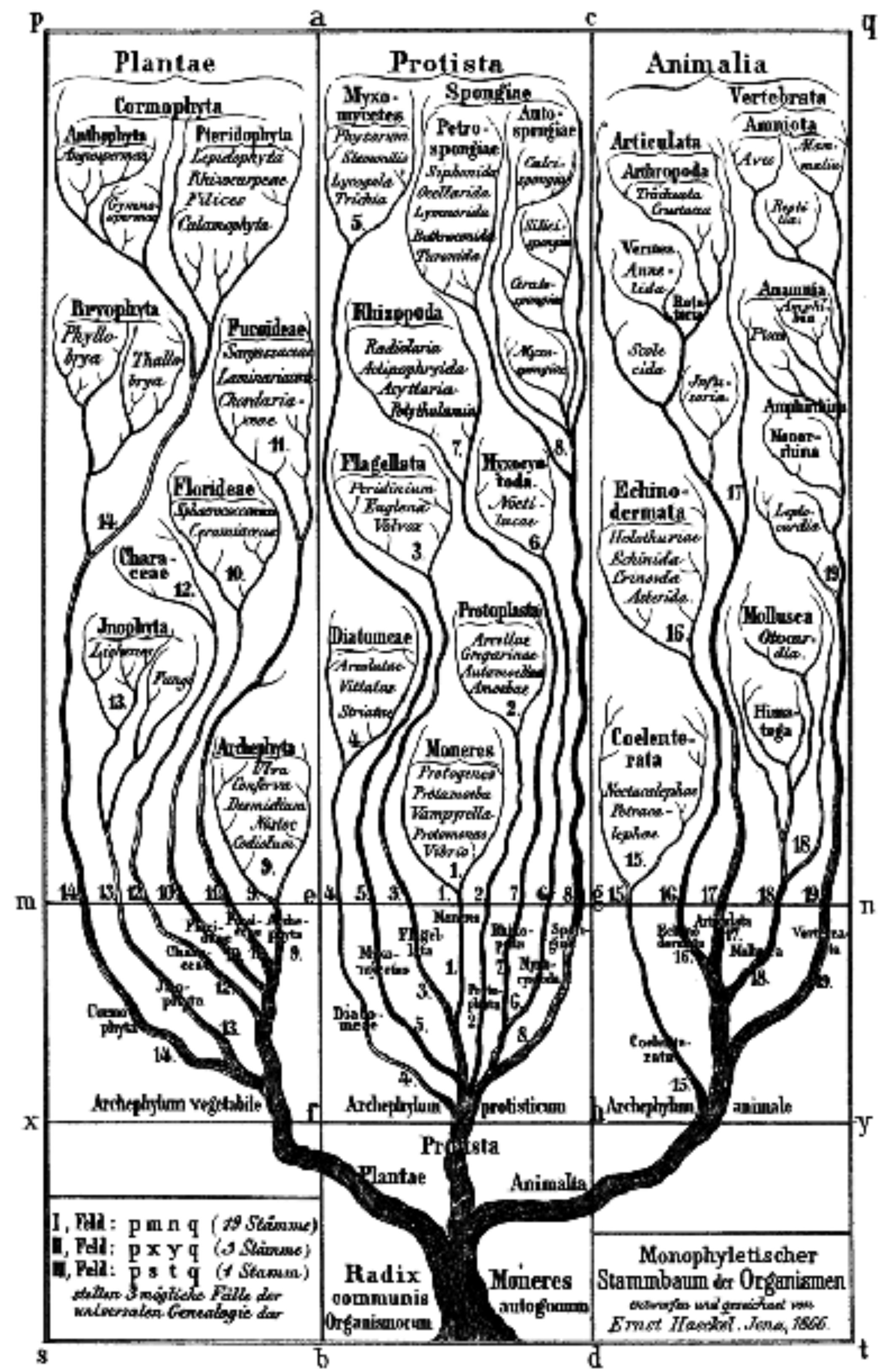
A thermodynamic threshold for Darwinian evolution

Evolution of Complexity from the Statistical Physics Perspective, June 2022



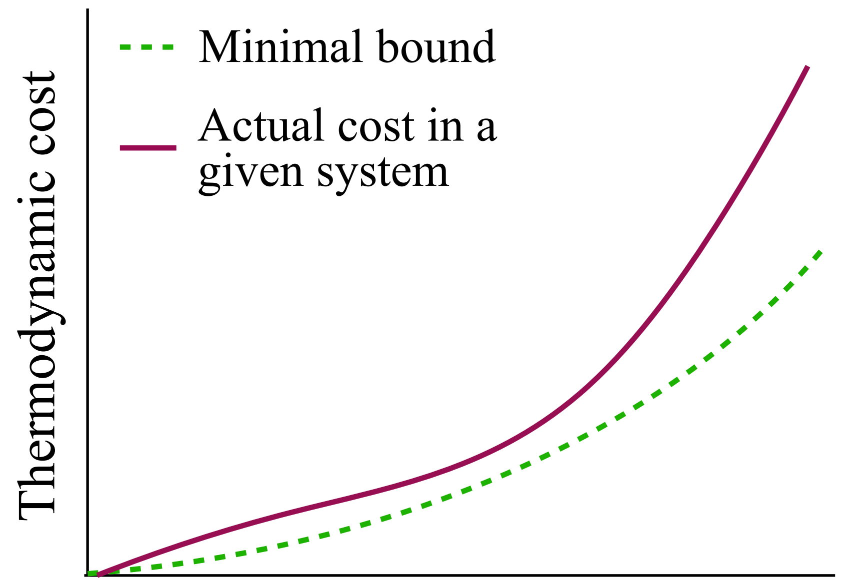
Artemy Kolchinsky artemyk@gmail.com
Universal Biology Institute, University of Tokyo

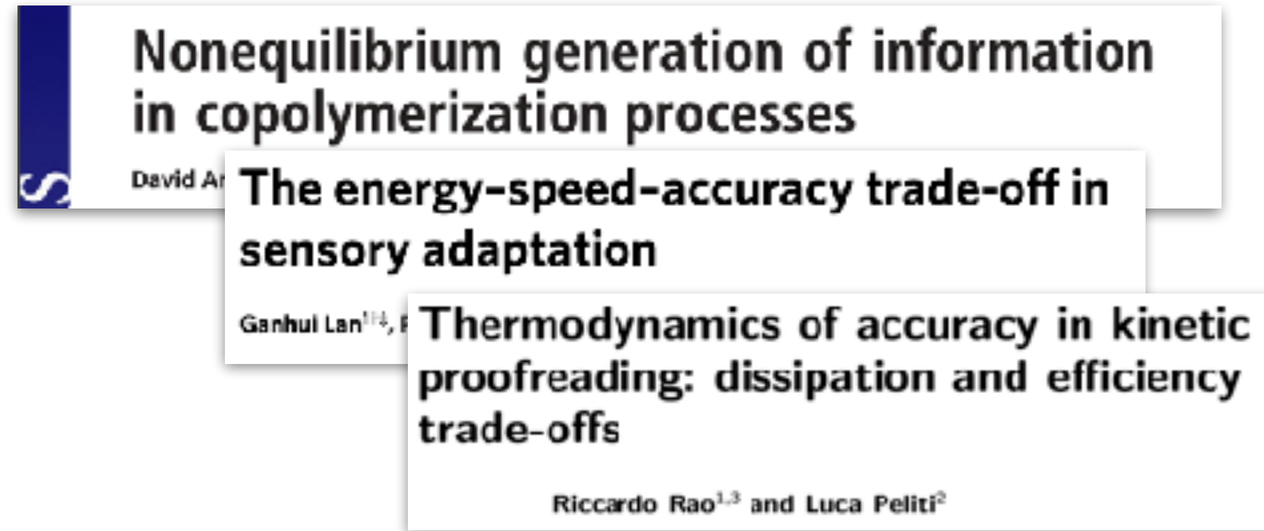
Roadmap

- Introduction: thermodynamics tradeoffs and thresholds
- Main result
- Illustration with data + example
- Other issues + future work

Introduction

Thermodynamic tradeoffs and thresholds





Nonequilibrium generation of information in copolymerization processes

David A

The energy-speed-accuracy trade-off in sensory adaptation

Ganhui Lan[1,4]

Thermodynamics of accuracy in kinetic proofreading: dissipation and efficiency trade-offs

Riccardo Rao[1,3] and Luca Peliti[2]

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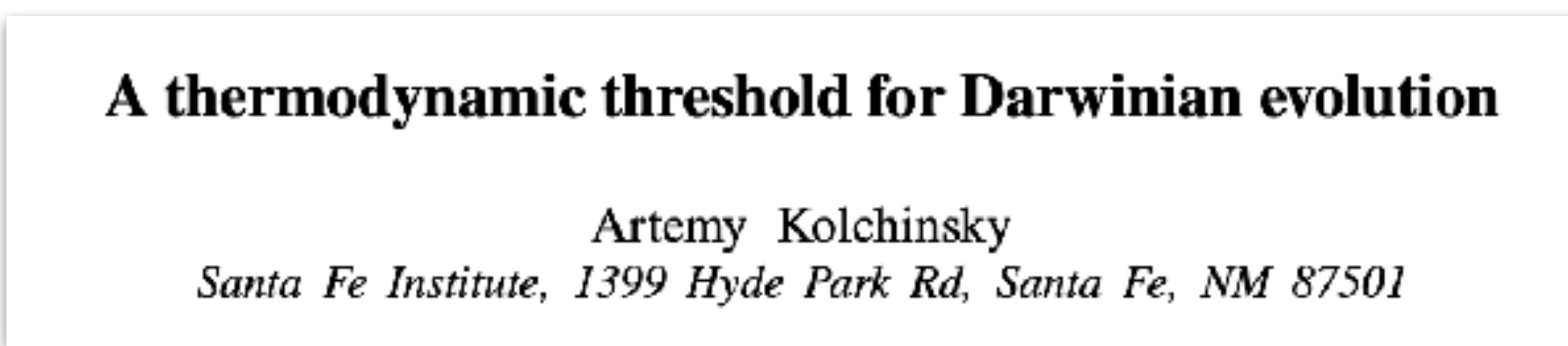
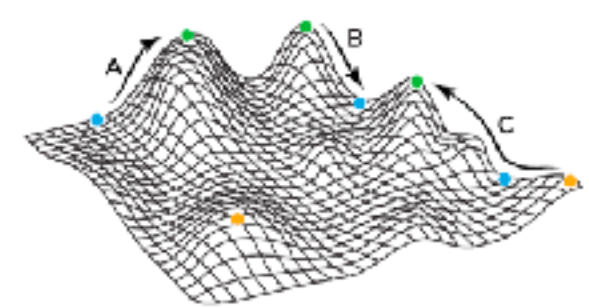


A thermodynamic threshold for Darwinian evolution

Artemy Kolchinsky

Santa Fe Institute, 1399 Hyde Park Rd, Santa Fe, NM 87501

https://arxiv.org/abs/2112.02809



Darwinian evolution

Thermodynamic threshold for Darwinian evolution

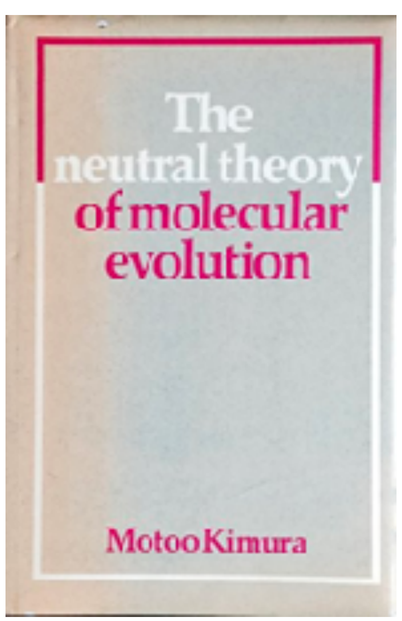
Darwinian evolution: when, in a population of replicators, replicators with higher fitness outcompete those with lower fitness

Selection coefficient $s \in [-1,1]$: measure of relative fitness difference between replicators ($s = 0$ for no difference)

"Strength of selection" can be quantified via a lower bound on s, the critical selection coefficient that is "visible" to selection

Finite population sizes

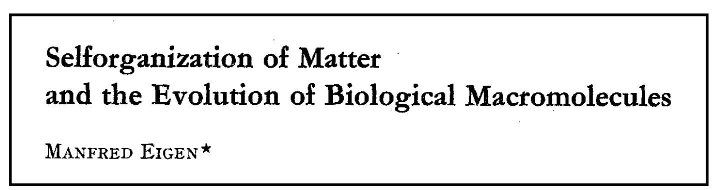
$s \gg 1/N_{\mathrm{eff}}$



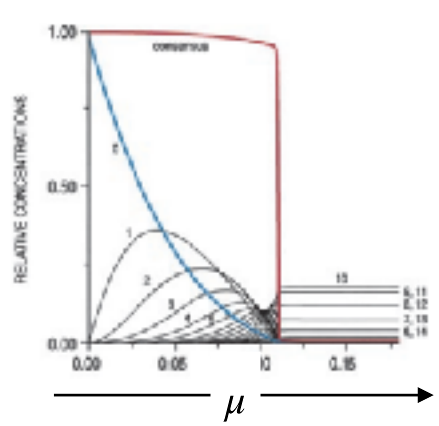
Finite mutation rate μ

(Eigen's "error catastrophe")

$s > \mu$


Selforganization of Matter and the Evolution of Biological Macromolecules

Manfred Eigen*



doi:10.1073/pnas.212514799

Preview of main result: a thermodynamic threshold for molecular replicators

$$s \geq e^{-\sigma}$$

s : selection coefficient $(1 - f'/f)$ (between 0 and 1)

σ : Gibbs free energy dissipated by fitter replicator (kT/copy)

Why do we care?

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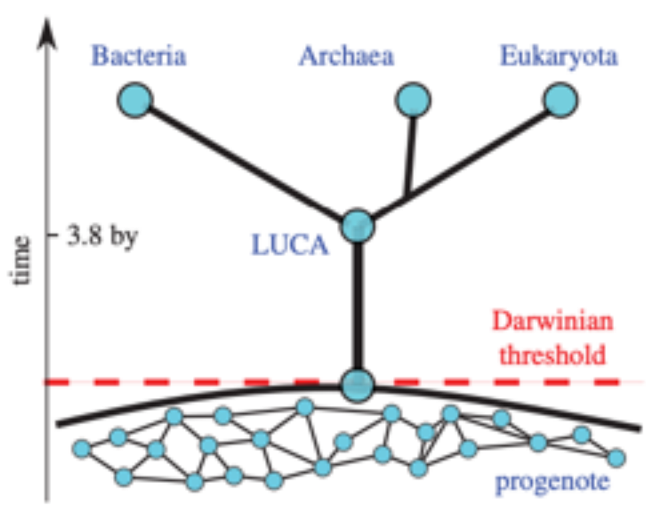
Perspective

Thresholds in Origin of Life Scenarios

Cyrille Jeancolas,[1,2] Christophe Malaterre,[3,*] and Philippe Nghe[1,*]



Goldenfeld et al, 2017

Threshold Examples	System State before Threshold	System State after Threshold	Variables Triggering the Transition (In Model or Experiment)	Naturalized Variables Posited to Have Triggered the Transition in an Origin of Life Scenario
Chirality symmetry breaking (Budin and Szostak, 2010; Hawbaker and Blackmond, 2019)	Racemic state of a solution	Homochiral state of a solution	Enantiomeric excess	Presence of circularly polarized light, stereospecific crystallization, isotopic enantioselective initiators, auto-catalysis
Spontaneous polymerization (Monnard et al., 2003; Baaske et al., 2007; Lambert, 2008)	Solution of monomers	Solution of polymers	Concentrations of monomers, chemical activation	Ponds evaporation, freeze-thaw cycle, mineral surfaces, thermophoresis in hydrothermal vents, in situ closure in vesicles
Self-assembly of compartments (Bachmann et al., 1992; Todisco et al., 2018)	Solution of free constituents	Solution of molecular self-assembled compartments	Concentration of the constituents, salinity, pH, temperature, molecular crowding	Increase of CO_2 concentration, day-night temperature variations, wet-dry cycles
Catalytic closure threshold (Kauffman, 1986)	Solution of polymers with few catalysts	Closed collective autocatalytic sets	Number of catalysts and reactions catalyzed	Spontaneous and effective synthesis of diverse polymers
Error threshold (Eigen, 1971; Takeuchi et al., 2017)	Unreplicated polymers	Polymers copied by template-based replication	Selective advantage, copying error rate, polymers length	Selection of compartments, genotype-phenotype redundancy, mineral surfaces
Decay threshold (King, 1977; Szathmáry, 2006; Vasas et al., 2012)	No autocatalysis	Autocatalytic set	Kinetics, network topology, feedstock concentration	Transient depletion in reactants or rare product of pre-existing reactions
Darwinian threshold (Woese, 2002; Goldenfeld et al., 2017)	Progenotes with high Horizontal Gene Transfer (HGT)	Speciated individuals with high Vertical Gene Transfer	HGT strength (i.e., competence), fitness	Decrease in cell density, nutrient limitation, alkaline shift, toxic chemicals release

Table 1. Examples of Thresholds in Origin of Life Scenarios

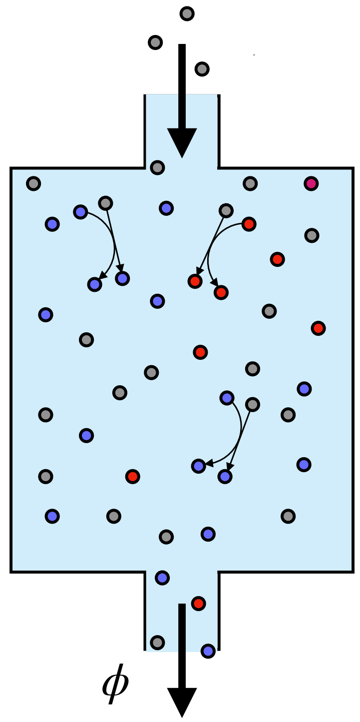
Systems states before and after crossing the threshold are listed, along with corresponding physico-chemical variables and prebiotically relevant phenomena.

Main results

Main results

Setup | Assumptions | Definition of fitness | (Non)elementary replicators | Derivation of main results

- Reaction volume contains n types of replicators
- Replicators flow out at dilution rate ϕ
- Consider (deterministic) concentrations in steady state



Each replicator X undergoes autocatalytic reaction:

$$X + \sum_i \alpha_i A_i \rightleftarrows X + X + \sum_i \beta_i A_i$$

Gibbs free energy of reaction

$$\sigma = -\ln x + \sum_i (\alpha_i - \beta_i) \ln a_i - \Delta G^\circ$$

Autocatalytic current

$$J(x, \mathbf{a}, \phi)$$

Outflow and autocatalysis balance

$$\phi x = J(x, \mathbf{a}, \phi)$$

ϕ: dilution rate x: concentration of replicator X $\mathbf{a} = (a_1, \ldots, a_k)$: concentrations of substrate/waste $A_1, \ldots, A_k$

Main results

J^+

$$X + \sum_i \alpha_i A_i \rightleftarrows X + X + \sum_i \beta_i A_i$$

J^-

$J(x, \mathbf{a}, \phi)$

Flux kinetics are "mass-action-like"

$$J^+ = \kappa^+(\mathbf{a}, \phi)x$$
$$J^- = \kappa^-(\mathbf{a}, \phi)x^2$$

Flux-force inequality

$$\sigma \geq \ln \frac{J^+}{J^-}$$

ϕ: dilution rate

x: concentration of replicator X

$\mathbf{a} = (a_1, \ldots, a_k)$: concentrations of substrate/waste $A_1, \ldots, A_k$

Main results

Fitness of replicator: maximum per-capita growth rate

$$f(\mathbf{a},\phi) := \sup_{x>0} J(x,\mathbf{a},\phi)/x$$

$$J(x,\mathbf{a},\phi) = \kappa^+(\mathbf{a},\phi)x - \kappa^-(\mathbf{a},\phi)x^2$$

$$\phi x = J(x,\mathbf{a},\phi)$$

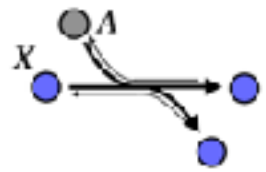
Fitness is the forward rate constant
$$f(\mathbf{a},\phi) = \kappa^+(\mathbf{a},\phi)$$

If $\phi > f(\mathbf{a},\phi)$, replicator must be extinct, $x = 0$
If $\phi < f(\mathbf{a},\phi)$, there is non-extinct steady state, $x > 0$

Main results

Setup | Assumptions | Definition of fitness | **(Non)elementary replicators** | Derivation of main results

Elementary replicator



Mass action current

$$J(x,\mathbf{a}) = k\prod_i a_i^{\alpha_i} x - k e^{\Delta G^\circ} \prod_i a_i^{\beta_i} x^2$$

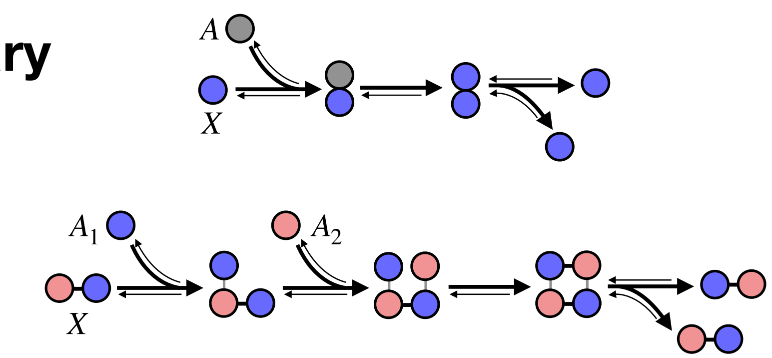
Flux-force equality

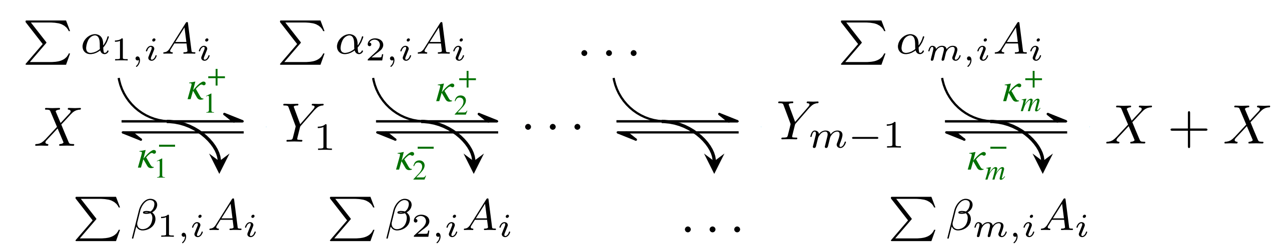
$$\sigma = \ln \frac{k\prod_i a_i^{\alpha_i} x}{k e^{\Delta G^\circ}\prod_i a_i^{\beta_i} x^2}$$

Fitness

$$f = k\prod_i a_i^{\alpha_i}$$

Non-elementary replicator





Mass-action-like current

$$J(x,\mathbf{a},\phi) = \kappa^+_{\text{eff}}(\mathbf{a},\phi)x - \kappa^-_{\text{eff}}(\mathbf{a},\phi)x^2$$

Flux-force inequality

$$\sigma \geq \ln \frac{\kappa^+_{\text{eff}}(\mathbf{a},\phi)x}{\kappa^-_{\text{eff}}(\mathbf{a},\phi)x^2}$$

Fitness

$$f(\mathbf{a},\phi) = k^+_{\text{eff}}(\mathbf{a},\phi)$$

$$\kappa^+_{\text{eff}}(\mathbf{a},\phi) = \kappa_1^+\left[\kappa_1^-(M+\phi I)^{-1}_{11} + 2\kappa_m^+(M+\phi I)^{-1}_{m-1,1} - 1\right]$$

$$\kappa^-_{\text{eff}}(\mathbf{a},\phi) = \kappa_m^-\left[2 - \kappa_1^-(M+\phi I)^{-1}_{m-1,m-1} + 2\kappa_m^+(M+\phi I)^{-1}_{1,m-1}\right]$$

$$M = \begin{bmatrix} \kappa_1^- + \kappa_2^+ & -\kappa_2^- & 0 & 0 & 0 & \dots \\ -\kappa_2^+ & \kappa_2^- + \kappa_3^+ & -\kappa_2^- & 0 & 0 & \dots \\ 0 & -\kappa_3^+ & \kappa_3^- + \kappa_4^+ & -\kappa_3^- & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix}$$

Main results

Setup | Assumptions | Definition of fitness | (Non)elementary replicators | **Derivation of main results**

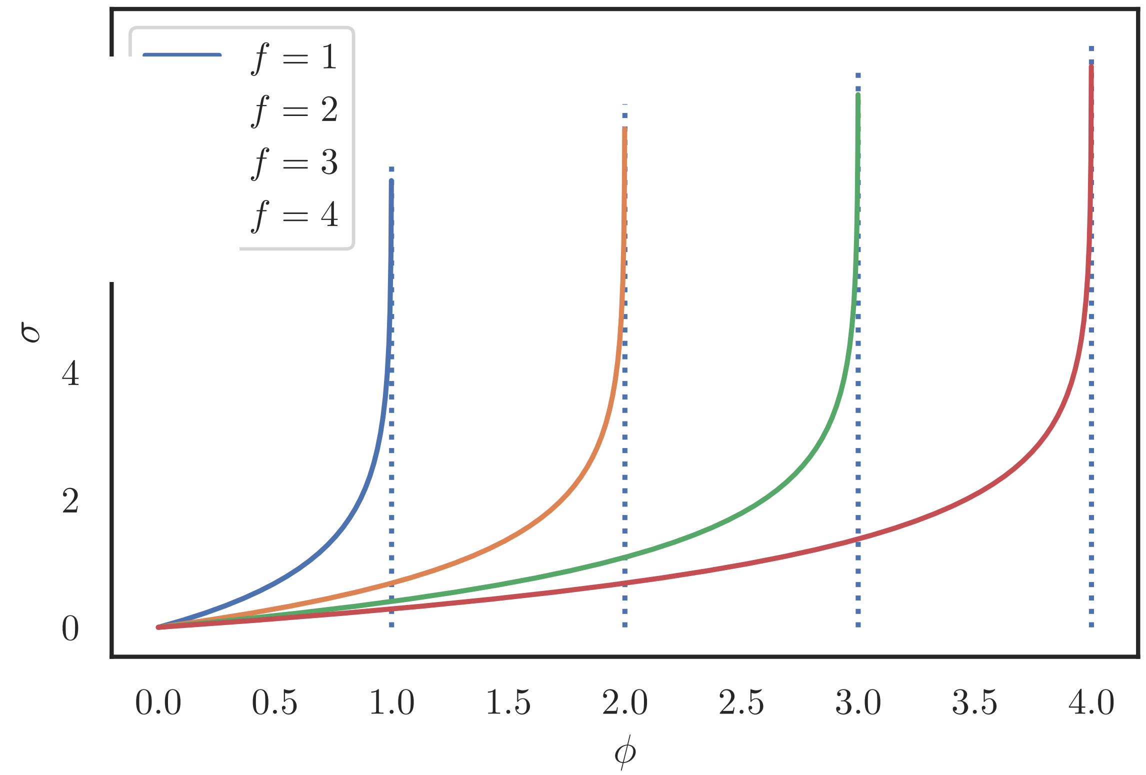
Flux-force inequality

Defi

Stea

ϕ

Defi



$$\sigma \geq -\ln\left(1-\frac{\phi}{f}\right)$$

$$\text{Dissipation} \geq -\ln\left(1-\frac{\text{Actual growth rate}}{\text{Max growth rate}}\right)$$

Main results

Consider two replicators:

1. Replicator X with fitness f that is not extinct, $x > 0$
2. Replicator X' with fitness f' that is extinct, $x' = 0$

If $\phi > f'$, replicator X' must be extinct, $x' = 0$

If $\phi < f'$, there is non-extinct steady state, $x' > 0$

$$\sigma \geq -\ln\left(1 - \frac{\phi}{f}\right)$$

$$\sigma \geq -\ln\left(1 - \frac{f'}{f}\right)$$

$$= -\ln s$$

$$s := 1 - f'/f$$

A thermodynamic bound on selection for molecular replicators

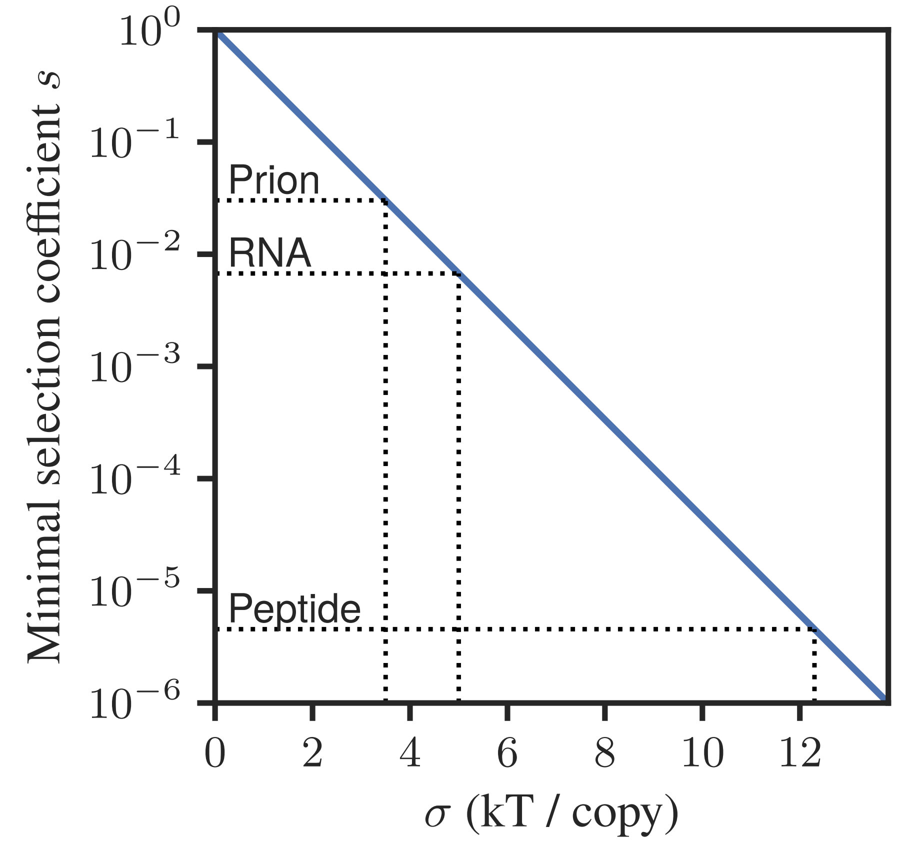
$$s \geq e^{-\sigma}$$

Illustration of result

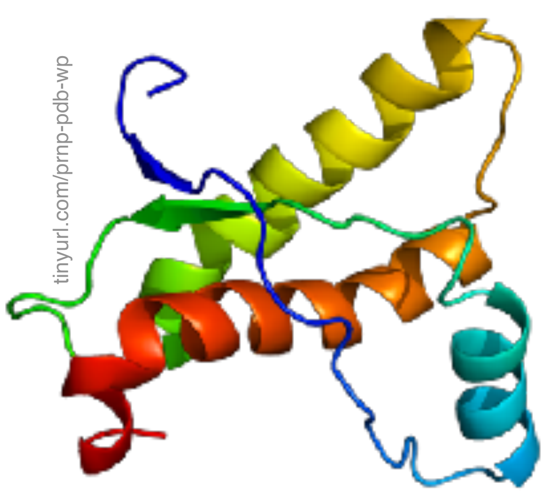
Comparison to real-world replicators

A thermodynamic bound on selection for molecular replicators

$$s \geq e^{-\sigma}$$



Self-replicating prion

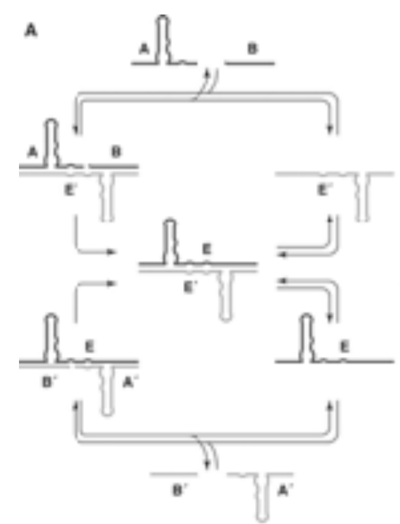


$3.5\ kT$

Baskakov et al, *J Bio Chem*, 2001

Self-replicating RNA

Lincoln & Joyce, Science, 2009

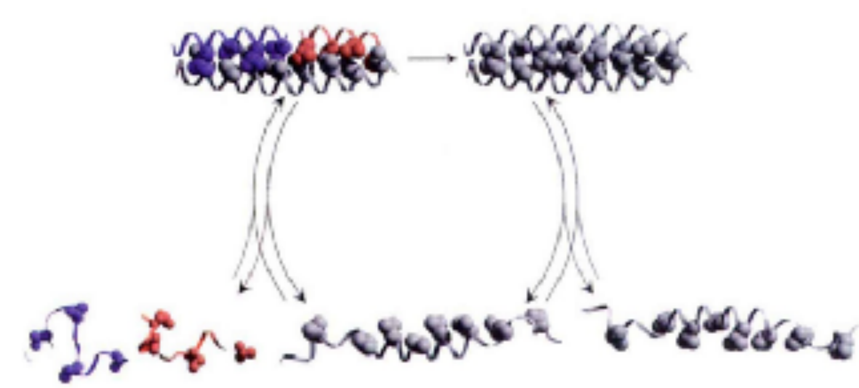


$5\ kT$

Jülicher & Bruinsma, *Biophys J*, 1998

Self-replicating peptide

Lee et al, Nature, 1996

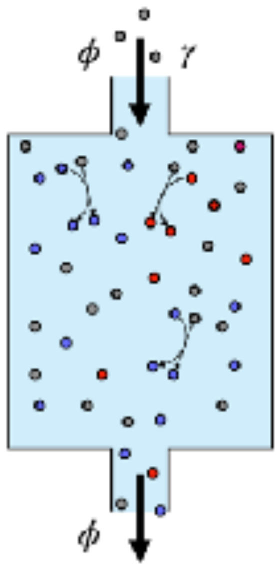


$12\ kT$

Wang et al, *Chem: Asian J*, 2011

Example: elementary replicators in a chemostat

Example: elementary replicators in a chemostat



$X_1 + A \rightleftarrows X_1 + X_1$

$X_2 + A \rightleftarrows X_2 + X_2$

$X_3 + A \rightleftarrows X_3 + X_3$

$X_4 + A \rightleftarrows X_4 + X_4$

$$\dot{x}_i(t) = k_i x_i(t)[a(t) - e^{\Delta G_i^\circ} x_i(t)] - \phi x_i(t)$$
$$\dot{a}(t) = \phi(\gamma - a(t)) - \sum_i k_i x_i(t)[a(t) - e^{\Delta G_i^\circ} x_i(t)]$$

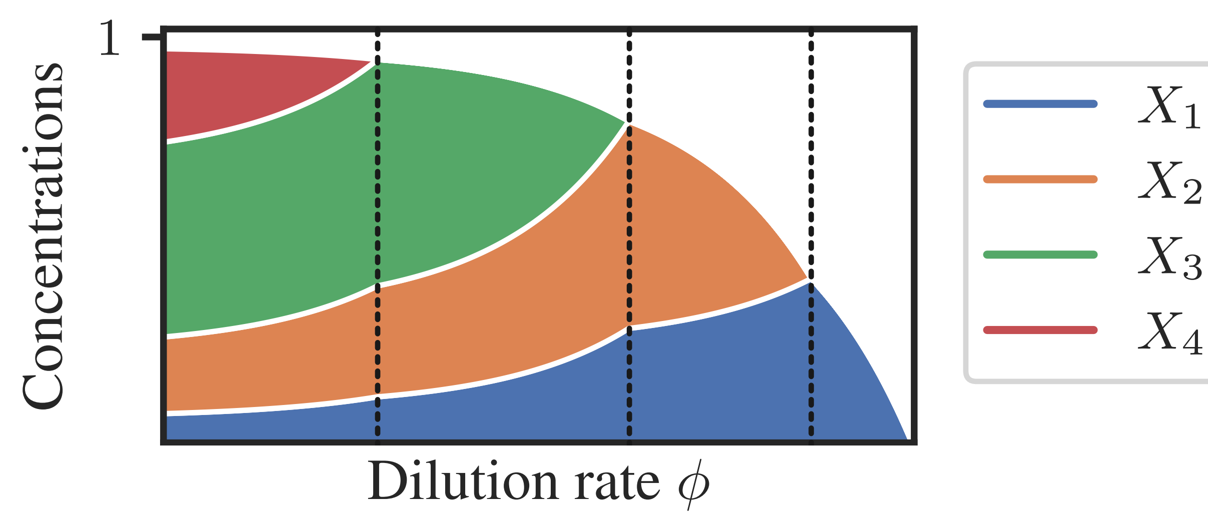
ϕ	dilution rate	k_i	rate constant of replicator X_i
γ	inflow substrate concentration	$-\Delta G_i^\circ$	standard Gibbs energy of X_i
$a(t)$	substrate concentration in volume	$x_i(t)$	concentration of replicator X_i

$$k_1 > k_2 > k_3 > k_4$$

Steady state:

$$a = \gamma - \sum_i x_i, \quad x_i = \max\{0, e^{-\Delta G_i^\circ}(a - \phi/k_i)\}$$

Schuster and Sigmund, Dynamics of Evolutionary Optimization, *Berichte der Bunsengesellschaft für physikalische Chemie*, 1985



$\sigma \geq -\ln s$

$$\sigma_i = \ln \frac{a}{x_i} - \Delta G_i^\circ$$
$$f_i = k_i a$$
$$s_i = 1 - f_i/f_1 = 1 - k_i/k_1$$

$$\sigma_1 \geq -\ln s_i = -\ln(1 - k_i/k_1)$$

σ increases with the dilution rate ϕ

Other issues + future work

Collectively autocatalytic systems (autocatalytic sets)

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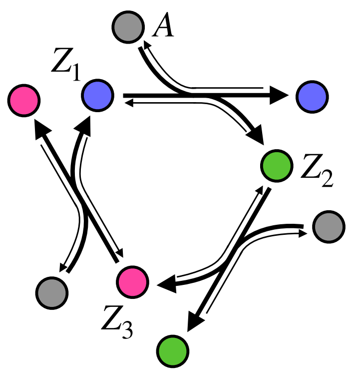
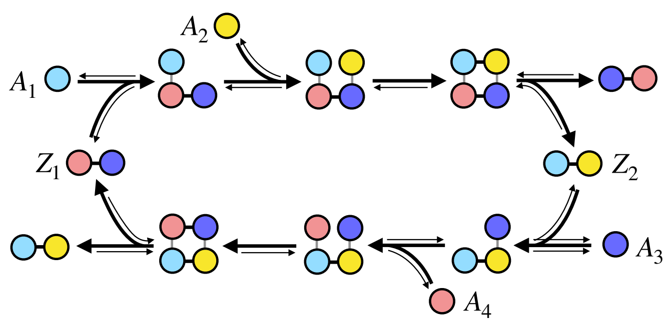
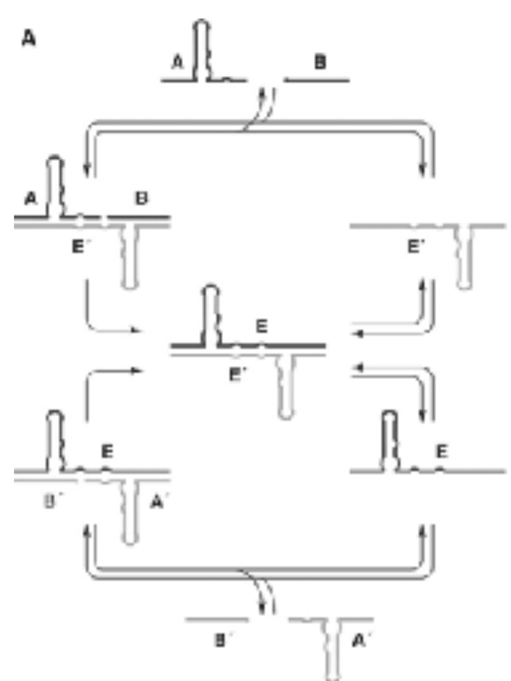


$$Z_{j-1} + \sum_i \alpha_{j,i} A_i \rightleftarrows Z_{j-1} + Z_j + \sum_i \beta_{j,i} A_i$$
$$j \in \{1..m\} \qquad \text{mod } m$$





Self-replicating RNA
Lincoln & Joyce, Science, 2009

Fitness of a cross-catalytic cycle

$$f(\mathbf{a}, \phi) := \sup_{\lambda \geq 0, \mathbf{z} \in \mathbb{R}_+^m} \lambda \quad \text{such that} \quad J_j(\mathbf{z}, \mathbf{a}, \phi) = \lambda z_j$$

$$f(\mathbf{a}, \phi) = \prod_j \kappa_j^+(\mathbf{a}, \phi)^{1/m}$$

$$\langle \sigma \rangle = \frac{1}{m} \sum_j \sigma_j(\mathbf{z}, \mathbf{a})$$

$$\langle \sigma \rangle \geq -\ln\left(1 - \frac{\phi}{f}\right)$$

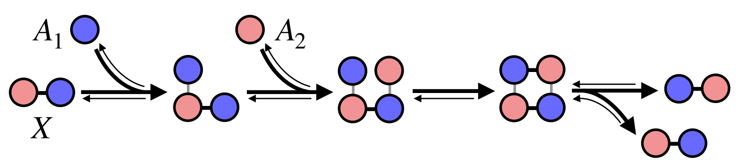
$$\langle \sigma \rangle \geq -\ln\left(1 - \frac{f'}{f}\right)$$

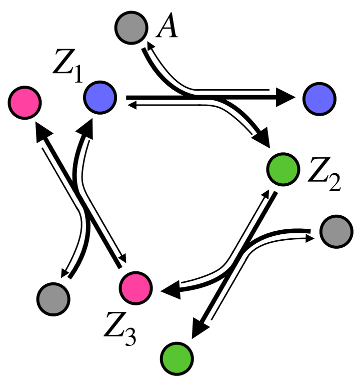
Future work

1. Stochastic fluctuations

2. Mutations

3. More general topologies for nonelementary replicators and for autocatalytic sets

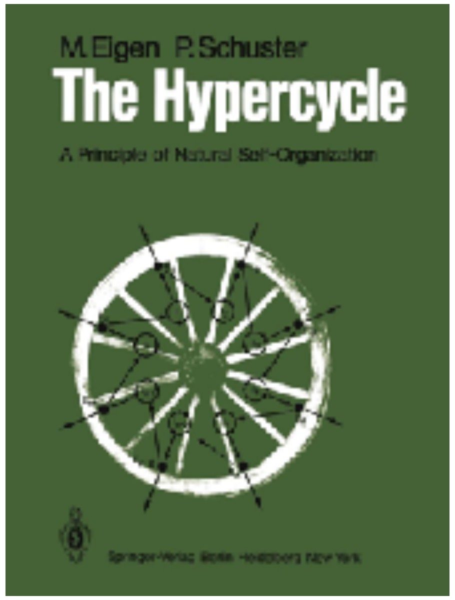




4. Second-order replicators

"The Shlögl Model"

$$2X + A \rightleftarrows 3X$$



Thank you!

artemyk@gmail.com

arxiv.org/abs/2112.02809