On the power of oritatami cotranscriptional folding with unary bead sequence [1]

Szilard Zsolt Fazekas[1], Kohei Maruyama[2], Reoto Morita[2], Shinnosuke Seki[2]

[1]Akita University, [2]University of Electro-Communications

TAMC2019

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

What is oritatami system?

Oritatami system is a mathematical model for cotranscriptional folding(CF). (C. Geary, P.E. Meunier, N. Schabanel and S. Seki.)

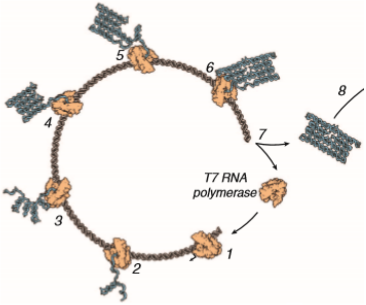


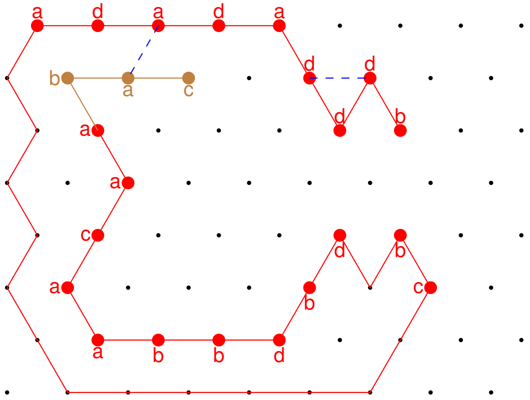
Figure: RNA tile is self-assembly(RNA Origami)

(C. Geary, P.W.K. Rothemund and E.S. Anderson. Science 345(6198), 2014)

How oritatami system works?

An example

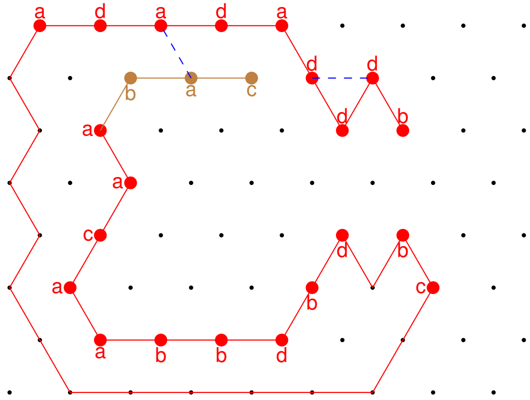
$\Sigma = \{a, b, c, d\}$, $R = \{(a,a), (b,b), (c,c), (d,d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = \underline{bac}bcadbcbab$



How oritatami system works?

An example

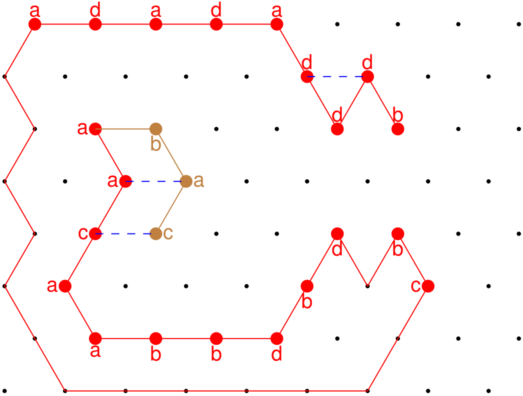
$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = \underline{bac}bcadbcbab$



How oritatami system works?

An example

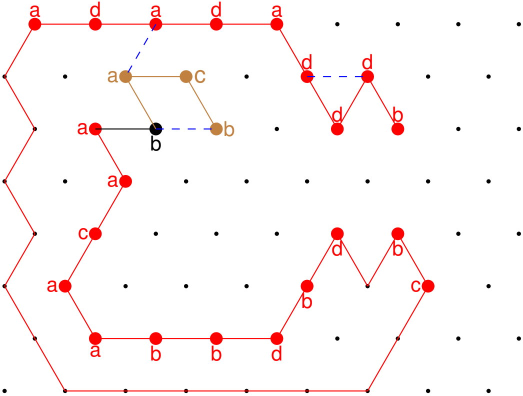
$\Sigma = \{a, b, c, d\}$, $R = \{(a,a), (b,b), (c,c), (d,d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = \underline{bac}bcadbcbab$



How oritatami system works?

An example

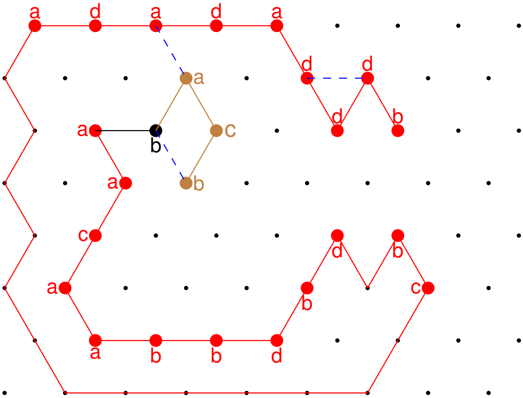
$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = b\underline{acb}cadbcbab$



How oritatami system works?

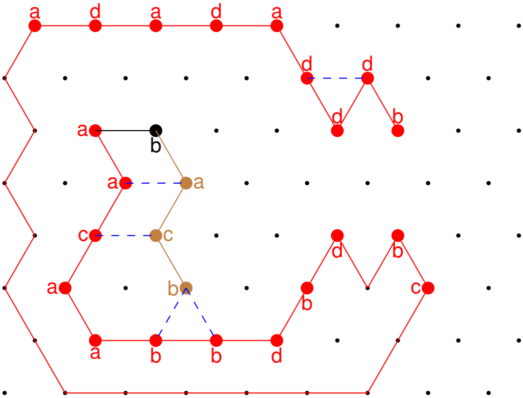
An example

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



An example

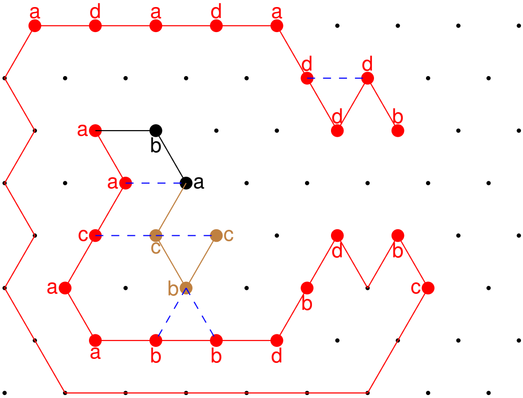
$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = b\underline{acb}cadbcbab$



How oritatami system works?

An example

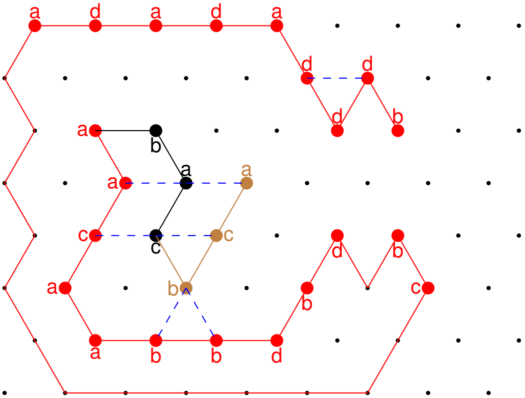
$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = ba\underline{cbc}adbcbab$



How oritatami system works?

An example

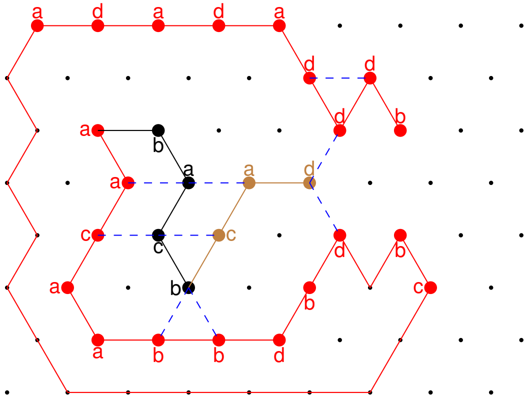
$\Sigma = \{a, b, c, d\}$, $R = \{(a,a), (b,b), (c,c), (d,d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = bac\underline{bca}dbcbab$



How oritatami system works?

An example

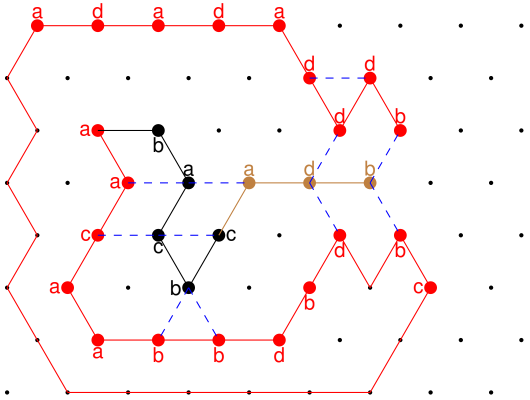
$\Sigma = \{a, b, c, d\}$, $R = \{(a,a),(b,b),(c,c),(d,d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = bacb\underline{cad}bcbab$



How oritatami system works?

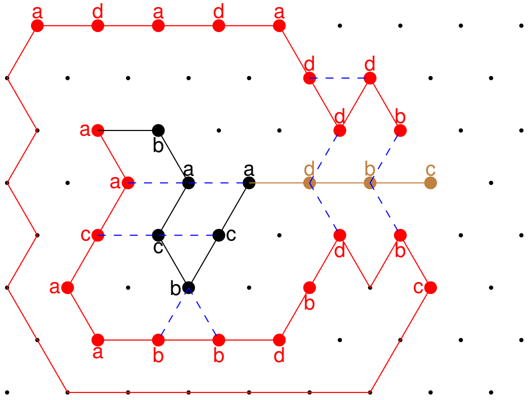
An example

$\Sigma = \{a, b, c, d\}$, $R = \{(a,a),(b,b),(c,c),(d,d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = bacbc\underline{adb}cbab$



An example

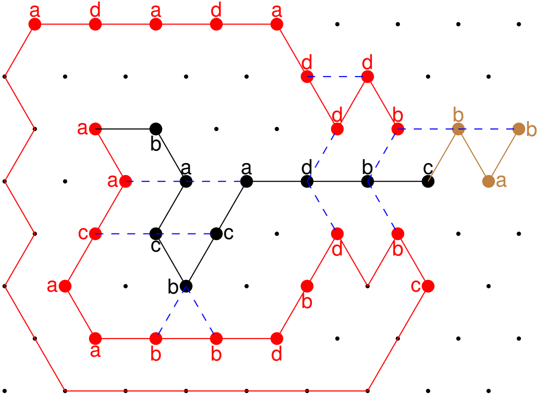
$\Sigma = \{a, b, c, d\}$, $R = \{(a, a), (b, b), (c, c), (d, d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = bacbca\underline{dbc}bab$



A deterministic oritatami system

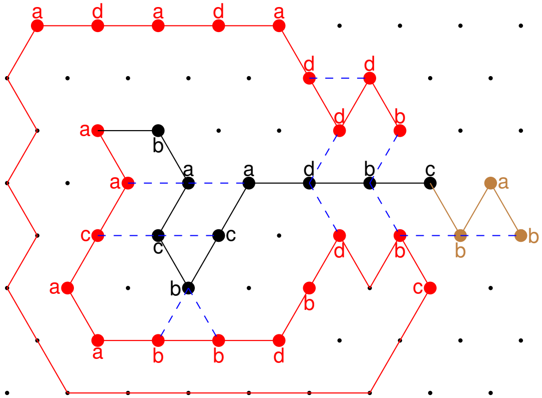
An example

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



An example

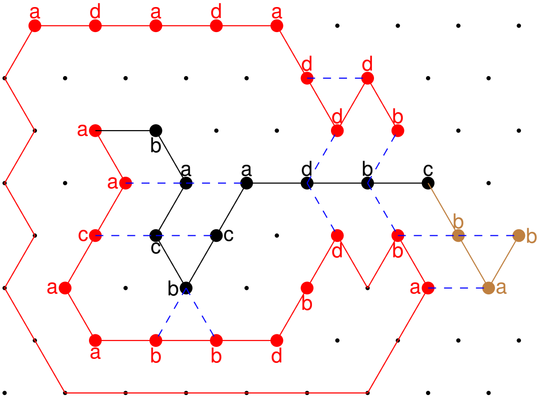
$\Sigma = \{a, b, c, d\}$, $R = \{(a,a),(b,b),(c,c),(d,d)\}$,
arity $\alpha = 2$, *delay* $\delta = 3$, $w = bacbcadbc\underline{bab}$



A deterministic oritatami system

An example

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



Turing universal

Theorem (C. Geary *et al*. ISAAC, 2018)

Oritatami system at *delay* $\delta = 3$ which employs 542 types of beads is Turing universal.

Theorem

Polynomial length of conformations $\longrightarrow$ Non-Turing-universal

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*.

Oritatami System

input : *delay* δ, *arity* α, seed, rule, transcript
output : conformation

Why unary?

Because we considered the unary oritatami system is good for a first step towards the characterization of non-Turing-universal oritatami systems.

Cases of non-Turing-universal oritatami systems

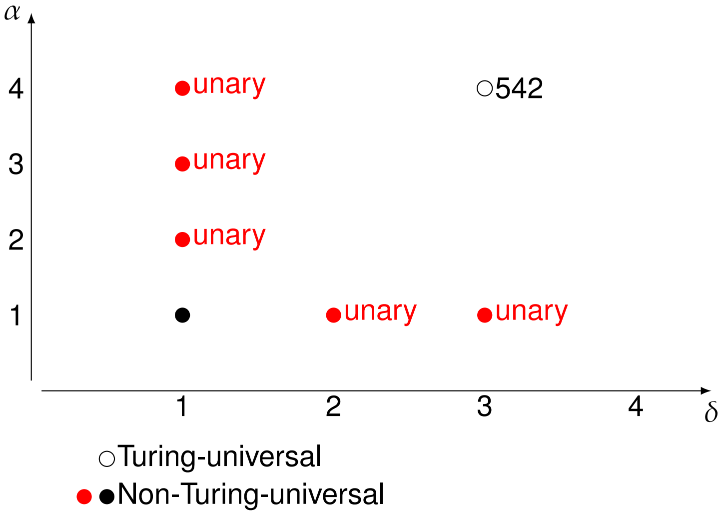


Figure: Cases of non-Turing-universal oritatami systems

Cases of non-Turing-universal oritatami systems

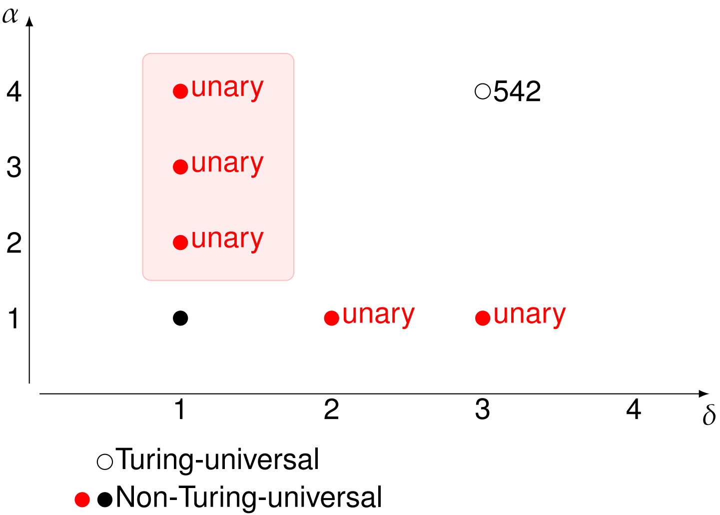
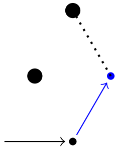


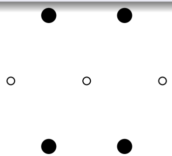
Figure: Cases of non-Turing-universal oritatami systems

Two ways for a bead stabilization

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



Bond

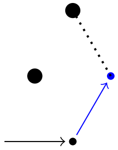


Tunnel section

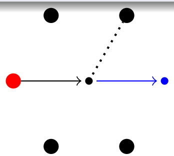
Deterministic unary oritatami systems at delay 1

Two ways for a bead stabilization

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



Bond



Tunnel section

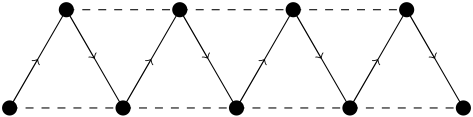
Deterministic unary oritatami systems at delay 1

Results ($\delta = 1$)

$\alpha = 4$	$3n^2+3n+1$
$\alpha = 3$	$4n+14$
$\alpha = 2$	∞ but zigzag after $(27n^2+9n+1)$

*[a]

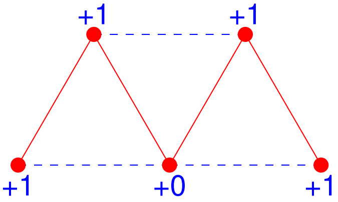
[a] c.f. $\alpha = 1$: $10n$ (Demaine et al. 2018 DNA24)



$\alpha = 2$

zig-zag conformation

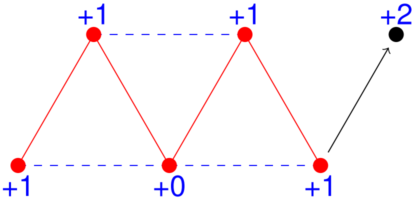
Deterministic oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag conformation



$\alpha = 2$

zig-zag conformation

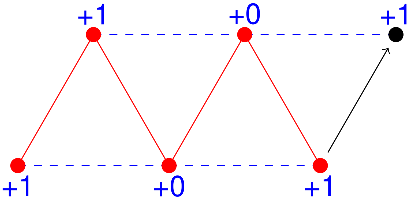
Deterministic oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag conformation



$\alpha = 2$

zig-zag conformation

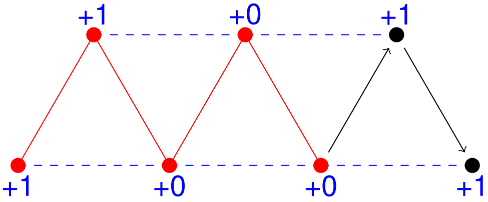
Deterministic oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag conformation



$\alpha = 2$

zig-zag conformation

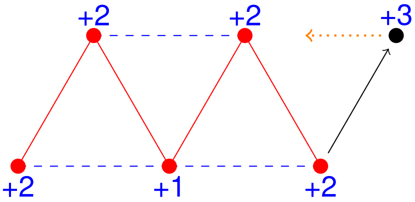
Deterministic oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag conformation



$\alpha = 2$

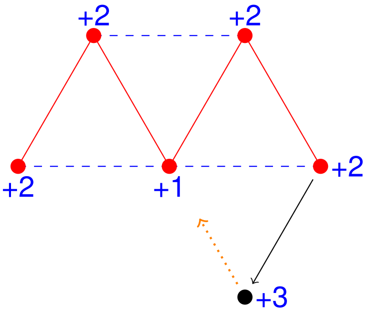
zig-zag conformation

Deterministic oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag conformation



$\alpha = 3$

Deterministic oritatami system at $\delta = 1$ and at $\alpha = 2$ can make zig-zag conformation



$\alpha = 3$

Deterministic unary oritatami systems at delay 1

Results ($\delta = 1$)

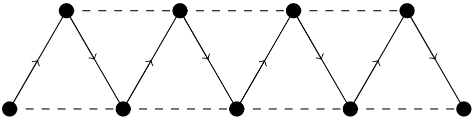
$\alpha = 4$ $3n^2+3n+1$

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

$\alpha = 2$ ∞ but zigzag after $(27n^2+9n+1)$

$*$[a]

[a] c.f. $\alpha = 1$: $10n$ (Demaine et al. 2018 DNA24)

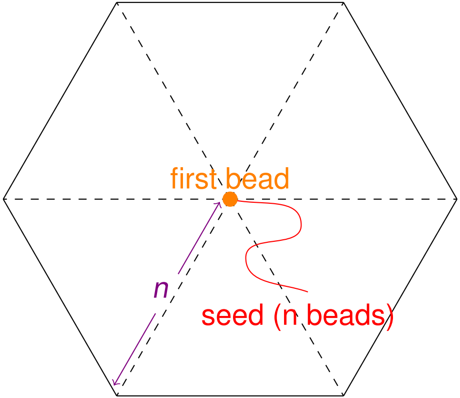


$\alpha = 2$

Deterministic unary oritatami systems at delay 1

$\alpha = 4$

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

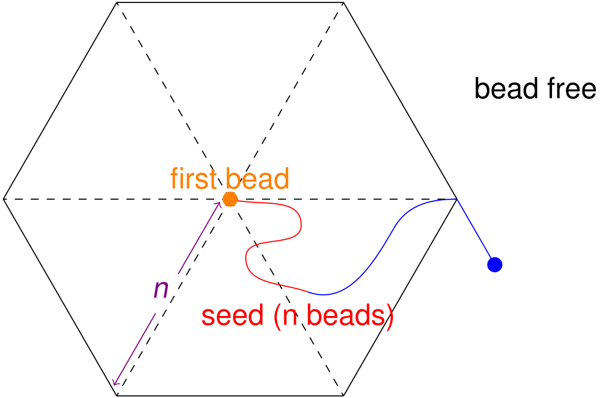


bead free

Deterministic unary oritatami systems at delay 1

$\alpha = 4$

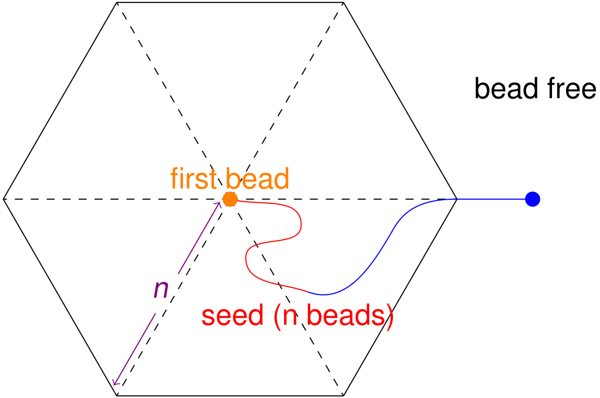
The terminal conformation at $\alpha = 4$ is of length at most $3n^2 + 3n + 1(\hexagon^n_O)$.



Deterministic unary oritatami systems at delay 1

$\alpha = 4$

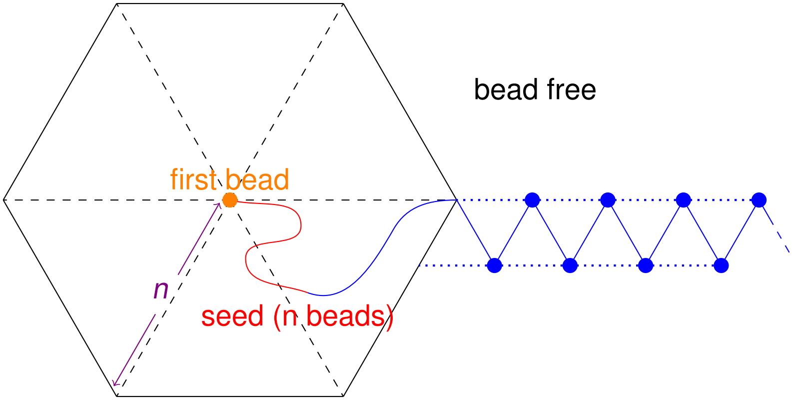
The terminal conformation at $\alpha = 4$ is of length at most $3n^2 + 3n + 1(\hexagon_O^n)$.



Deterministic unary oritatami systems at delay 1

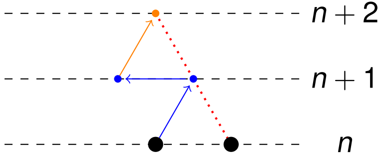
$\alpha = 2$ ($\delta = 1$)

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

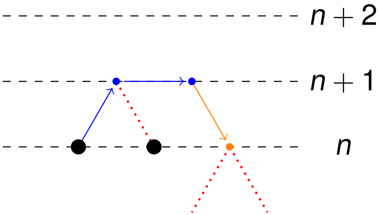


$\alpha = 2$ ($\delta = 1$)

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



zig-zag conformation

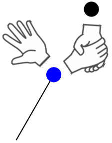


free hands ≤ 2

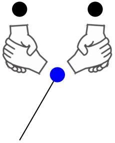
Deterministic unary oritatami systems at delay 1

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

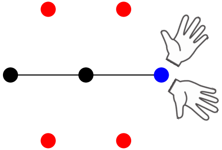
A transcript folds into the zig-zag conformation after its $(27n^2 + 9n + 1)$-th bead ($\hexagon_O^{3n}$).



free hands = ± 0



free hands = -2

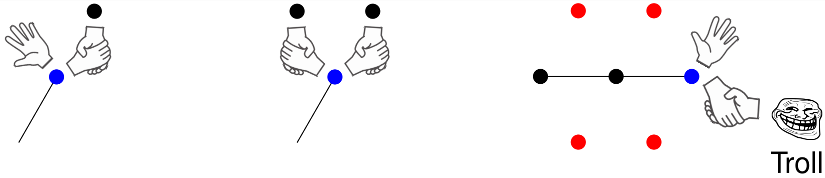


free hands $\leq +2$

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 ($\hexagon^{3n}_{O}$).



free hands = ± 0 free hands = -2 free hands $\leq +2$

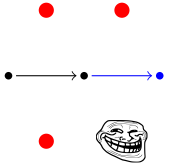
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

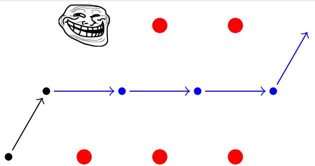
$\alpha \geq 4$ No free hand supplies / tunnel section.

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

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



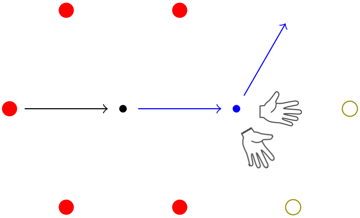
Tunnel section

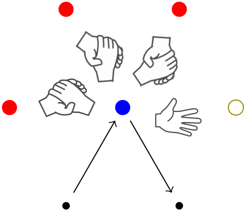


Tunnel

Tunnel Troll Theorem

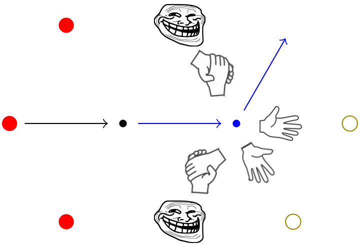
$\alpha \geq 4$ Any hands are not supplied with using a tunnel section.



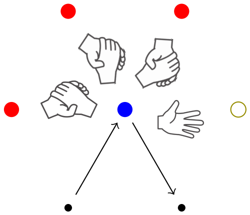


Tunnel Troll Theorem

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

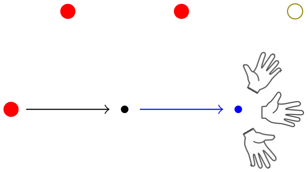


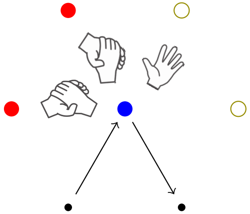
free hands ≤ 0



Tunnel Troll Theorem

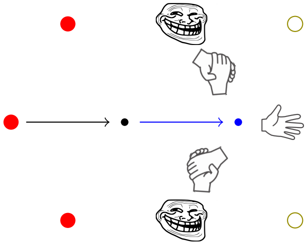
$\alpha = 3$ At least one free hand is decreased / tunnel section.



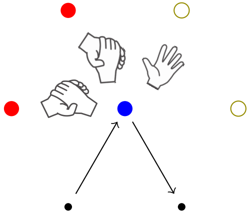


Tunnel Troll Theorem

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



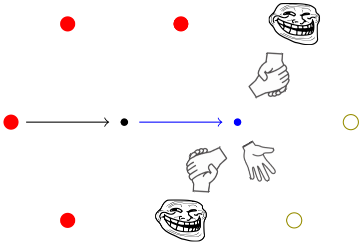
free hands ≤ -1

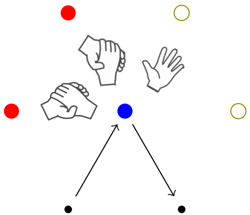


Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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



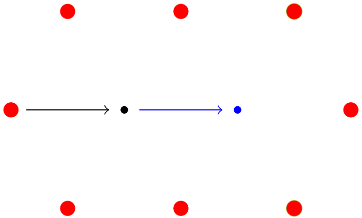


free hands ≤ -1

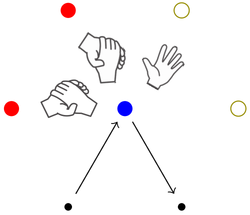
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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



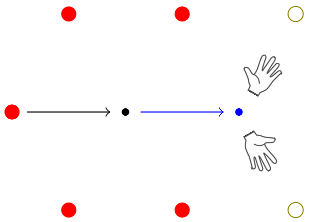
terminal conformaion

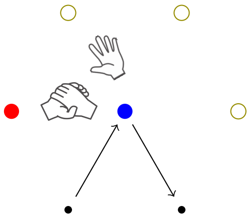


Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

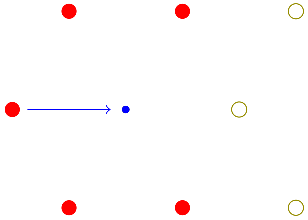
$\alpha = 2$ At least one free hand is decreased / tunnel.

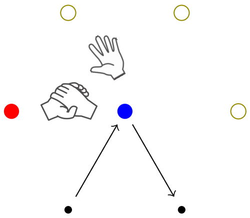




Tunnel Troll Theorem

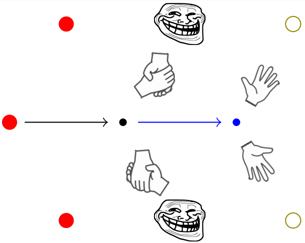
$\alpha = 2$ At least one free hand is decreased / tunnel.



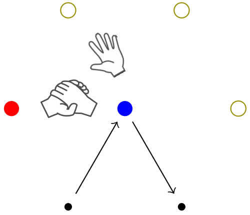


Tunnel Troll Theorem

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



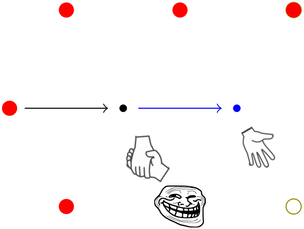
free hands ≤ 0



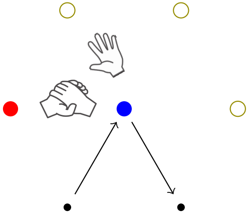
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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



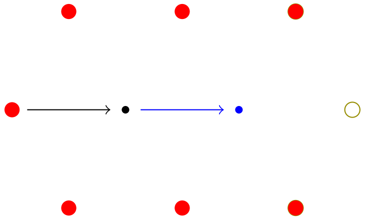
free hands ≤ 0



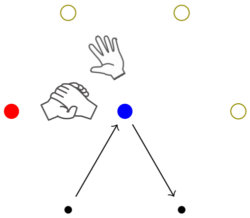
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem

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

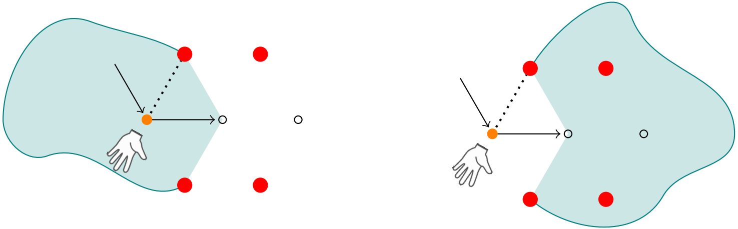


inside tunnel



Jordan curve theorem (Hales 2007)

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



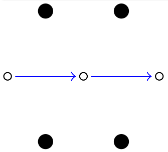
At $\alpha = 2$, Troll consumes free hands an entrance of tunnel, too.

Thank you for listening!!

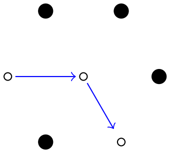
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

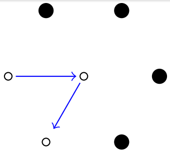
Type of tunnel sections



Straight



Obtuse

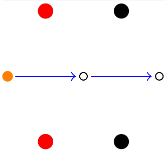


Accute

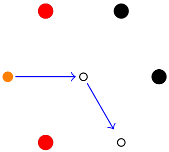
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

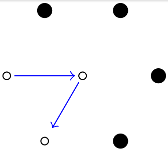
Type of tunnel sections



Straight



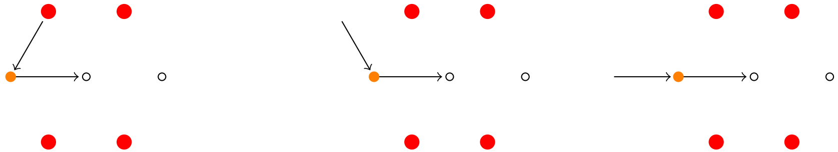
Obtuse



Accute

Tunnel Troll Theorem ($\alpha = 2$)

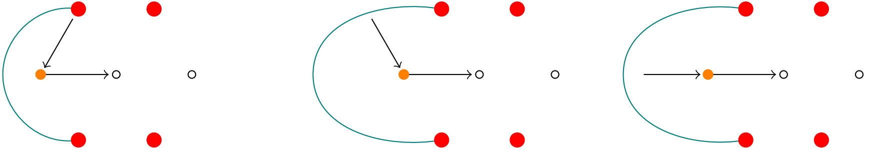
Directions to enter a tunnel



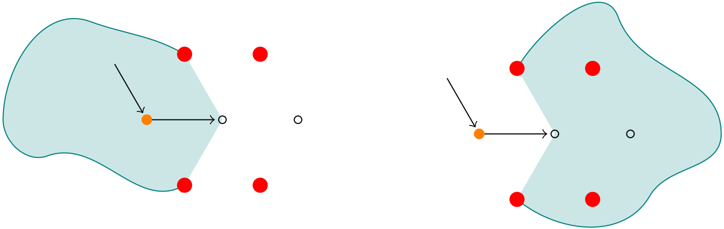
Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

Directions to enter a tunnel



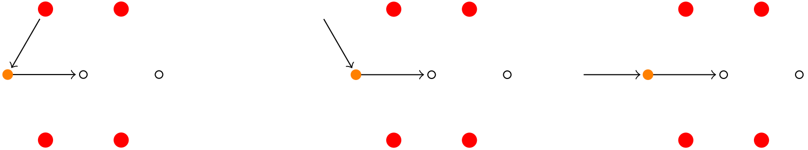
freehands $\leq \pm 0$



Deterministic unary oritatami systems at delay 1

Tunnel Troll Theorem ($\alpha = 2$)

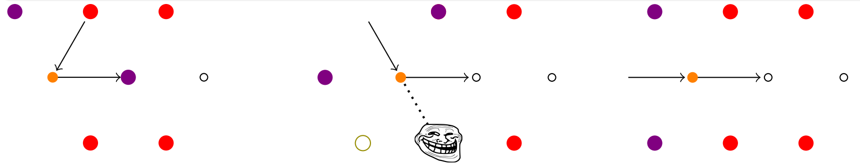
If this orange bead is stabilized by bonds, total bonds decrease.



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

References I