Extending computational complexity theory to include thermodynamic resource costs

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with

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For continuous-time Markov chains sending p(0) to $p(1) = \sum_j P(i \mid j)\, p_j(0)$

Van denBroeck and Esposito, *Physica A*, 2015

For many non-Markvonian chains sending p(0) to $p(1) = \sum_j P(i \mid j)\, p_j(0)$

Ptaszynski and Esposito, *PRL*, 2019

$$-\Delta Q = \Delta\Sigma - \Delta S$$

- $\Delta S = S(p_1) - S(p_0)$ is gain in Shannon entropy of p
- $-\Delta Q$ is (Shannon) entropy flow from system between t = 0 and t = 1
- $\Delta\Sigma$ is total entropy production in system between t = 0 and t = 1
  - ***cannot be negative***

  (I.e., the second law of thermodynamics)

GENERALIZED LANDAUER BOUND

- System connected to multiple reservoirs, e.g., heat baths at different temperatures. (So "$k_B T$" not defined.)
- Arbitrary number of states
- Arbitrary initial distribution p_0
- Arbitrary dynamics $P(x_1 \mid x_0)$

$$-\Delta Q = \Delta\Sigma + S(p_0) - S(p_1)$$

Entropy Production ($\Delta\Sigma$) is non-negative. So:

"*Generalized Landauer's bound*"

$$-\Delta Q \geq S(p_0) - S(p_1)$$

BOOLEAN CIRCUITS

- Currently, all mass-produced computers are implemented with circuits.

- The simplest circuit is one without loops or branches (a "straight-line program")

- If set of allowed gates are a universal basis (e.g., NAND gates), then can build a circuit with them to implement any desired Boolean function.

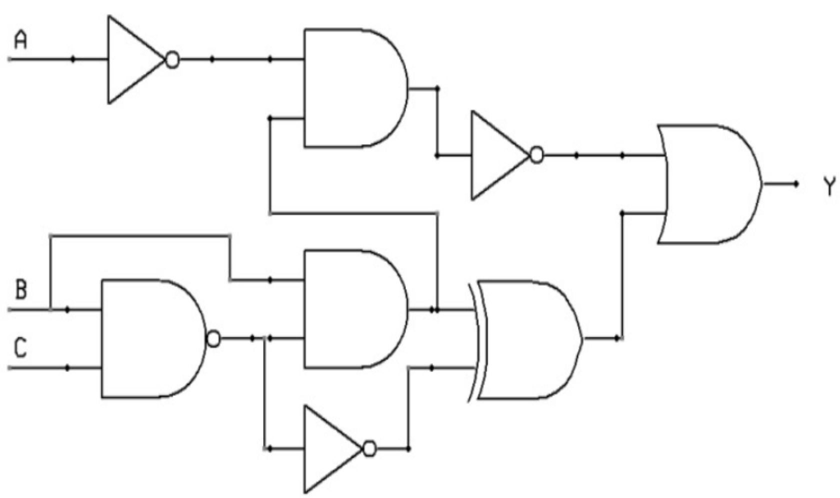
$$-\Delta Q = \Delta\Sigma + S(p_0) - S(p_1)$$

- For fixed $P(x_1 \mid x_0)$, changing p_0 changes Landauer cost, $S(p_0) - S(p_1)$

- N.b., the same $P(x_1 \mid x_0)$ - e.g., same AND gate - has different p_0, depending on where it is in a circuit.

- So *even for a thermo. reversible gate* ($\Delta\Sigma(p_0) = 0$), ***changing the gate's location in a circuit*** (changes $S(p_0) - S(p_1)$ and so) ***changes*** $-\Delta Q(p_0)$

A	B	C	Y
0	0	0	
0	0	1	
0	1	0	
0	1	1	
1	0	0	
1	0	1	
1	1	0	
1	1	1	



- Changing a gate's location in a circuit changes $S(p_0) - S(p_1)$, and so changes the heat it produces, $-\Delta Q(p_0)$

- Sum those heats over all gates to get minimal heat flow of that circuit

Different circuits implementing *same* Boolean function on *same* input distribution have *different* minimal heat

- Formally, those differences in minimal heat of the circuits are differences in EPs of the circuits, arising due to modularity of gates

➢ A new circuit design optimization problem

A	B	C	Y
0	0	0	
0	0	1	
0	1	0	
0	1	1	
1	0	0	
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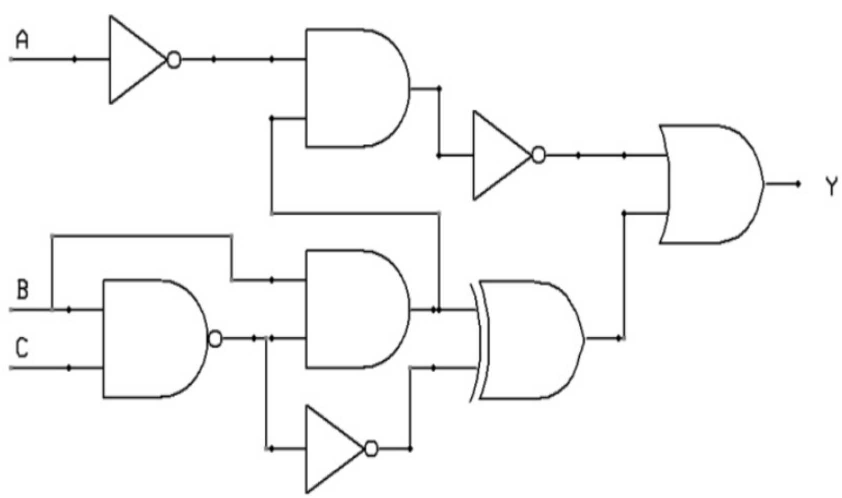

Demaine, E., et al., *Comm. ACM*, 2016

- Considers a similar problem - but incorrectly sets Landauer cost at each gate to same value, KT ln(2).

WHAT IS *REALLY* IMPORTANT THERMODYNAMICALLY?

$$-\Delta Q = \Delta\Sigma + S(p_0) - S(p_1)$$

- System evolves while connected to *single* heat bath at temperature *T*
  - Then heat flow into environment = $-k_B T\, \Delta Q$

- At scale of real computers and brains, $k_B T[S(p_0) - S(p_1)]$ is small

- At scale of real computers and brains, $\Delta\Sigma$ **is dominant cost**
  - Generalized Landauer's bound often irrelevant (it assumes $\Delta\Sigma = 0$!)

What determines $\Delta\Sigma$?

BEYOND GENERALIZED LANDAUER

- System connected to multiple reservoirs, e.g., heat baths at different temperatures. (So "$k_B T$" not defined.)
- Arbitrary number of states
- Arbitrary initial distribution p_0
- Arbitrary dynamics $P(x_1 \mid x_0)$

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Entropy Production ($\Delta\Sigma$) is non-negative.

Are there broadly applicable non-negative lower bounds on $\Delta\Sigma$, to complement Landauer's bound?

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- Yes.

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Entropy Production ($\Delta\Sigma$) is non-negative.

Are there broadly applicable non-negative lower bounds on $\Delta\Sigma$, to add to the lower bound $-\Delta Q \geq S(p_0) - S(p_1)$?

- Yes.

  - Focus on two: ***Speed limit theorem*** (SLT) and ***Mismatch cost***

Use them to investigate
the (thermodynamic) resource costs of
computational machines

Original speed limit theorem (SLT): $$\Delta\Sigma \geq \frac{L(p(0), p(1))}{A_{0,1}}$$

- $L(p(0), p(1))$: L_1 distance from distribution p(0) to distribution p(1)
- $A_{0,1}$: total number of (stochastic) state jumps from t = 0 to t = 1

Since introduced, SLT has been strengthened several ways

(more complicated formulas).

Shiraishi, N., Funo, K.; Saito, K., *PRL* (2018)
Delvenne, J., Falasco, G.; arXiv:2110.13050
Lee, J., et al.; *PRL* (2022)
Van Vu, T., Saito, K.; *PRL* (2023)

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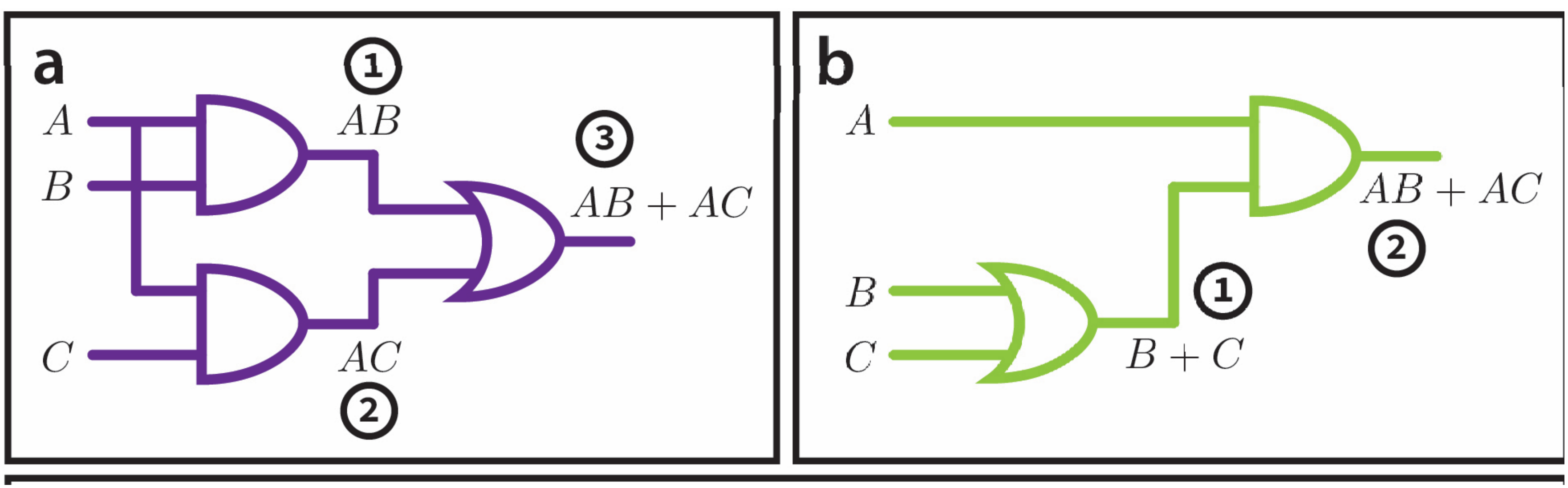
- Suppose uniform initial distribution over all gates and input bits;
- How does the (Lee et al.) SLT bound vary with error rate of gates, for two logically equivalent circuits?



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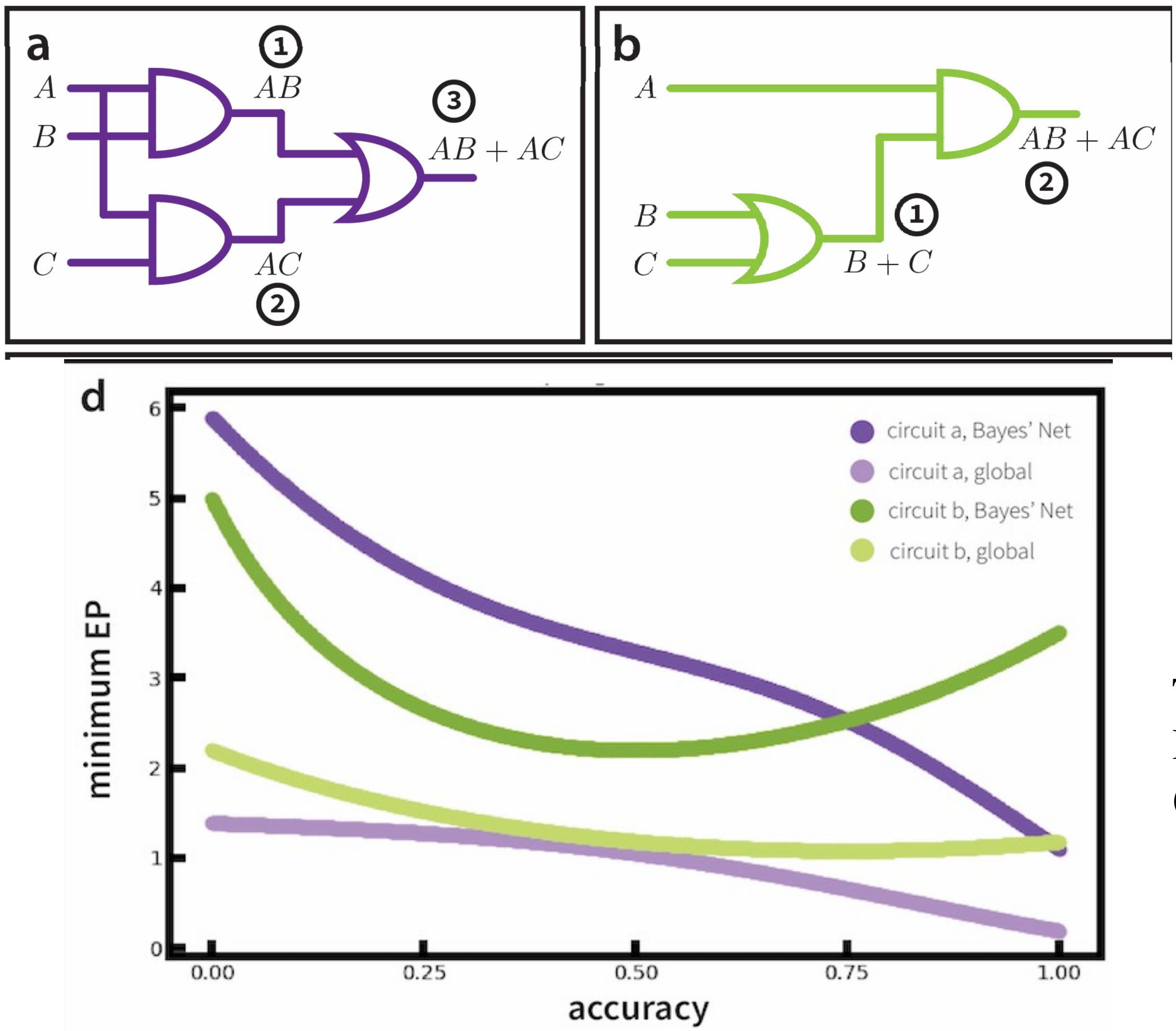

Tasnim, F., Wolpert, D., Korbel J., Lynn, C., et al. (2023)

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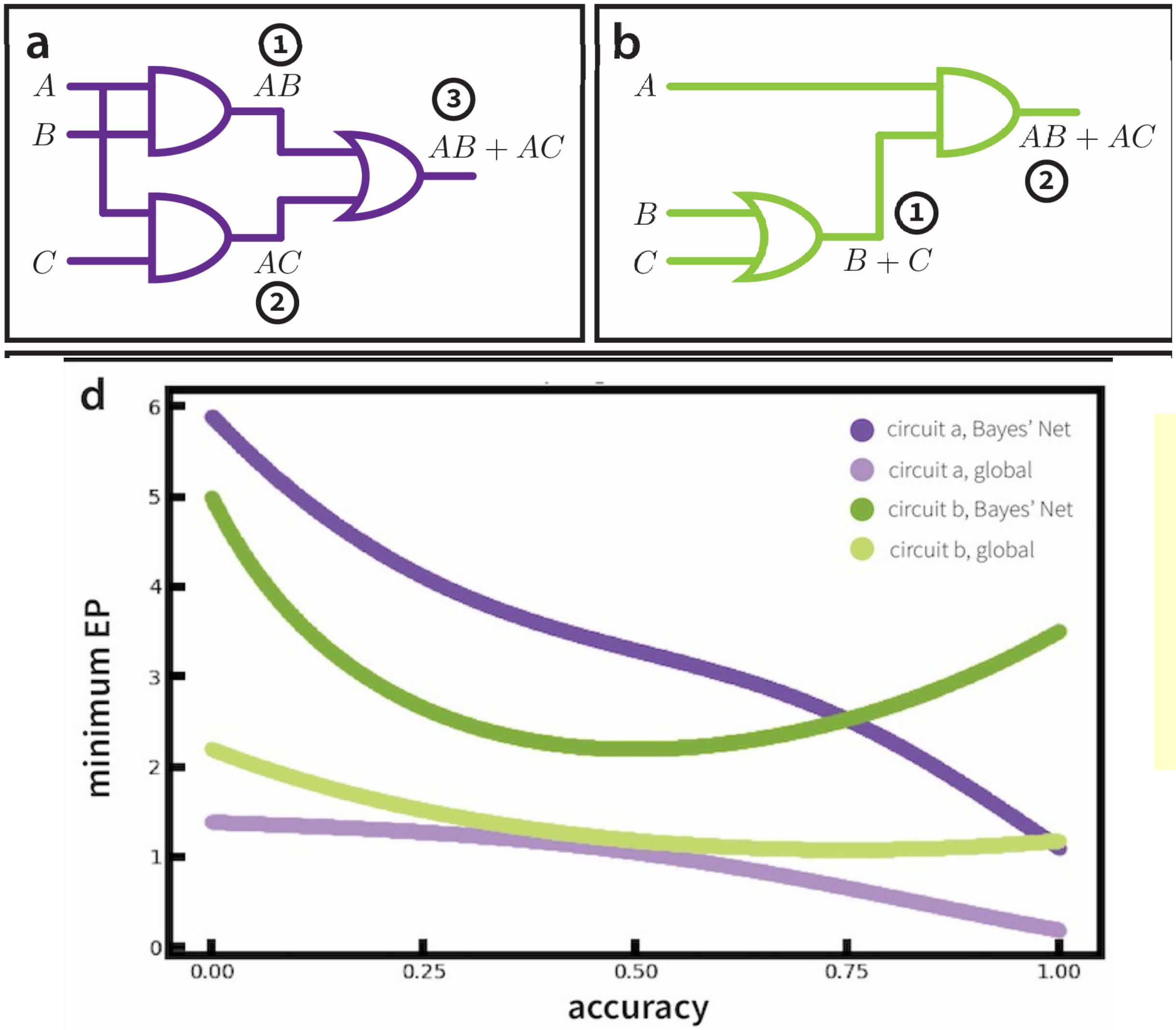

What causes the curves to have these shapes? What are curves for other circuits?

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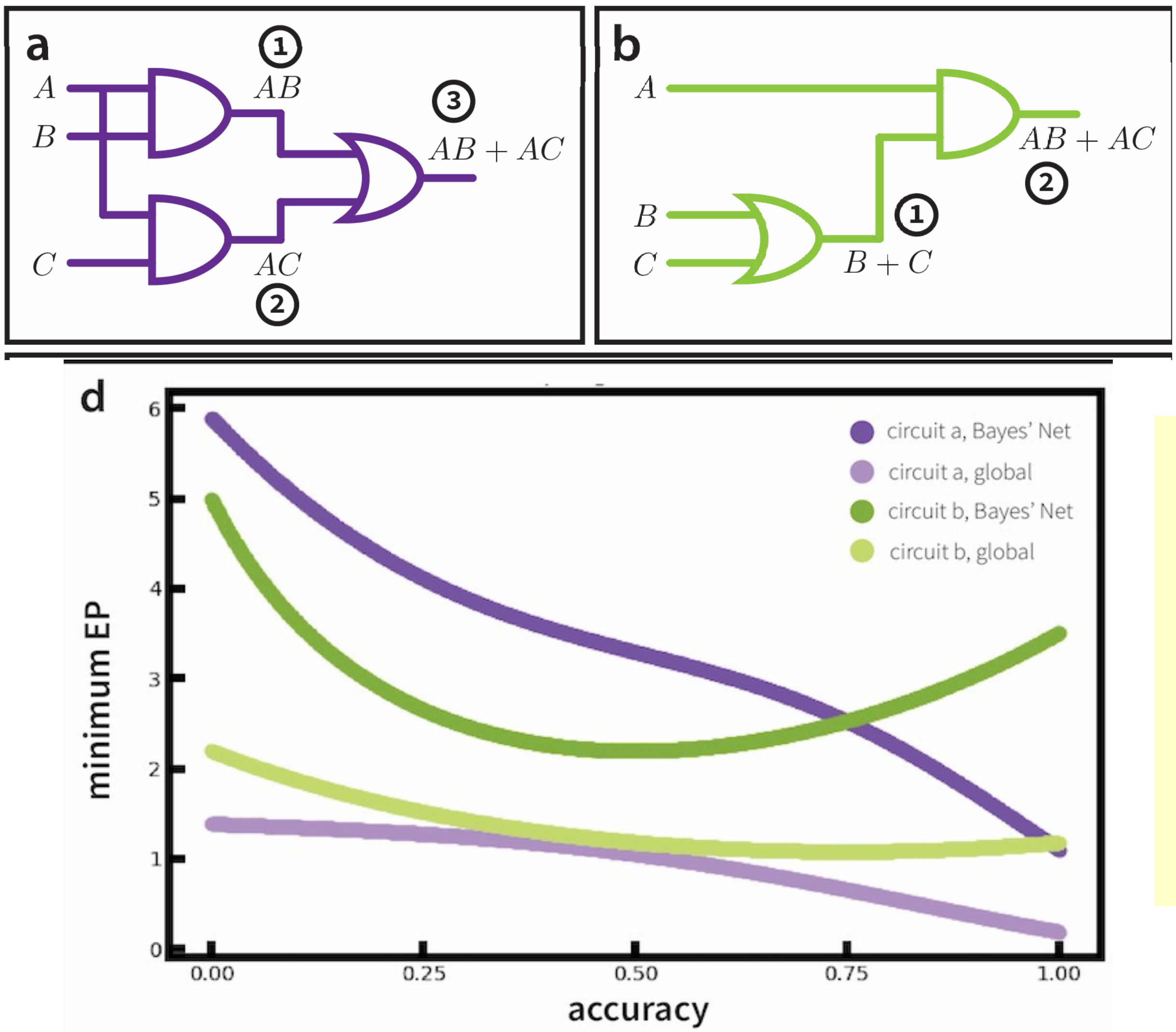

What causes the curves to have these shapes? What are curves for other circuits?

A: Who knows!

DEPENDENCE OF EP ON INITIAL DISTRIBUTION

- Arbitrary dynamics $P(x_1 \mid x_0)$
- ***Assume system is thermo. reversible for initial distribution q_0***

  I.e., $\Delta\Sigma(q_0) = 0$

- Run that system with initial distribution $p_0 \neq q_0$ instead:

$$\Delta\Sigma(p_0) = D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1) \geq 0$$

where D(. || .) is relative entropy (KL divergence)

Kolchinsky, A, Wolpert D., *J. Stat. Mech.* (2017)
Wolpert, D., Kolchinsky, A., *New J. Phys.* (2020)
Riechers, P., Gu, M., *Phys. Rev. E* (2021)
Kolchinsky, A., Wolpert D., *arxiv:2103.05734*

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$D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1)$ is called ***mismatch cost***

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Any nontrivial process that is thermodynamically reversible for one initial distribution ***will be costly*** for any other initial distribution

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Holds for master equations, Langevin dynamics, (open) quantum thermodynamics, inclusive (Hamiltonian) dynamics – pretty much everything.

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Same formula (just different prior q) for nonadiabatic EP, net lost free energy, etc.

EXAMPLE: Mismatch cost for parallel bit erasure

- ***Two*** distinct bit-erasing gates, each with thermo. rev. initial distribution q_0
- Run gates in parallel, on bits x^A and x^B, with initial distribution $p_0(x^A, x^B)$
- Assume $p_0(x^A) = q_0(x^A)$ and $p_0(x^B) = q_0(x^B)$.

- So each gate, by itself, generates zero EP. But:

If $p_0(x^A, x^B)$ statistically couples the bits, then full system is **not** *thermo. reversible, and generates nonzero EP*

- **Formally**: Since gates are distinct, the thermo. rev. *joint* distribution is

$$q_0(x^A, x^B) = q_0(x^A)q_0(x^B)$$

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$q_0(x^A, x^B) = q_0(x^A)q_0(x^B)$. So $D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1) \neq 0$

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- Intuition: **Running two thermo. reversible gates in parallel loses information in their initial coupling, and so is not thermo. reversible**.

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- **Broader lesson**: ***Modularity increases EP***

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- **Broader lesson**: Whatever its practical benefits might be,

modularity is thermodynamically costly (!)

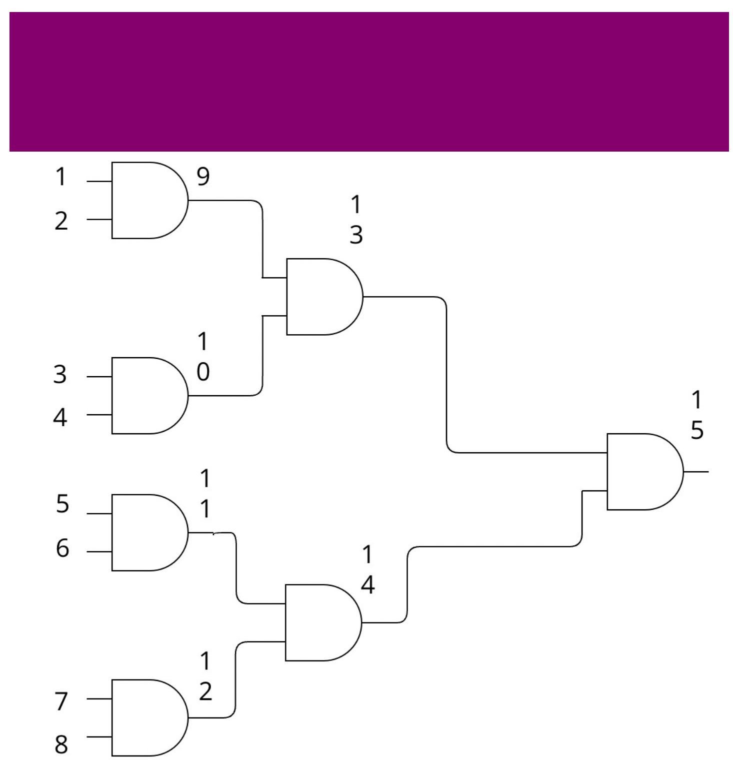
EXAMPLE: Mismatch cost for reusing a Boolean circuit

Over N periods, the sum-total mismatch cost (lower bound on EP) is:

$$\sum_{t=0}^{N-1} \left[D(P^t p_0 \,||\, q) - D(P^{t+1} p_0 \,||\, Pq) \right]$$

Gates are not reinitialized after being run; have old values when next run.
So assuming IID generation of input, $R(x_0)$, initially, joint distribution is

$$R(x) = R(x_0)\, R(x_{1,2,3} \mid x_0)$$



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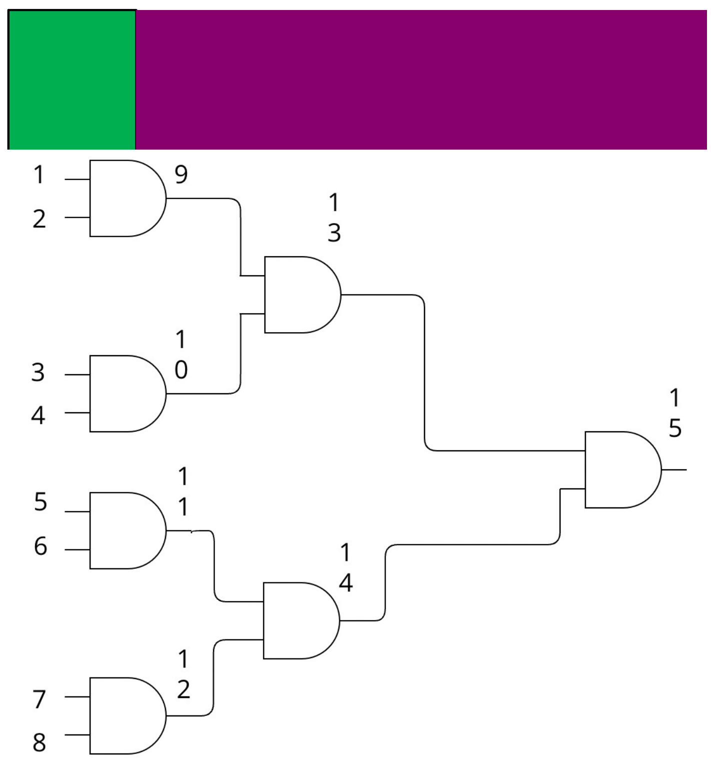
So assuming IID generation of input, $R(x_0)$, after running 1st layer, joint distribution is

$$R(x) \;=\; R(x_0)\, R(x_{1,2,3})$$



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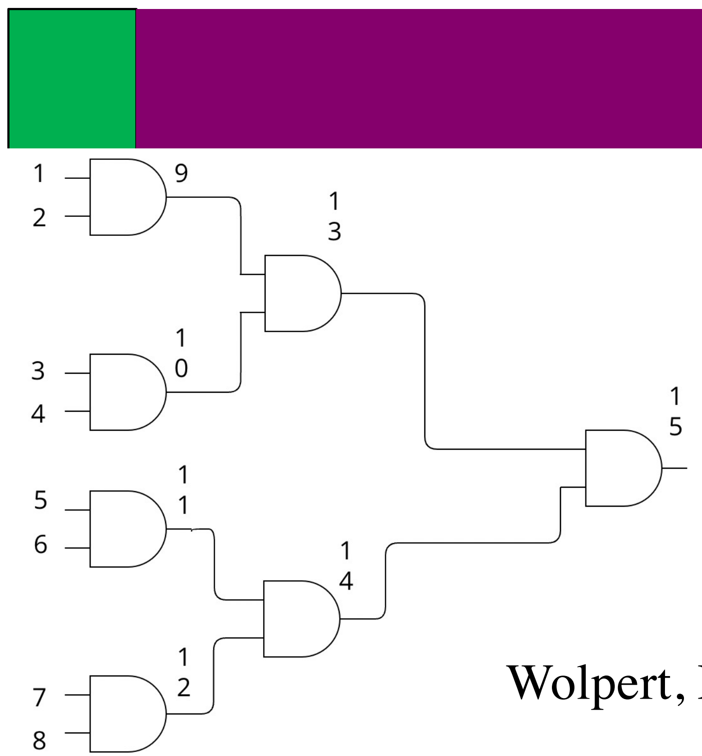
So running 1st layer gives mismatch cost

$$D\big(R(x_0)\, R(x_{1,2,3} \mid x_0) \,||\, q(x_0)\, q(x_{1,2,3} \mid x_0)\big) \; - \; D\big(R(x_0)\, R(x_{1,2,3}) \,||\, R(x_0) q(x_{1,2,3})\big)$$

$$\geq$$

$$I_R(X_0\, ; X_1, X_2, X_3)$$



Wolpert, D.H. *Phys. Rev. Letters*, **125**, (2020)

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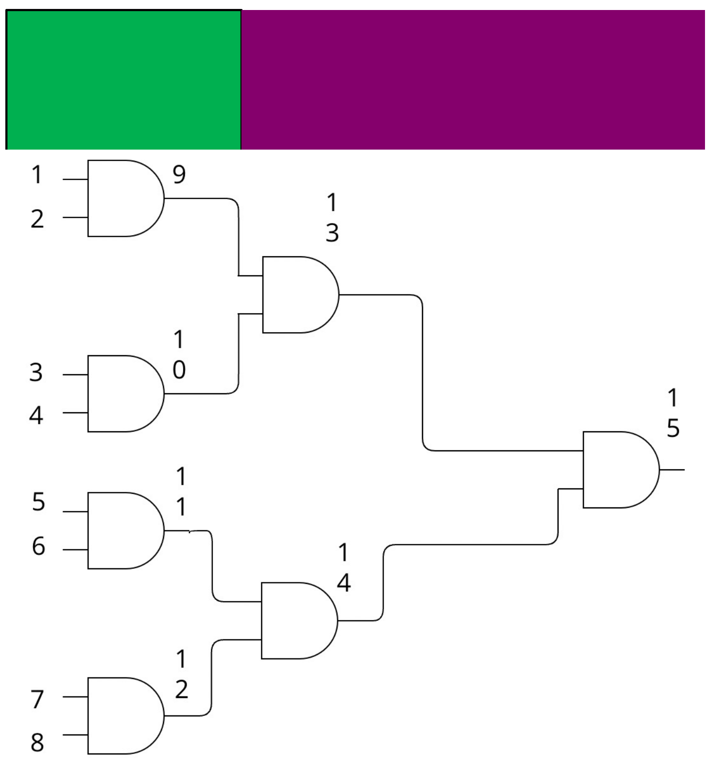
So assuming IID generation of input, $R(x_0)$, after running 2nd layer, joint distribution is

$$R(x) = R(x_{0,1})\, R(x_{2,3})$$



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So running 2nd layer gives mismatch cost

$$D(R(x_0)\, R(x_{1,2,3}) \,||\, R(x_0)\, q(x_{1,2,3})) \;-\; D(R(x_{0,1}) R(x_{2,3}) \,||\, R(x_{0,1}) q(x_{2,3}))$$

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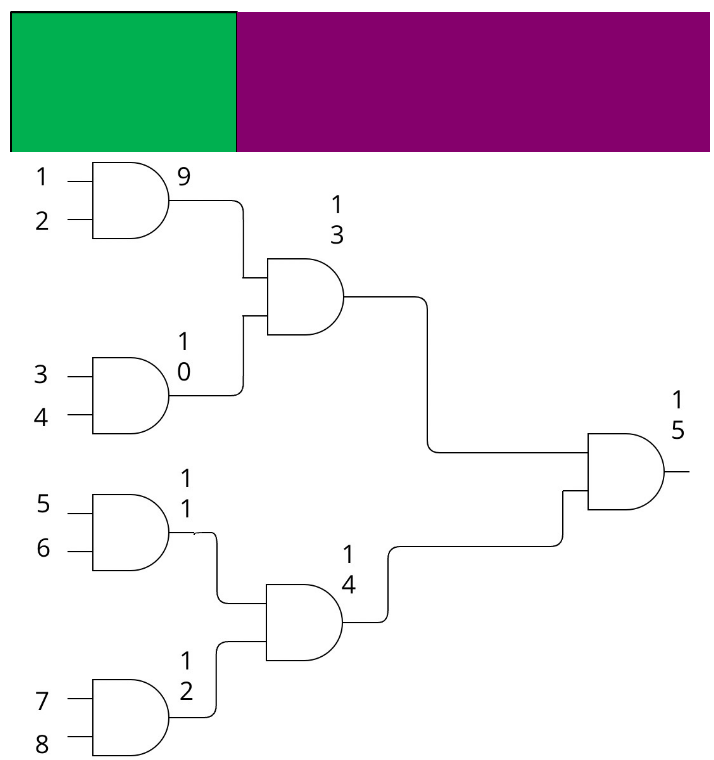

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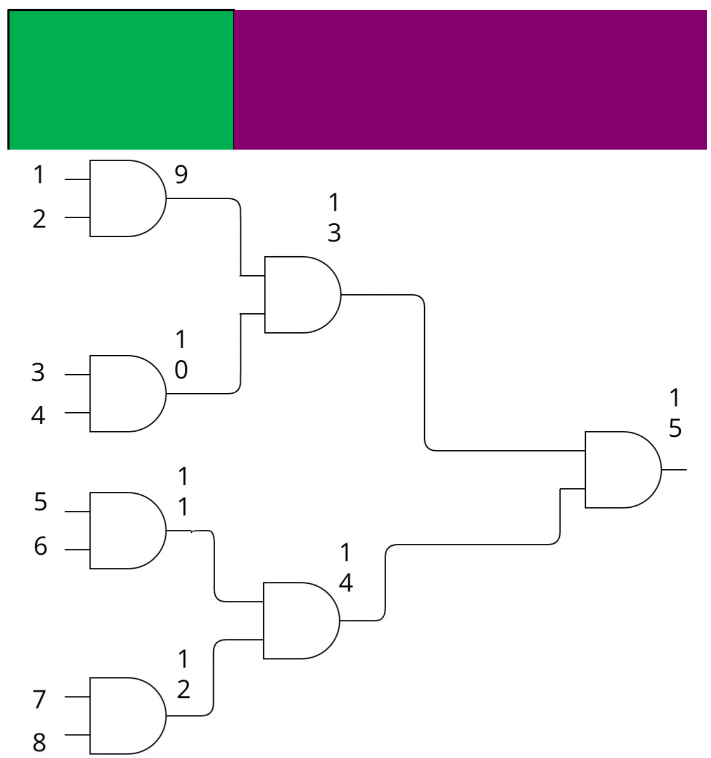

Technical detail: Also is a variable saying which layer is currently being updated, which increments in each iteration

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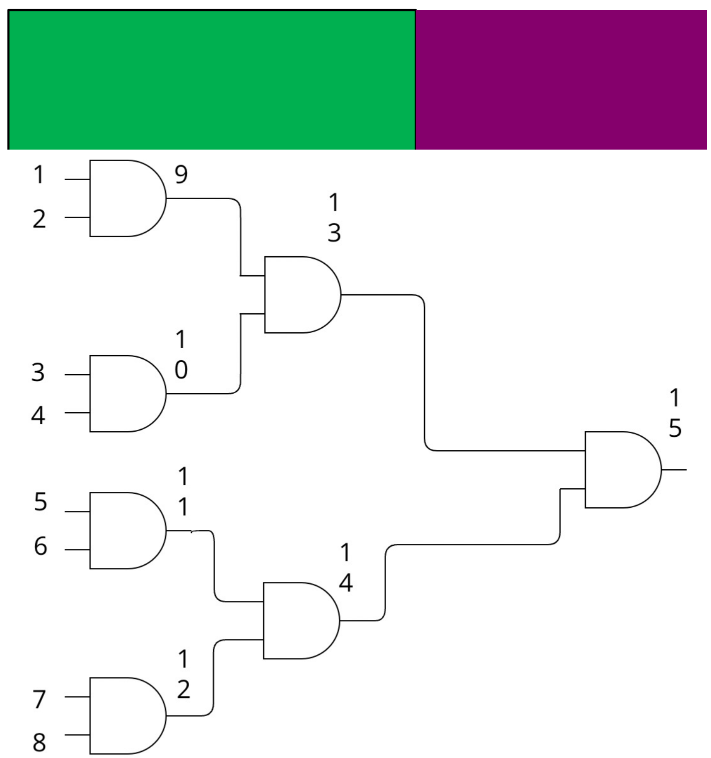
So assuming IID generation of input, $R(x_0)$, after running 3rd layer, joint distribution is

$$R(x) = R(x_{0,1,2})\, R(x_3)$$



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So running 3rd layer gives mismatch cost

$$D(R(x_{0,1})R(x_{2,3}) \,||\, R(x_{0,1})q(x_{2,3})) \;-\; D(R(x_{0,1,2})R(x_3) \,||\, R(x_{0,1,2})q(x_3))$$

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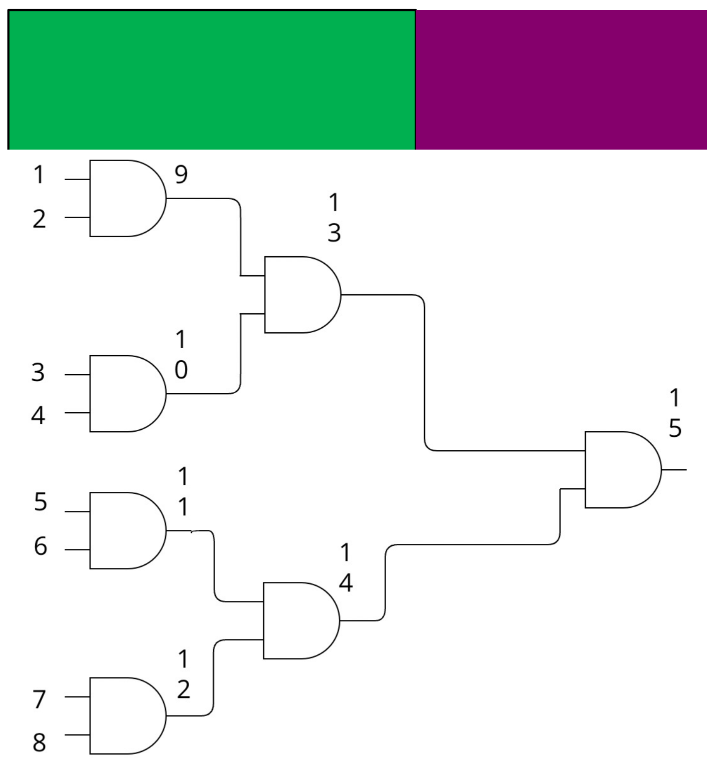

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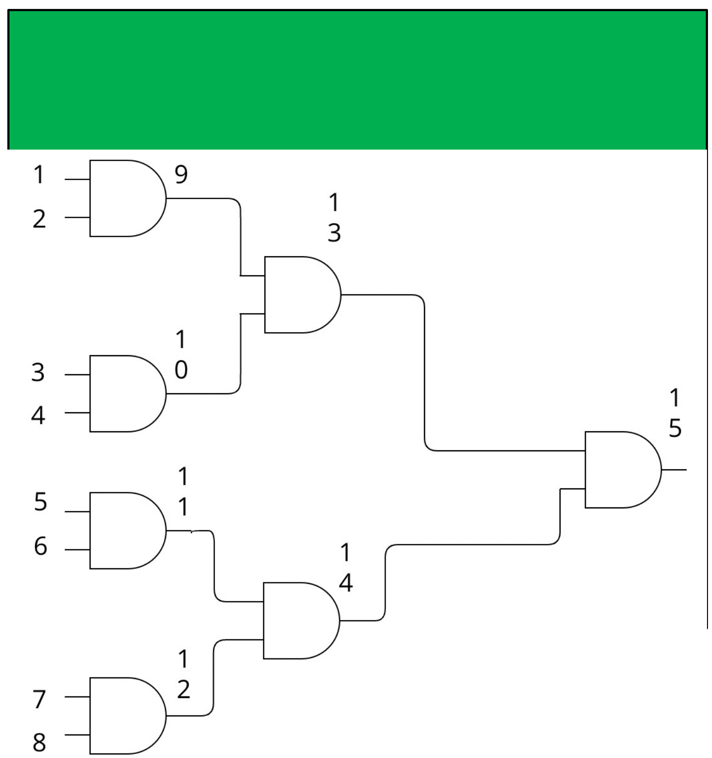
So assuming IID generation of input, $R(x_0)$, after running 4th layer, joint distribution is

$$R(x) \;=\; R(x_{0,1,2,3}) \;=\; R(x_{0,1,2,3})$$



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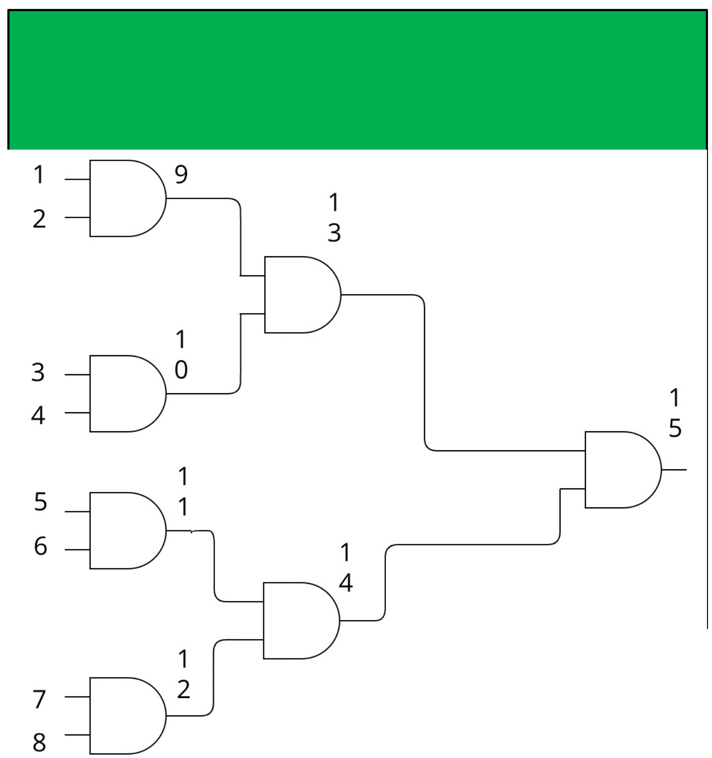
So running 4th layer gives mismatch cost

$$D(R(x_{0,1,2})R(x_3) \,||\, R(x_{0,1,2})q(x_3)) \; - D(R(x_{0,1,2,3}) \,||\, R(x_{0,1,2,3}))$$



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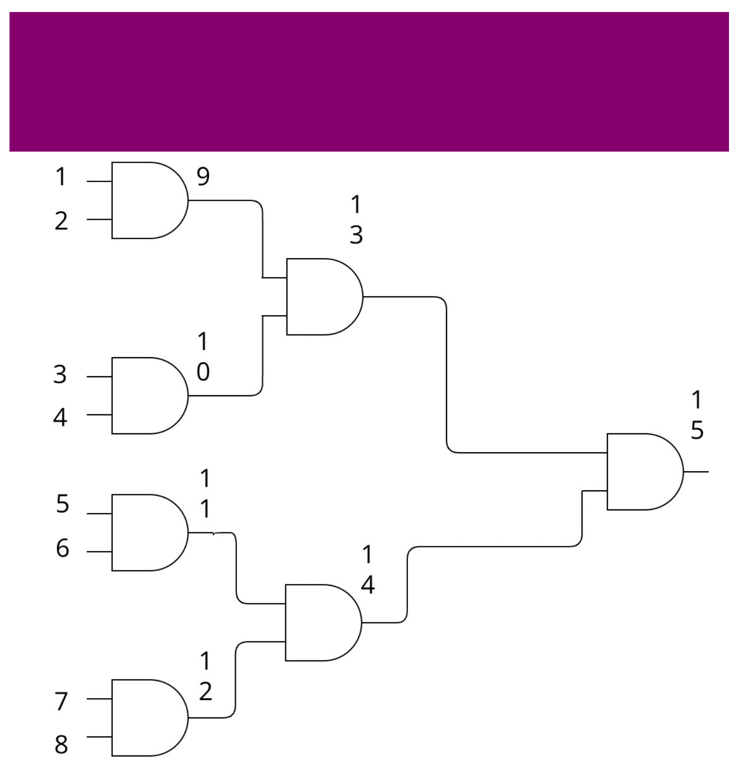
So assuming IID generation of input, $R(x_0)$, after 4th layer, joint distribution is

$$R(x) \;=\; R(x_0)R(x_{1,2,3} \mid x_0) = R(x)$$



MISMATCH COST IN PERIODIC PROCESSES

A process over a space X that is periodic, with period **λ**. So for all n,

$$P\left(x(n\lambda) \mid x((n-1)\lambda)\right) = P\left(x(\lambda) \,|\, x(0)\right)$$

So over N periods, the sum-total mismatch cost (lower bound on EP) is:

$$\sigma(N\lambda) \geq \inf_{q \in \Delta_X} \sum_{t=0}^{N-1} \left[D(P^t p_0 \,||\, q) - D(P^{t+1} p_0 \,||\, Pq)\right]$$

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A new strictly positive lower bound on EP for *any* periodic process

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So over N periods, the sum-total mismatch cost (lower bound on EP) is:

$$\sigma(N\lambda) \geq N\Delta JS(\{P^t p_0\})$$

- JS is Jensen-Shannon divergence for uniform distribution over N periods

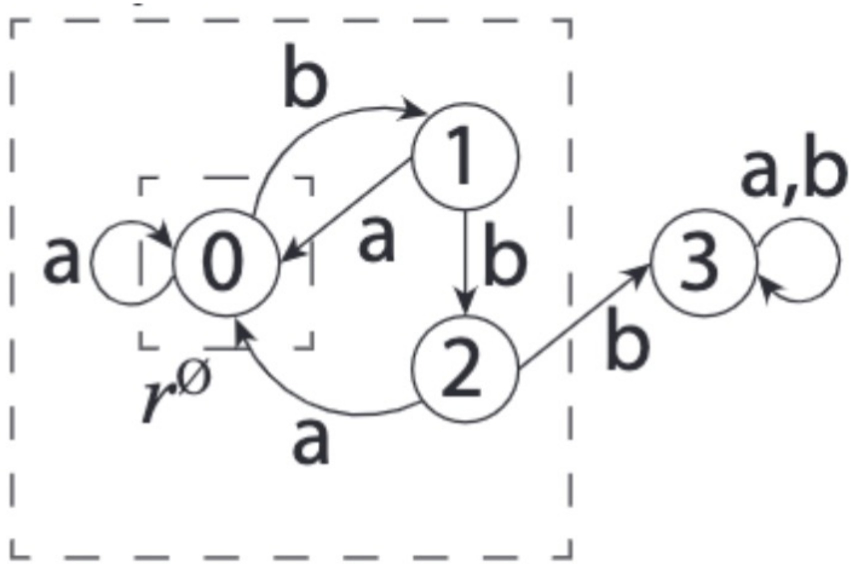
A new strictly positive lower bound on EP for *any* periodic process

Wolpert, D.H. *Phys. Rev. Letters*, **125**, (2020)
Ouldridge, T.; Wolpert, D.H., arxiv:2208.06895 (2022)
Tasnim, F.; Wolpert, D.H. *Entropy*, (2023)
Manzano, G., Kardes, G.; Roldan, E.; Wolpert, D.H., arxiv: 2307.05713 (2023)

DETERMINISTIC FINITE AUTOMATA (DFA)

- **Simplest computational machine in Chomsky hierarchy**
  - Finite number of states; one initial state, multiple "accept states"
  - Feed in a finite string of bits;
  - Each (bit, state) pair maps to a new state, after which next bit is read
  - A DFA "accepts" a string if it causes the DFA to end in an accept state
  - "Language" of a DFA is all input strings that it accepts
  - Many languages that are not accepted by *any* DFA

- **Example**: DFA that accepts any string with no more than two successive 'b' bits:



- *Every* digital computer is a **sequence of solitary processes**
    - Only part of the memory is physically to any processor at any time
    - So evolving subsystem is processor and current part of memory

- Results in **modularity (mismatch) cost** – just like parallel bit erasure
    - State space = {joint state of *full* memory and processor}

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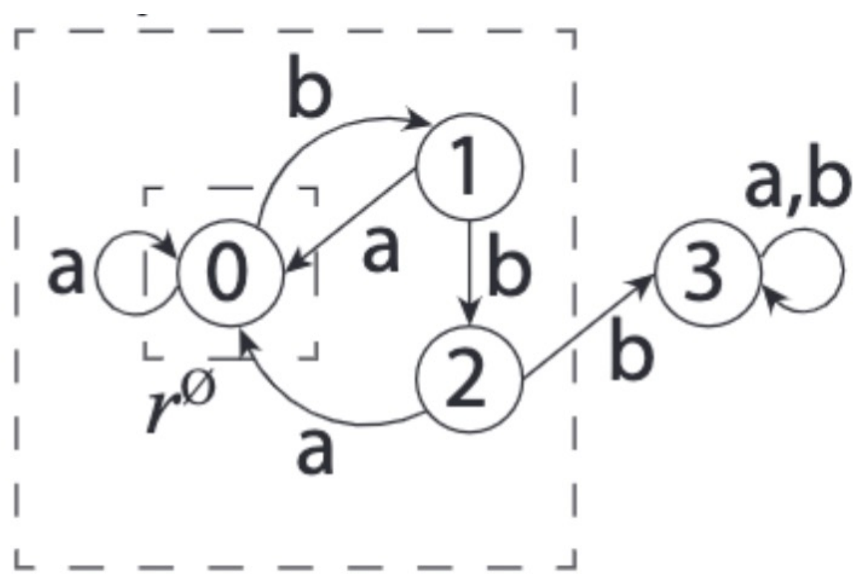
    - State space = {joint state of *full* memory and processor}

Example: In a DFA, memory contains *entire* string of input symbols
However, DFA state only physically coupled to *current* input symbol, **not** earlier or later symbols in the string

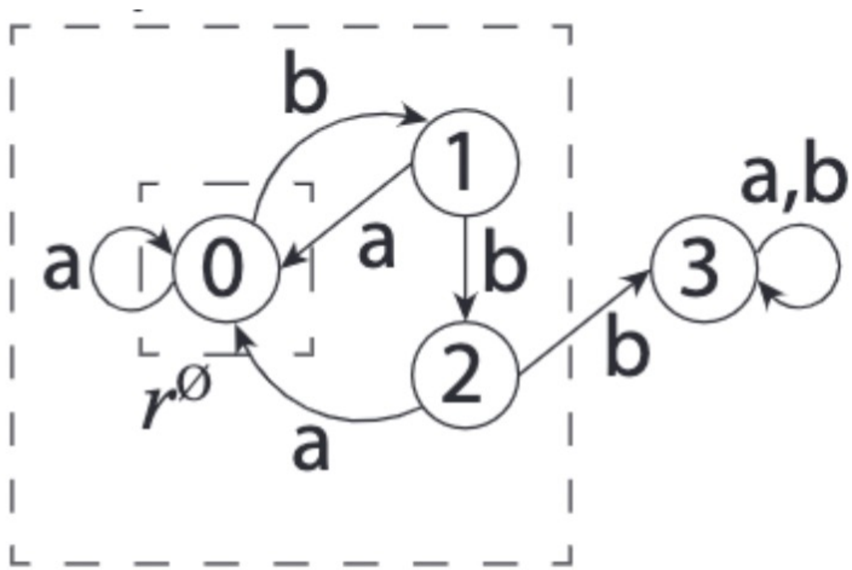


- *Every* (synchronous) digital computer is "**periodic**"
  - Every successive iteration is the same physical process.
  And so every iteration **has the same prior**

- E.g., in a DFA, every iteration has same prior

- So if prior distribution = actual distribution for iteration i, there is zero mismatch cost for iteration i .... ***But***:
  The distributions will differ for iteration i + 1 in general

- Results in "**periodicty (mismatch) cost**"



- *Every* (synchronous) digital computer is "**periodic**"
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- E.g., in a DFA, every iteration has same prior

- So if prior distribution = actual distribution for iteration i, there is
  zero mismatch cost for iteration i .... ***But***:
  The distributions will differ for iteration i + 1 in general

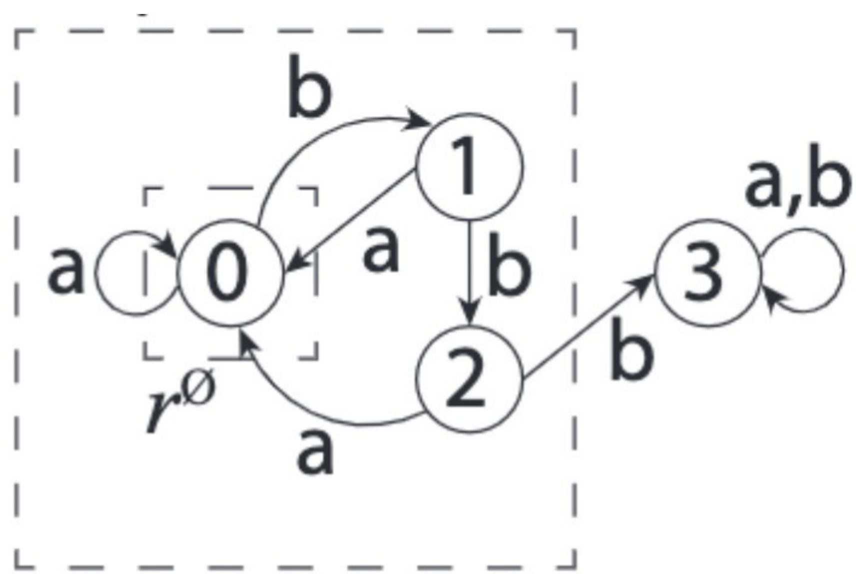
- Results in "**periodicity (mismatch) cost**"

- So, for any p_0 and any update conditional distribution P,

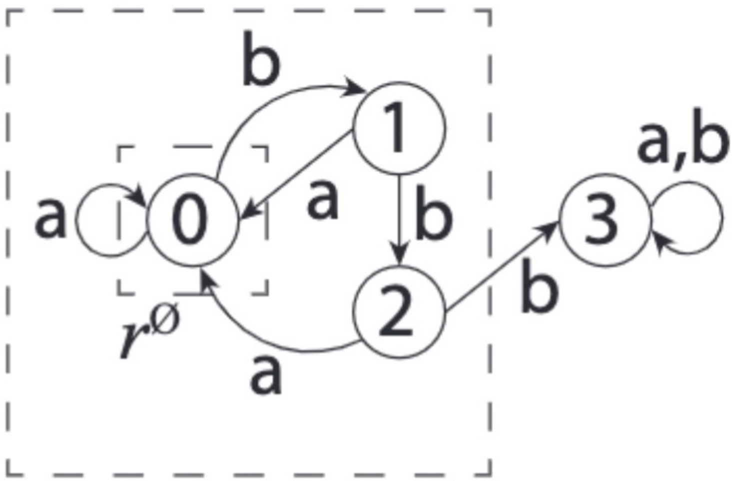
$$EP \geq \operatorname{argmin}_q \sum_{i=0}^{n} \left[D(P^i p_0 || q) - D(P^{i+1} p_0 || Pq) \right]$$

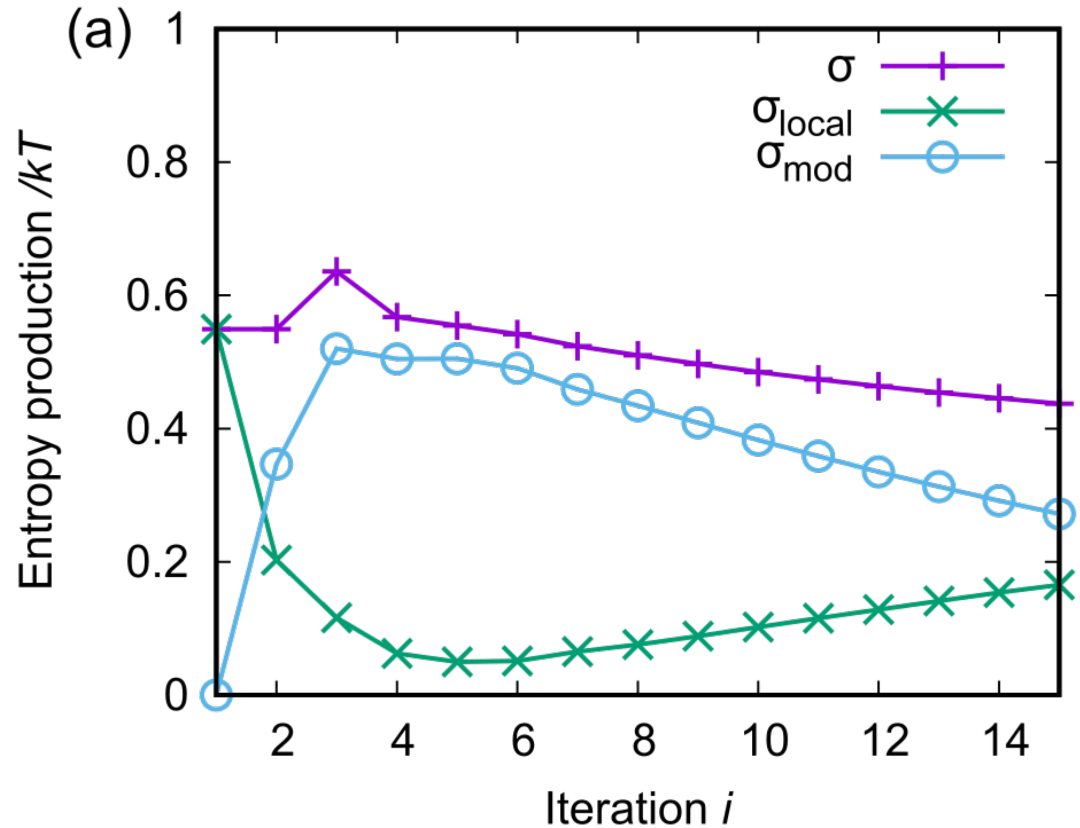
  - *Independent of the physical details of the underlying process*
    (just like generalized Landauer bound)
  - In general, RHS is strictly positive

- Total mismatch cost = modularity cost + periodicity cost



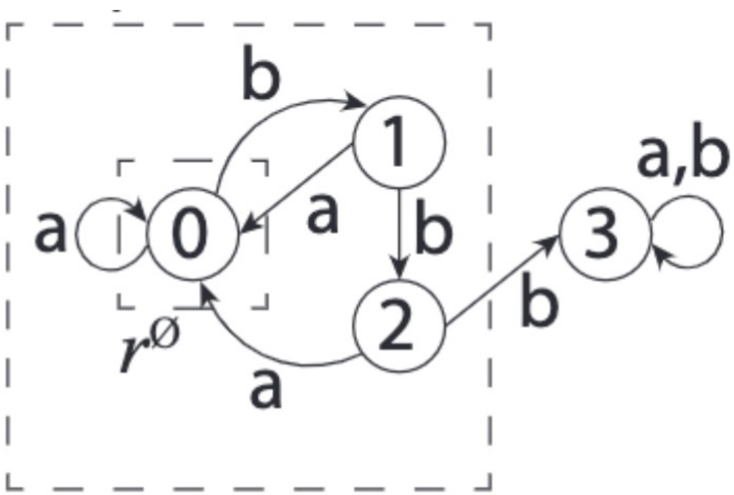
EXAMPLE

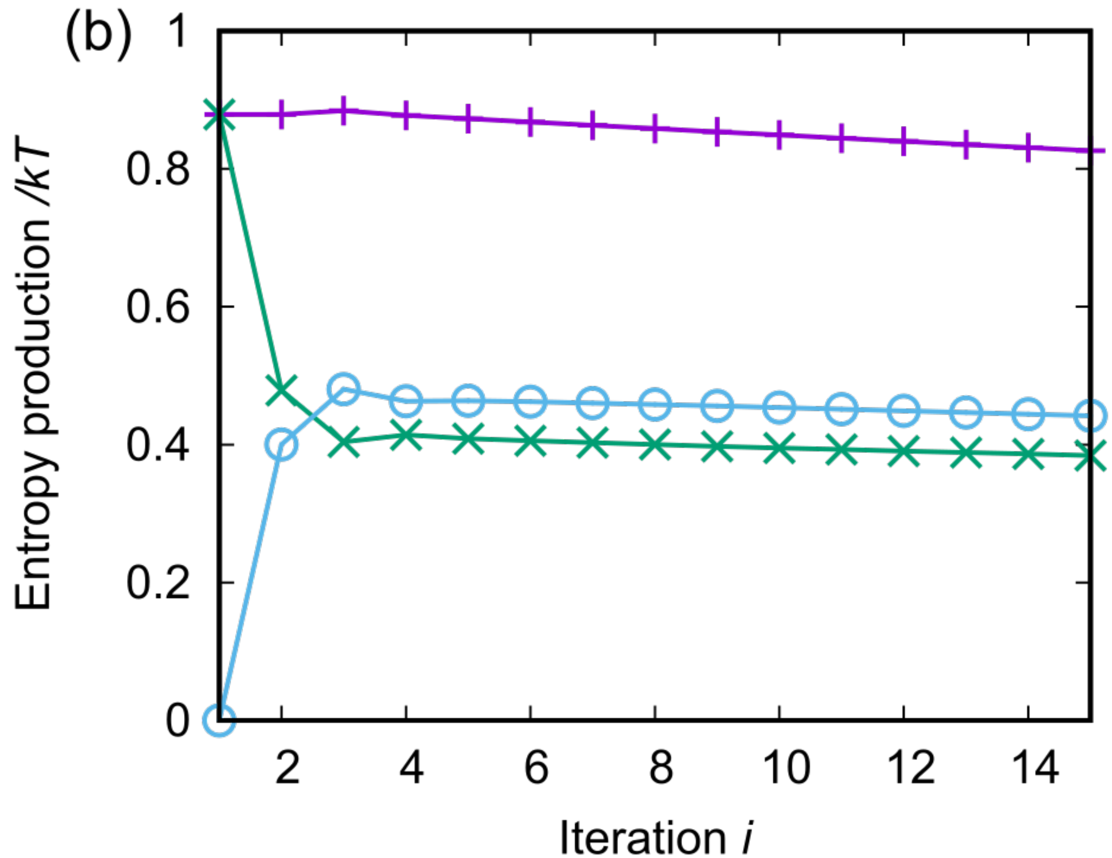




- Input strings have IID symbols with equal probability of a and b
- Uniform prior

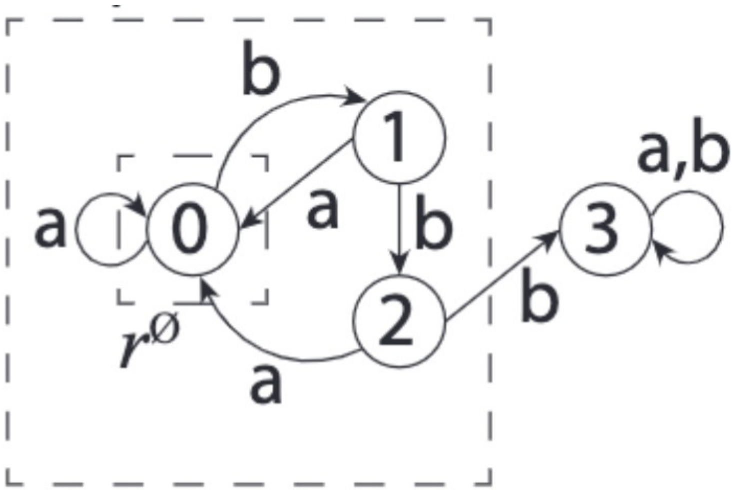
EXAMPLE

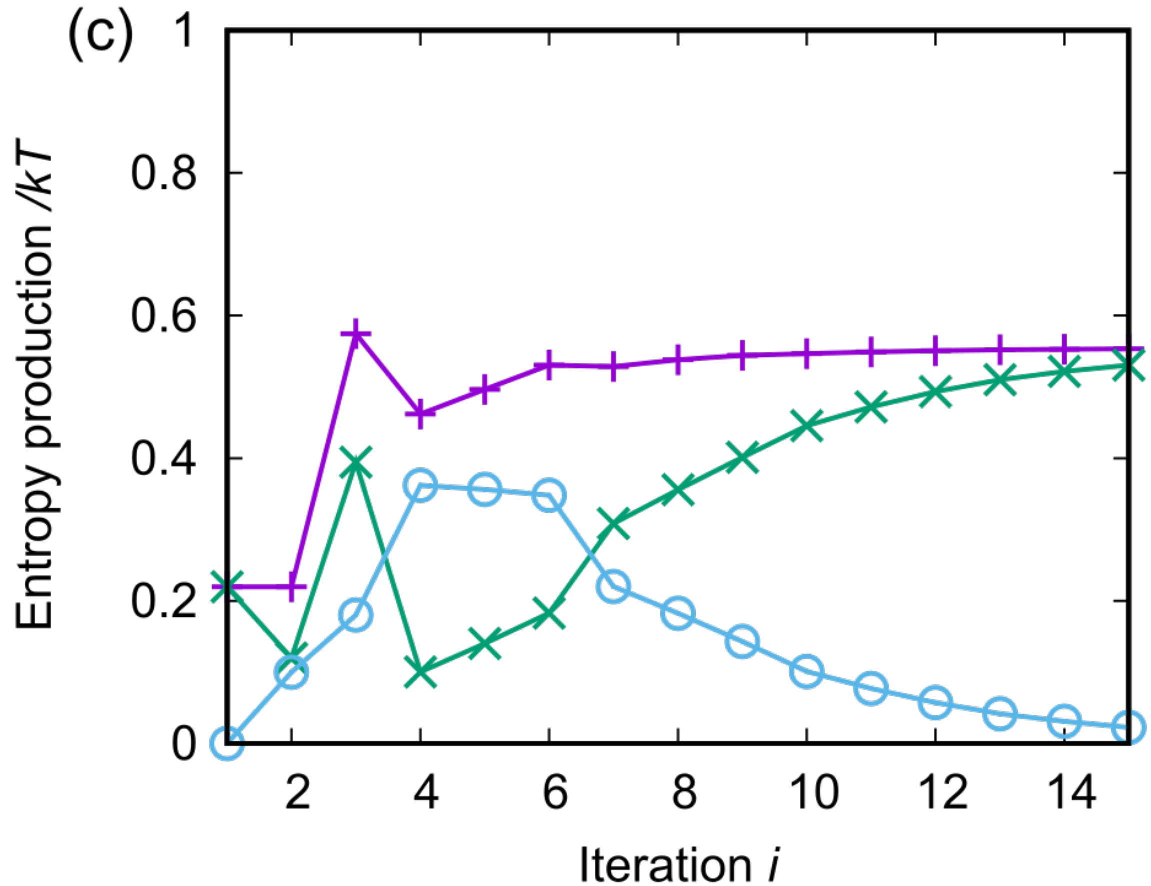




- Input strings have IID symbols with probability of a = 0.8

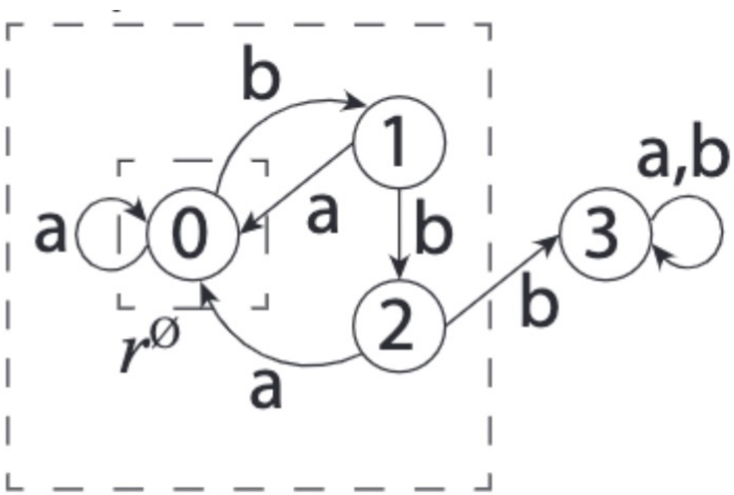
EXAMPLE

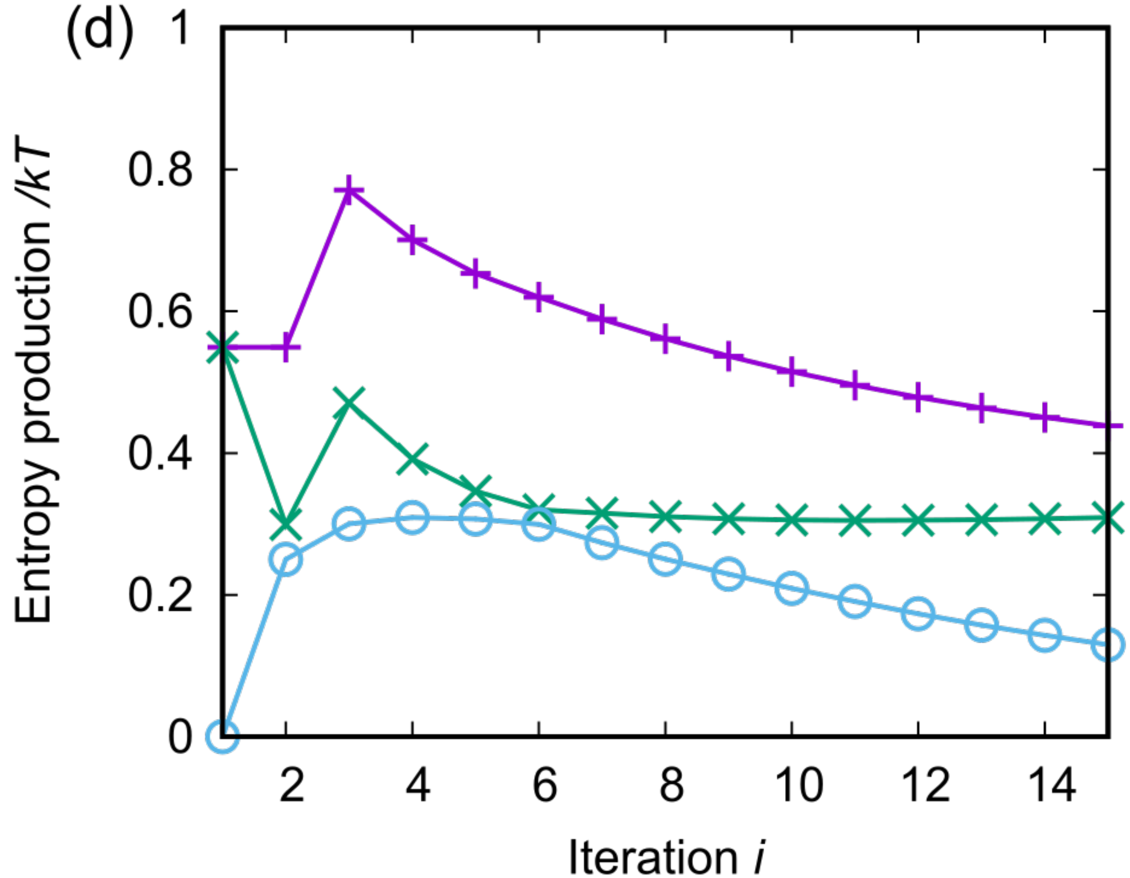




- Input strings have IID symbols with probability of a = 0.2

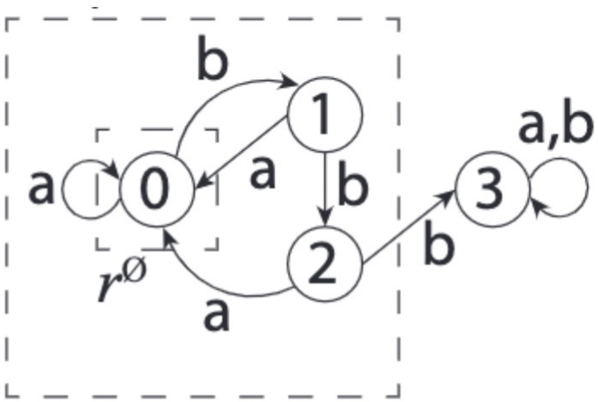
EXAMPLE

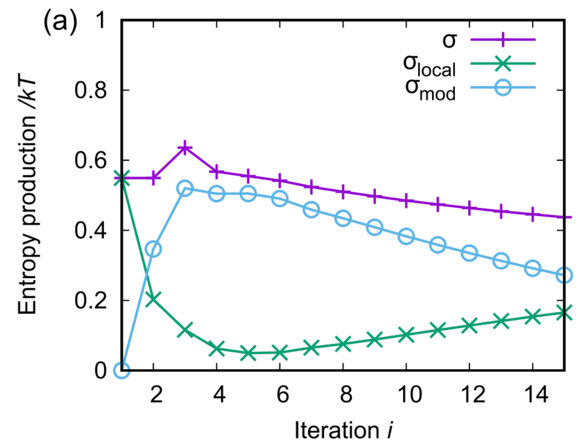


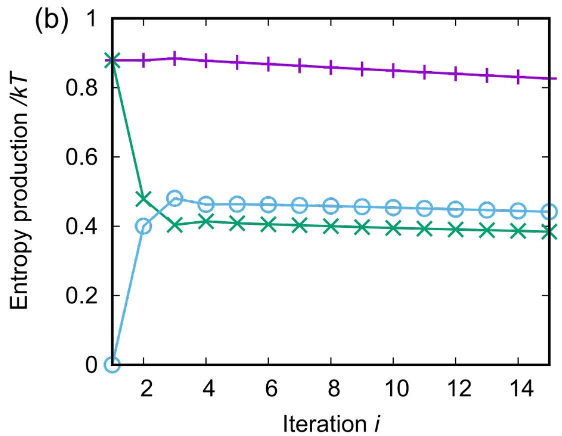


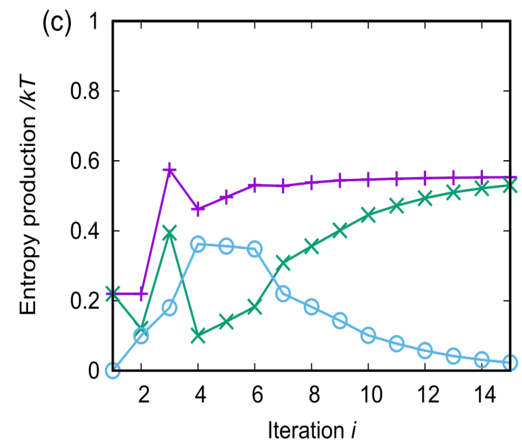
- Input strings are first order Markov chains (starting from uniform probability)

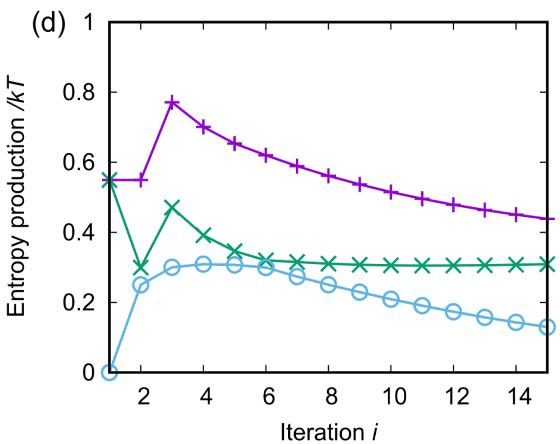
EXAMPLE





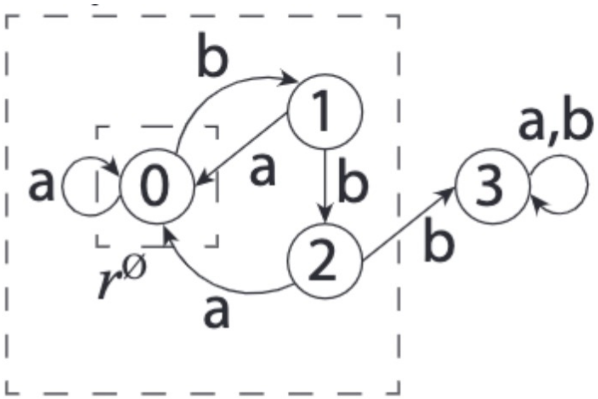


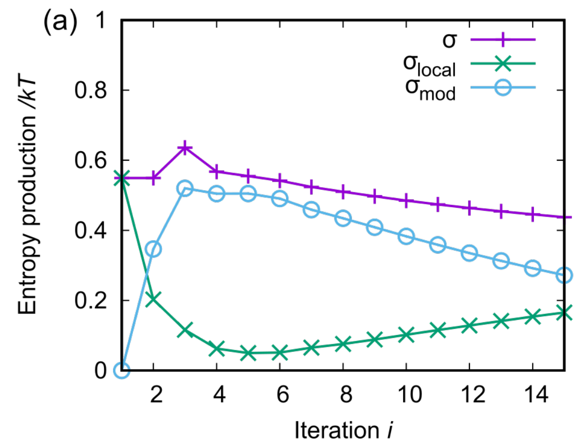


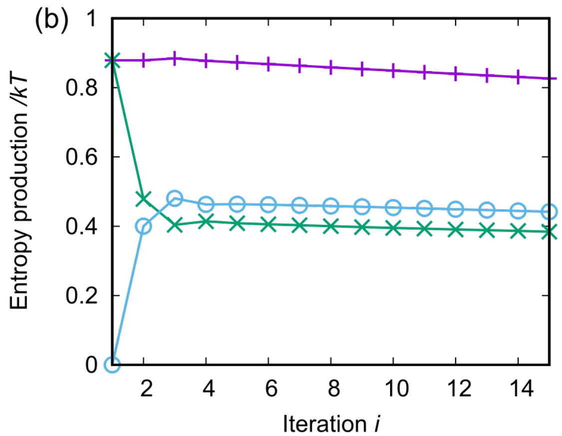


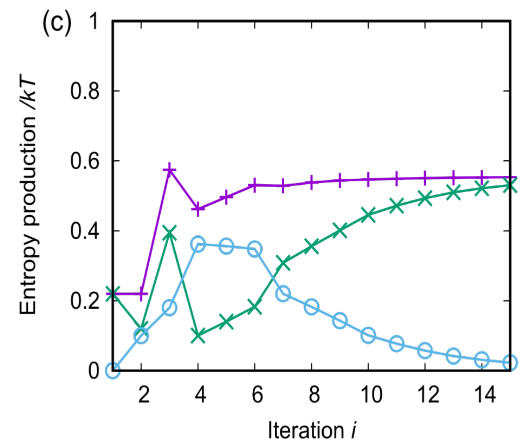
Ouldridge, T., Wolpert, D., arxiv:2208.06895 (2022)

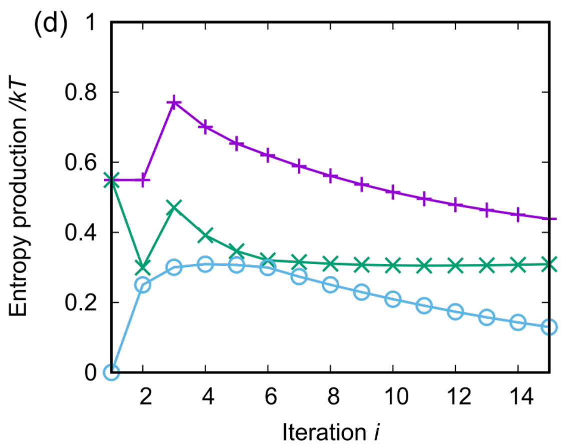
EXAMPLE











What causes curves to have these shapes?
What are curves for other DFAs?

A: Who knows!

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