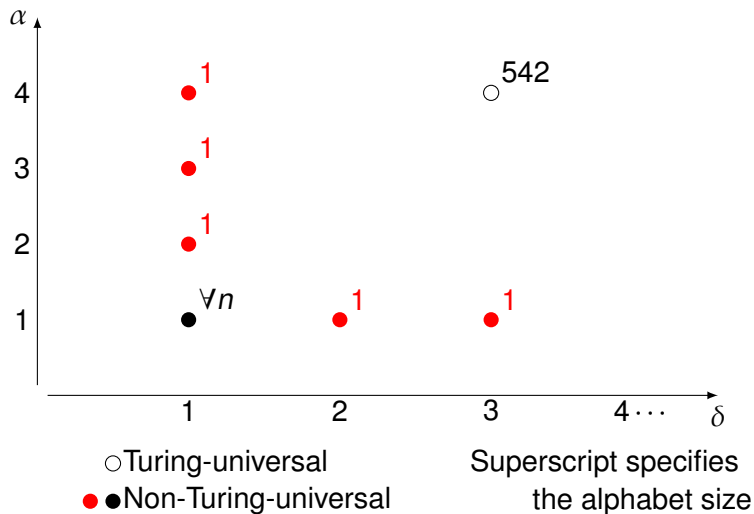
Unary variant

Let's focus on **unary**.

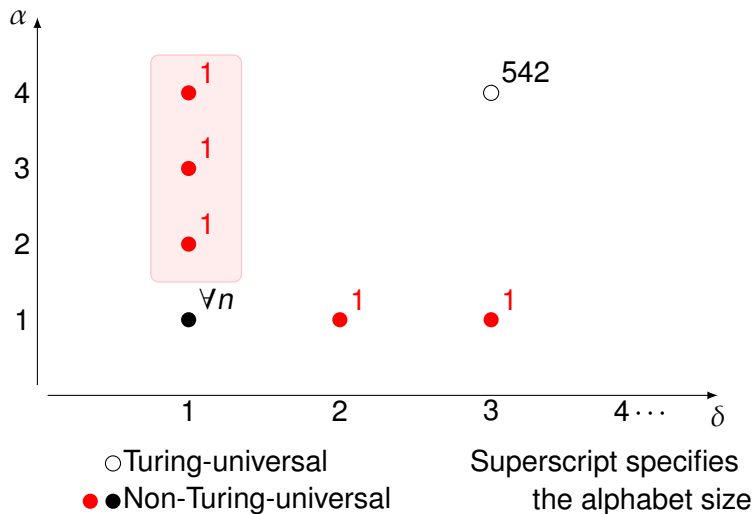
Turing-universal oritatami systems



Turing-universal oritatami systems



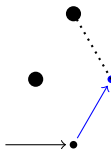
Turing-universal oritatami systems



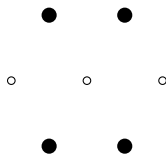
Oritatami systems at delay 1

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

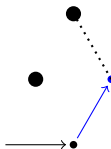


Tunnel section

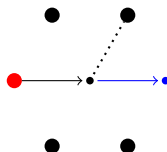
Oritatami systems at delay 1

The two ways to stabilize a bead at delay 1

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



Bond



Tunnel section

Deterministic unary oritatami systems at delay 1

Results ($\delta = 1$)

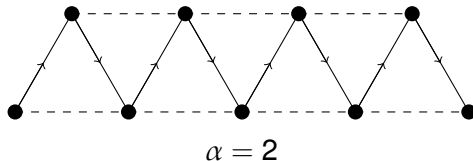
$$\alpha = 4 \quad 3n^2 + 3n + 1$$

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

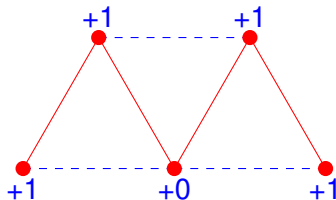
$$\alpha = 2 \quad \infty \text{ but zigzag after } (27n^2 + 9n + 1)$$

^a a

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

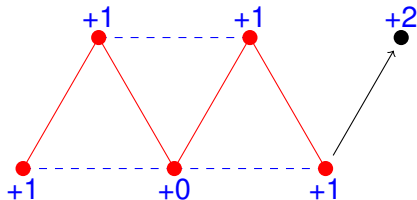


Deterministic **unary** oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag but cannot at larger arity



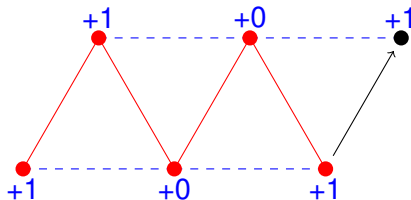
$$\alpha = 2$$

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



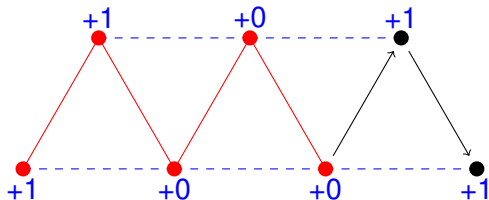
$$\alpha = 2$$

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



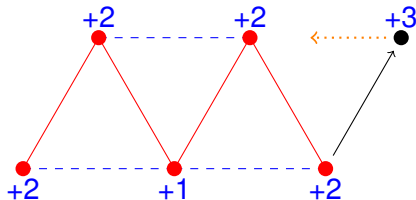
$$\alpha = 2$$

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



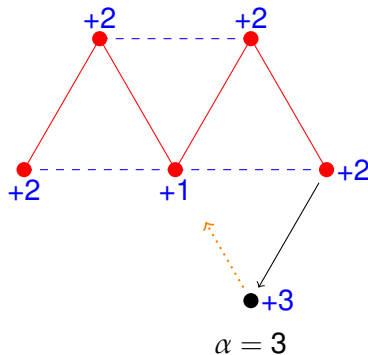
$$\alpha = 2$$

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 ($\delta = 1$)

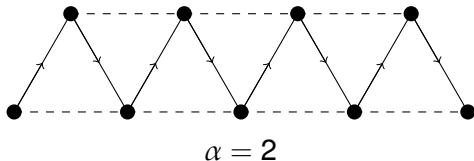
$$\alpha = 4 \quad 3n^2 + 3n + 1$$

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

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

^a a

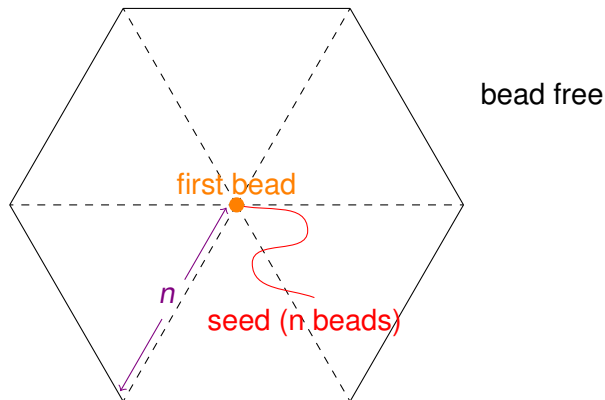
^ac.f. $\alpha = 1$: $10n$ (Demaine et al. 2018 DNA24)



Deterministic unary oritatami systems at delay 1

$$\alpha = 4$$

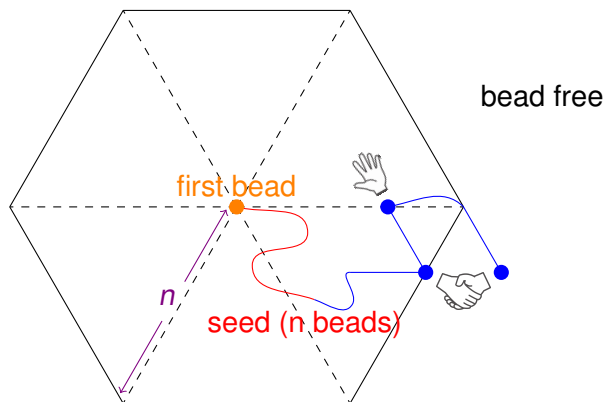
The terminal conformation at $\alpha = 4$ is of length at most $3n^2 + 3n + 1(\odot_O^n)$.



Deterministic unary oritatami systems at delay 1

$$\alpha = 4$$

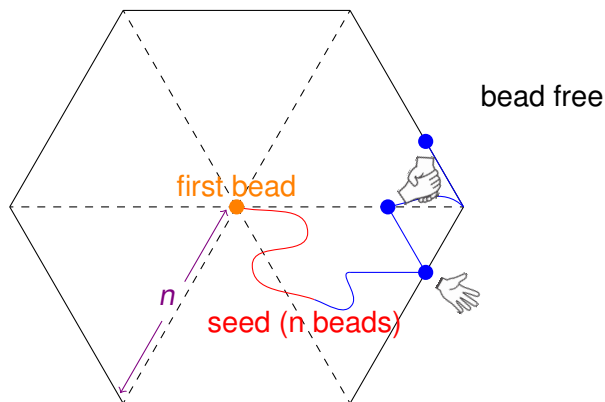
The terminal conformation at $\alpha = 4$ is of length at most $3n^2 + 3n + 1(\odot_O^n)$.



Deterministic unary oritatami systems at delay 1

$$\alpha = 4$$

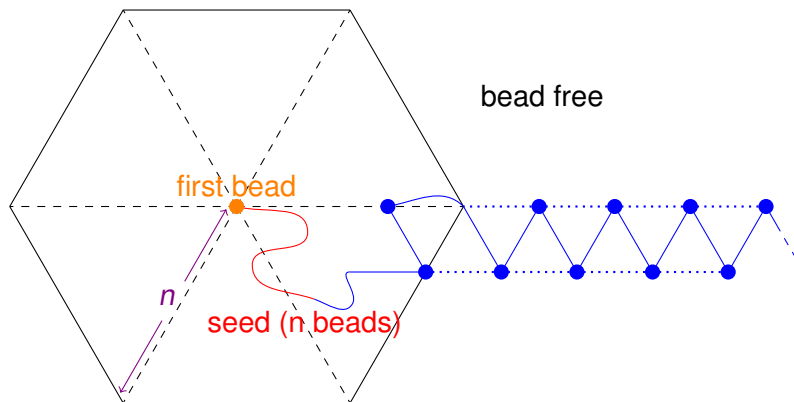
The terminal conformation at $\alpha = 4$ is of length at most $3n^2 + 3n + 1(\odot_O^n)$.



Deterministic unary oritatami systems at delay 1

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

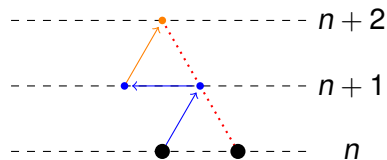
A transcript folds into the zig-zag conformation after its $(27n^2 + 9n + 1)$ -th bead ($\odot_{\mathcal{O}}^{3n}$).



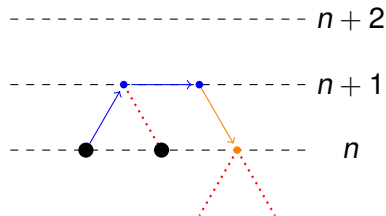
Deterministic unary oritatami systems at delay 1

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

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



zig-zag

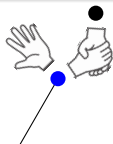


free hands: -2

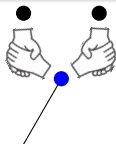
Deterministic unary oritatami systems at delay 1

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

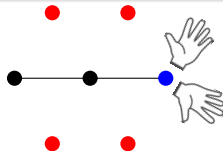
A transcript folds into the zig-zag conformation after its $(27n^2 + 9n + 1)$ -th bead (\hexagon_O^{3n}).



free hands: ± 0



free hands: -2

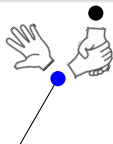


free hands: $\leq +2$

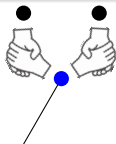
Deterministic unary oritatami systems at delay 1

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

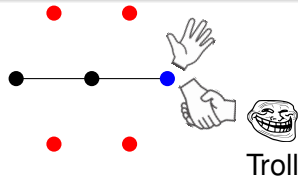
A transcript folds into the zig-zag conformation after its $(27n^2 + 9n + 1)$ -th bead (\square_O^{3n}).



free hands: ± 0



free hands: -2



free hands: ± 0

Tunnel Troll Theorem



Illustrated by Gido

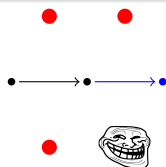
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

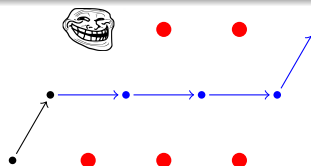
$\alpha \geq 4$ # of free hands does not increase / tunnel section.

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

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



Tunnel section

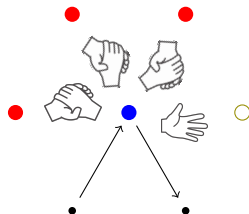
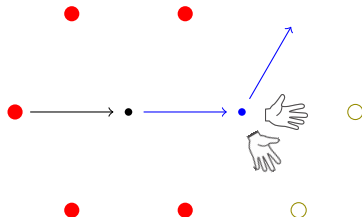


Tunnel

Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

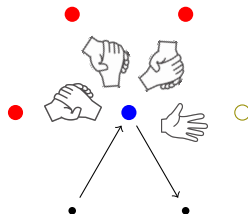
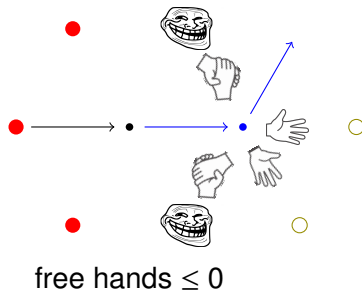
$\alpha \geq 4$ Any hands are not supplied with using a tunnel section.



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

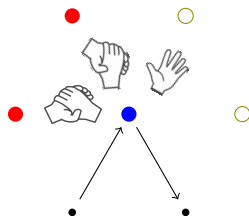
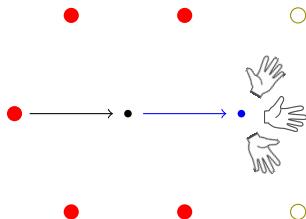
$\alpha \geq 4$ Any hands are not supplied with using a tunnel section.



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

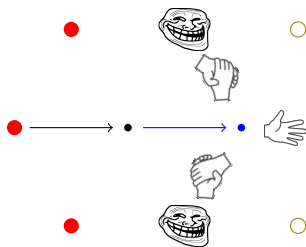
$\alpha = 3$ At least one free hand is decreased / tunnel section.



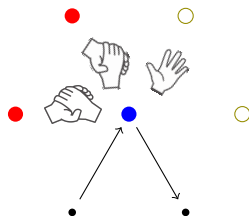
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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



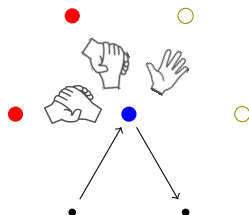
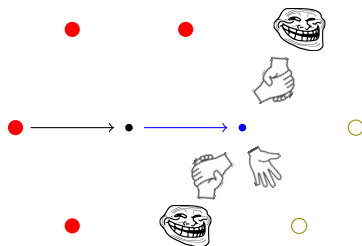
free hands ≤ -1



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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

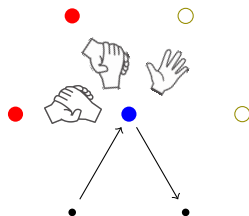
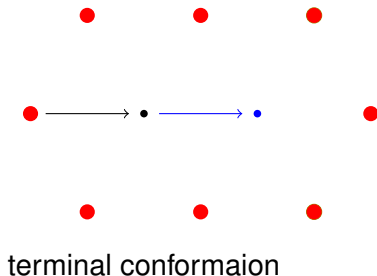


free hands ≤ -1

Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

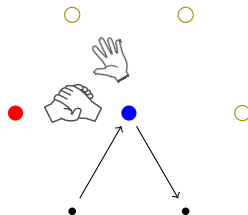
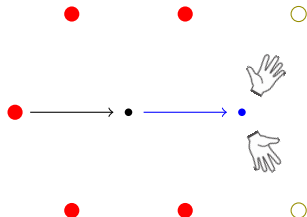
$\alpha = 3$ At least one free hand is decreased / tunnel section.



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

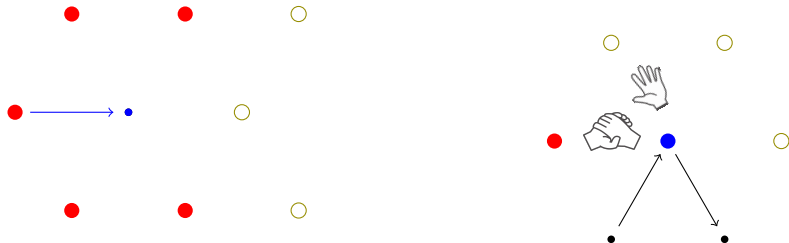
$\alpha = 2$ At least one free hand is decreased / tunnel.



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

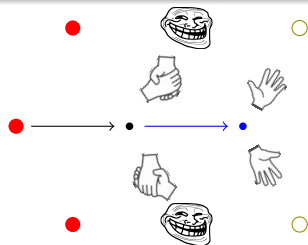
$\alpha = 2$ At least one free hand is decreased / tunnel.



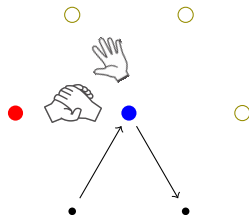
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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



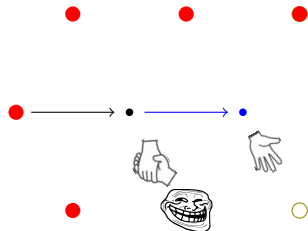
free hands ≤ 0



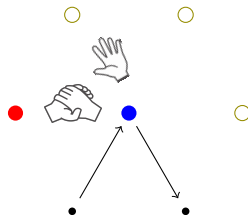
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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



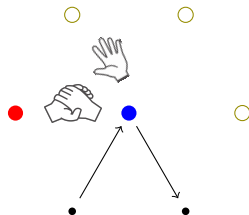
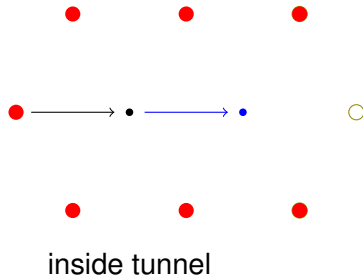
free hands ≤ 0



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

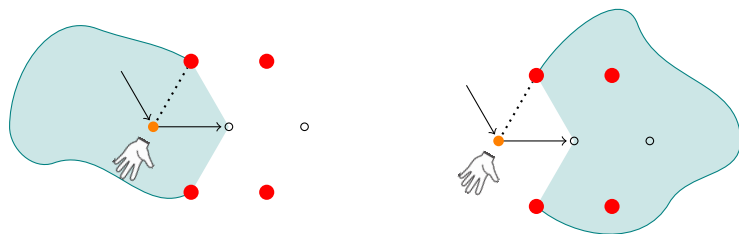
$\alpha = 2$ At least one free hand is decreased / tunnel.



Deterministic unary oritatami systems at delay 1

Jordan curve theorem

A closed curve which is a non-self-intersecting divides into inside and outside.



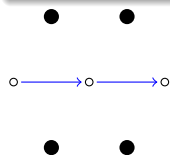
At $\alpha = 2$, Troll consumes free hands an entrance of tunnel, too.

Thank you for listening!!

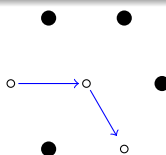
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

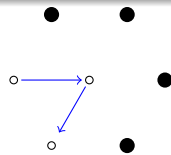
Type of tunnel sections



Straight



Obtuse

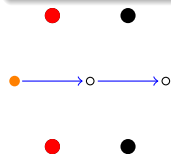


Accute

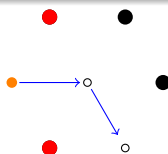
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

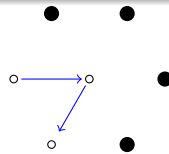
Type of tunnel sections



Straight



Obtuse

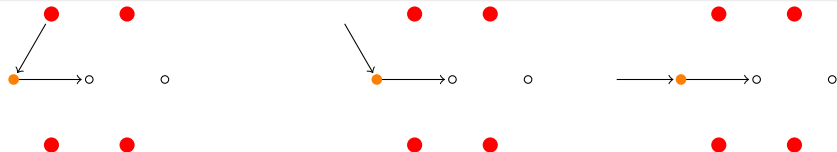


Accute

Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

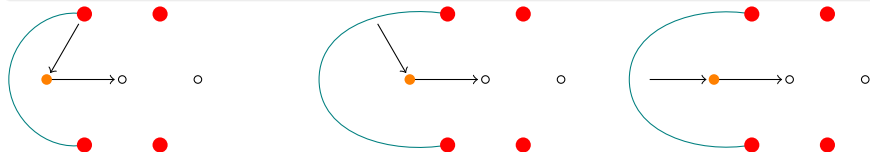
Directions to enter a tunnel



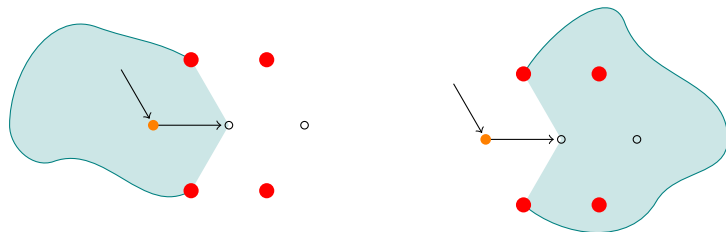
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

Directions to enter a tunnel



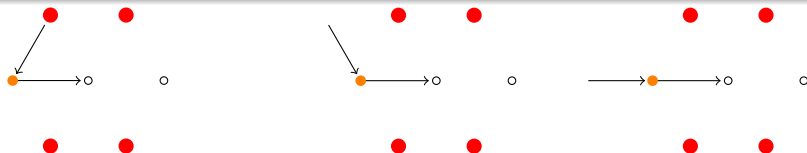
freehands $\leq \pm 0$



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

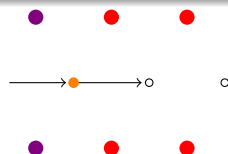
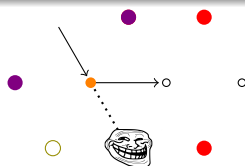
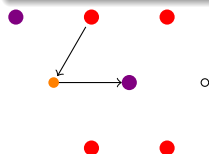
If this orange bead is stabilized by bonds, total bonds decrease.



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 ≤ -1

