On the power of oritatami cotranscriptional folding with unary bead sequence ⁰

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TAMC2019





)科学技術振興機構

O 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 cotranscriptional folding(CF). (Geary, Meunier, Schabanel and Seki.)

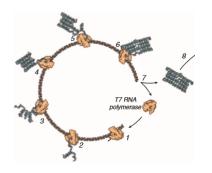
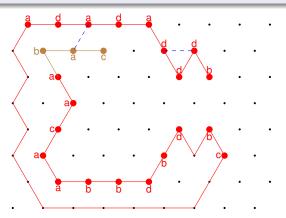


Figure: RNA tile is self-assembled (RNA Origami)

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

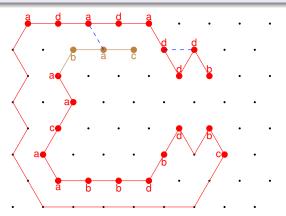
An example

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



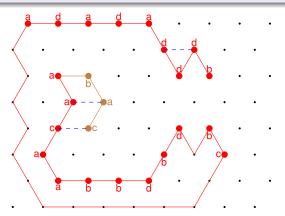
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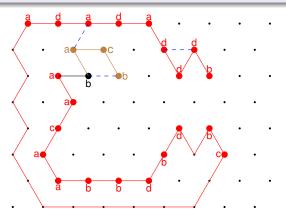
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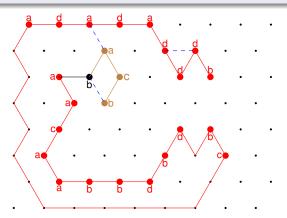
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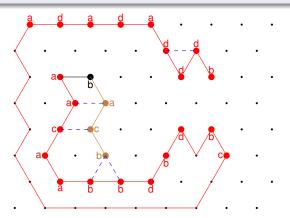
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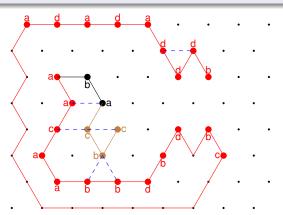
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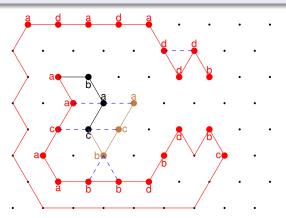
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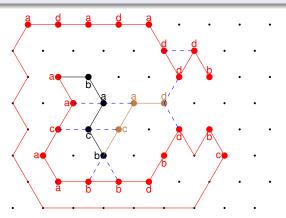
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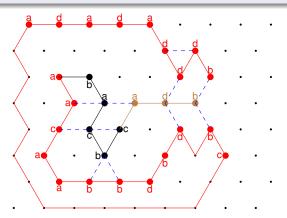
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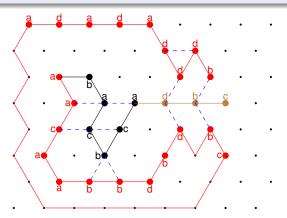
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An example

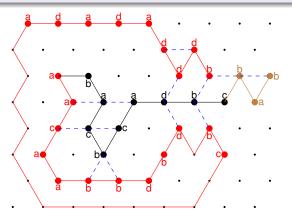
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A deterministic oritatami system

An example

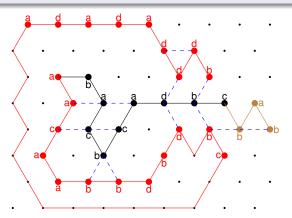
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A deterministic oritatami system

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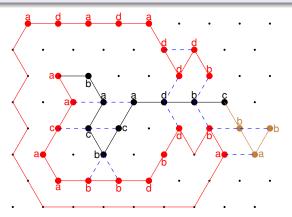
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A deterministic oritatami system

An example

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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 → 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

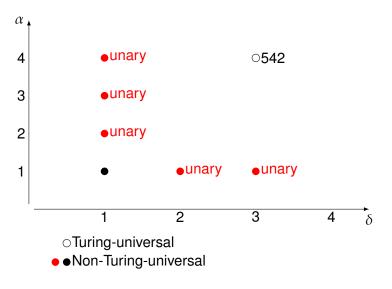


Figure: Cases of non-Turing-universal oritatami systems

Cases of non-Turing-universal oritatami systems

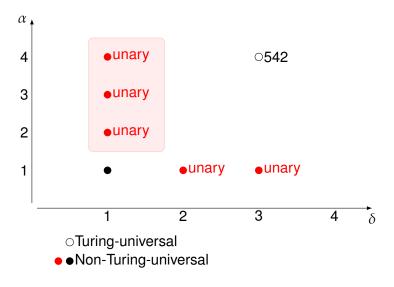
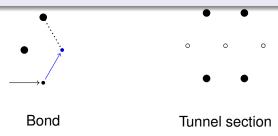


Figure: Cases of non-Turing-universal oritatami systems

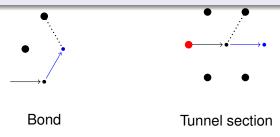
Two ways for a bead stabilization

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



Two ways for a bead stabilization

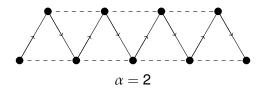
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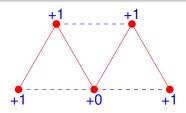


Results $\delta = 1$

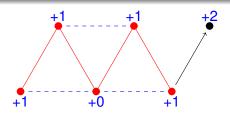
$$\alpha=4$$
 $3n^2+3n+1$
 $\alpha=3$ $4n+14$
 $\alpha=2$ ∞ but zigzag after $(27n^2+9n+1)$

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

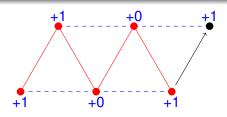




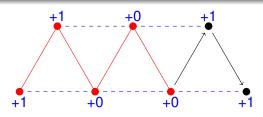
$$\alpha = 2$$



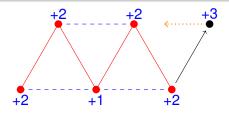
$$\alpha = 2$$



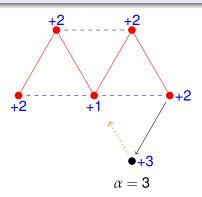
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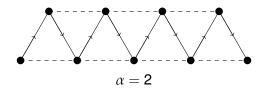
$$\alpha = 3$$



Results $\delta = 1$

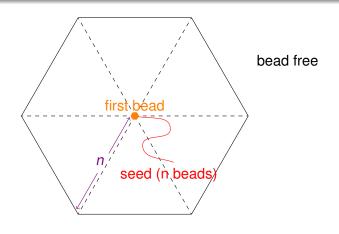
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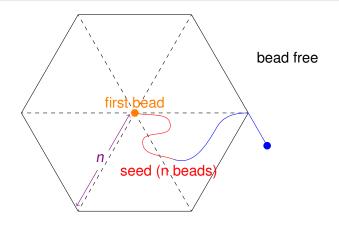
$$\alpha = 4$$

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



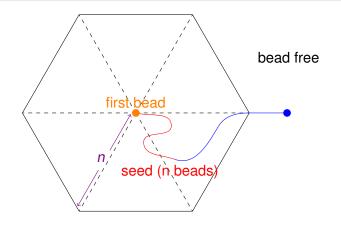
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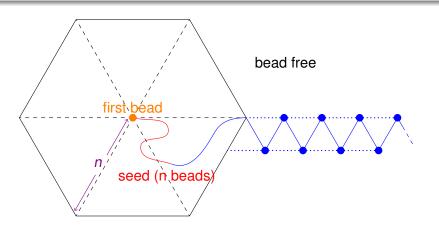
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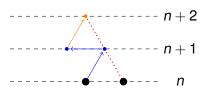
$$\alpha = 2 (\delta = 1)$$

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

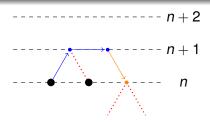


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zig-zag conformation



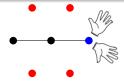
free hands ≤ 2

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

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







free hands =
$$\pm 0$$

free hands = -2

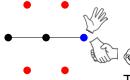
free hands
$$\leq +2$$

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

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







Troll

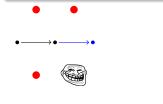
free hands =
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free hands =
$$-2$$

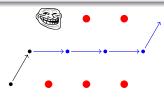
free hands
$$\leq +2$$

Tunnel Troll Theorem

- $\alpha \ge 4$ No free hand supplies / tunnel section.
- $\alpha = 3$ Troll consumes bonds / tunnel section.
- $\alpha = 2$ Troll consumes bonds / tunnel.



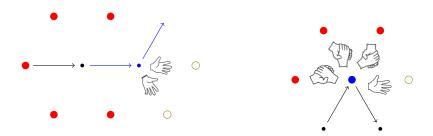
Tunnel section



Tunnel

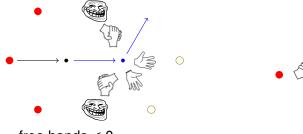
Tunnel Troll Theorem

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

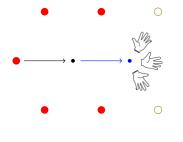


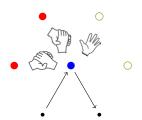
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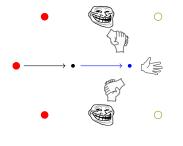
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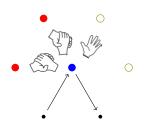




Tunnel Troll Theorem

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

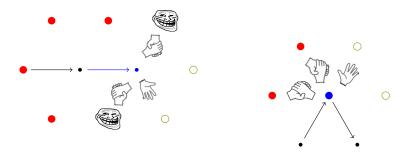




free hands < -1

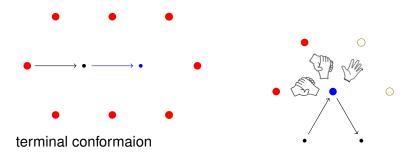
Tunnel Troll Theorem

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

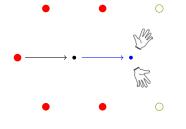


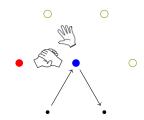
free hands ≤ -1

Tunnel Troll Theorem

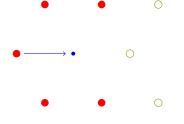


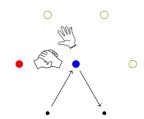
Tunnel Troll Theorem



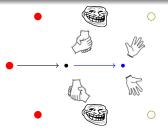


Tunnel Troll Theorem

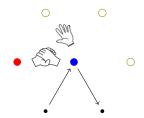




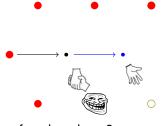
Tunnel Troll Theorem



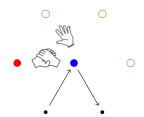




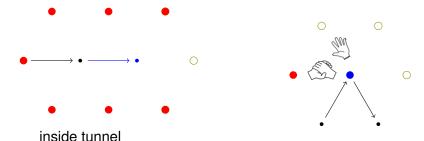
Tunnel Troll Theorem





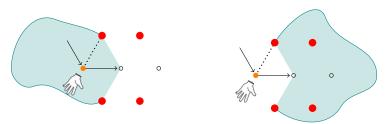


Tunnel Troll Theorem



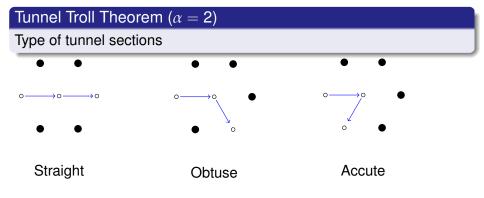
Jordan curve theorem (Hales 2007)

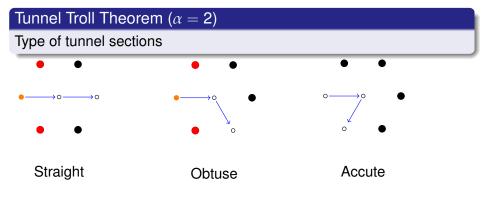
A closed curve which is a non-self-intersecting divides into inside and outside.

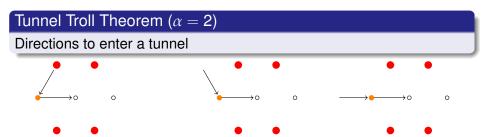


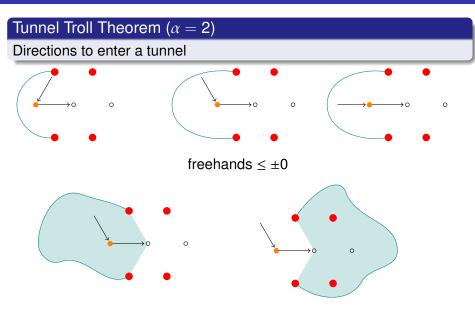
At $\alpha = 2$, Troll consumes free hands an entrance of tunnel, too.

Thank you for listening!!



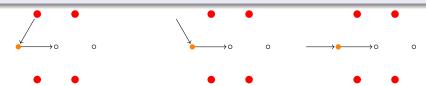


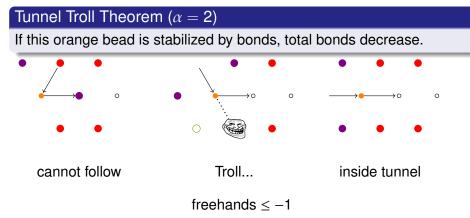




Tunnel Troll Theorem ($\alpha = 2$)

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





References I