

Concavity of the Second Law

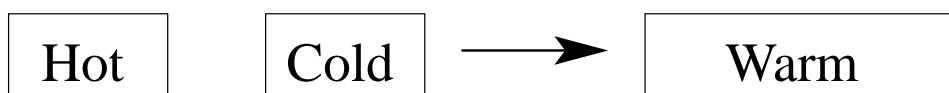
Motivation

First Law of Thermodynamics:

Energy is conserved.

Second Law:

Entropy increases (Useful energy decreases)



Question:

Is entropy increase “built into” stochastic processes?

Question:

How do you get time-asymmetric theorem (entropy increases) from time-symmetric physics.

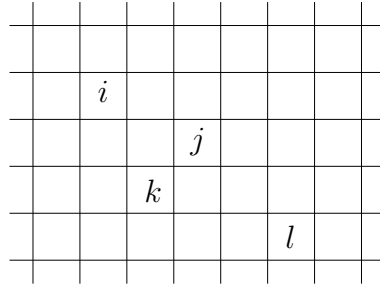
Second Law Consequences:

No perpetual motion.

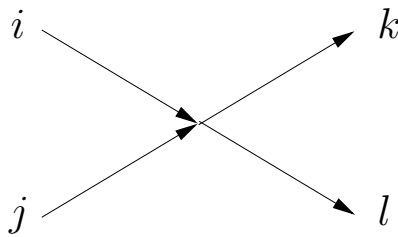
Black hole physics (Hawking radiation).

Boltzmann H theorem

Position, velocity space: $(x, y, z, v_x, v_y, v_z) \in \mathbb{R}^6$.



N_i particles in cell i . $\sum_i N_i = N$.



Number of collisions per unit time between molecules in cells i and j , and finally in k and l , is postulated to be

$$B_{ij}^{kl} N_i N_j$$

Thus,

$$\frac{dN_i}{dt} = \sum_j \sum_k \sum_l \left(B_{kl}^{ij} N_k N_l - B_{ij}^{kl} N_i N_j \right).$$

Boltzmann H theorem continued

Now suppose $(i, j) \rightarrow (k, l)$ and $(k, l) \rightarrow (i, j)$ have the same coefficient B (principle of microscopic reversibility), i.e.

$$B_{ij}^{kl} = B_{kl}^{ij}.$$

Then,

$$\frac{dN_i}{dt} = \sum_{j,k,l} B_{ij}^{kl} (N_k N_l - N_i N_j).$$

Now consider Boltzmann H function
(in statistical mechanics entropy $S = -kH_B$):

$$H_B = \sum_i N_i \log N_i$$

More H theorem

$$H_B = \sum N_i \log N_i; \quad \sum N_i = N$$

Then,

$$\begin{aligned} \dot{H}_B &= \sum \dot{N}_i \log N_i + \sum \dot{N}_i \\ &= \sum \dot{N}_i \log N_i \\ &= \sum_{i,j,k,l} B_{ij}^{kl} (N_k N_l - N_i N_j) \log N_i \\ &= \frac{1}{4} \sum_{i,j,k,l} B_{ij}^{kl} (N_k N_l - N_i N_j) (\log N_i N_j - \log N_k N_l) \\ &\leq 0. \end{aligned}$$

because $(x - y) \log \frac{y}{x} \leq 0$.

Thus $\dot{H}_B \leq 0$ (Boltzmann 1872).

Thus Boltzmann H function decreases and entropy increases.

Note: Implicit Markovity in proof.

Quantum H theorem

Assume weakly-interacting dilute gas.

Entropy

$$H = \sum_i \left(\alpha g_i \log \frac{g_i}{n_i} - (n_i + \alpha g_i) \log \left(\frac{g_i}{n_i} + \alpha \right) \right)$$

g_i = number of eigenstates of a particle in group i

n_i = number of particles occupying states in group i

$$\alpha = \begin{cases} 1, & \text{Bose-Einstein} \\ 0, & \text{Boltzmann} \\ -1, & \text{Fermi-Dirac} \end{cases}$$

$$\frac{dH}{dt} = \sum_i \frac{dn_i}{dt} \log \left(\frac{n_i}{g_i + \alpha n_i} \right)$$

Average number of transitions

$$(i, j) \rightarrow (k, l) : Z_{ij}^{kl} = A_{ij;kl} n_i n_j (g_k + \alpha n_k) (g_l + \alpha n_l)$$

$$(k, l) \rightarrow (i, j) : Z_{kl}^{ij} = A_{kl;ij} n_k n_l (g_i + \alpha n_i) (g_j + \alpha n_j)$$

Principle of microreversibility demands

$$A_{ij;kl} = A_{kl;ij}$$

Then $\frac{dH}{dt} \leq 0$.

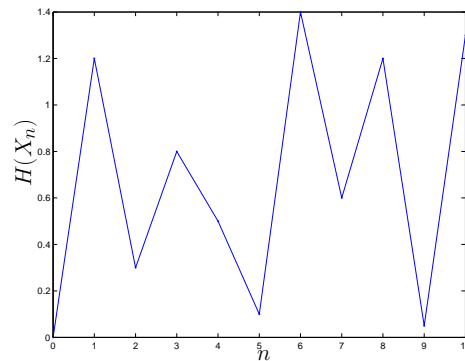
Main questions

- Is entropy increase a natural consequence of Markovity?
- Does entropy $H(X_n)$ increase for Markov chains?
 - $H(X_n|X_0)$?
 - $H(X_0|X_n)$?
 - Concavity?
- Implications in physics?

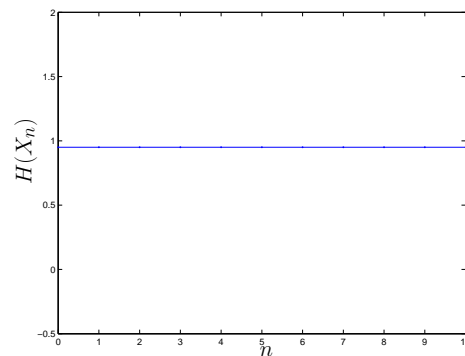
Entropy increase for stochastic processes

Stochastic process: $\{X_n\}$

- Arbitrary stochastic process: $H(X_n)$



- Stationary stochastic process: $H(X_n) \equiv \text{const.}$

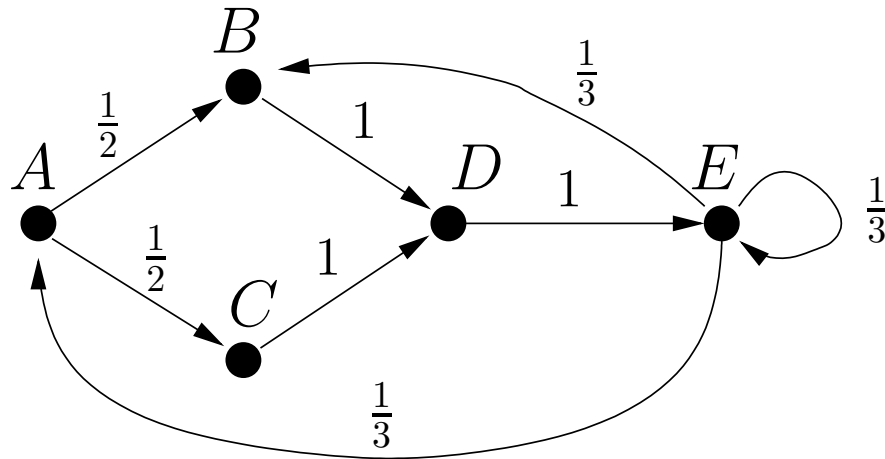


- Want conditional entropy $H(X_n|X_0)$.

Individual state behavior

What about $H(X_n|X_0 = i)$?

Consider:



Ex: ACDEBDEEEACDEBDEEEE...

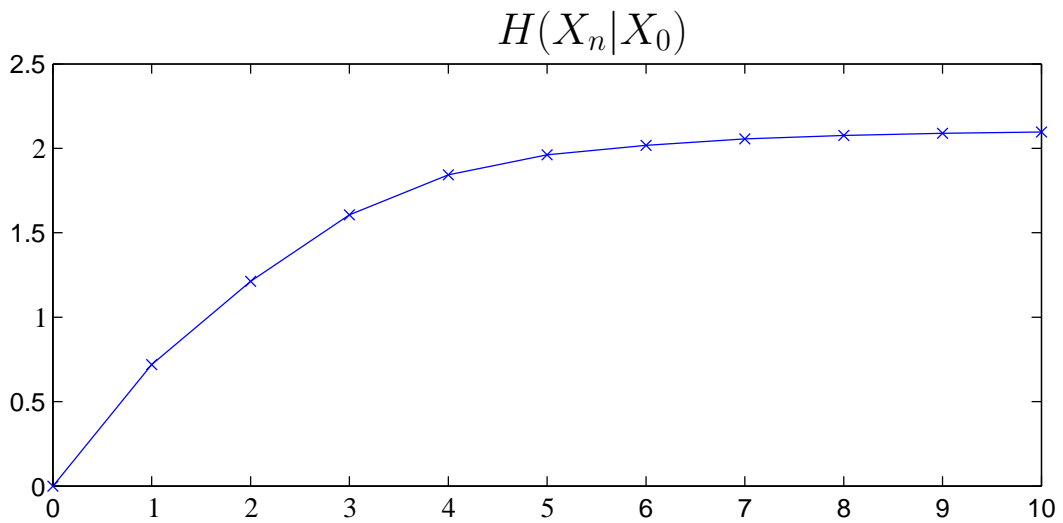
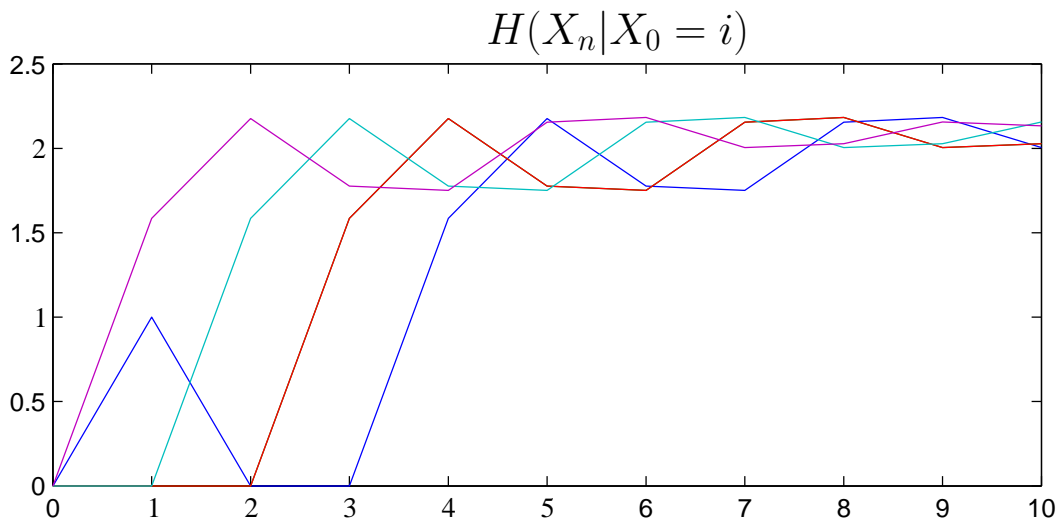
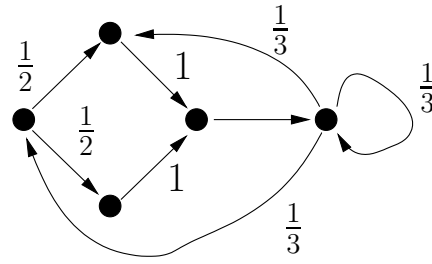
$H(X_n|X_0 = i)$ is not necessarily monotonic.

$\{X_n\}$ is not time reversible.

But we claim $H(X_n|X_0) \nearrow$, and $H(X_{-n}|X_0) = H(X_n|X_0)$ for *stationary Markov* processes.

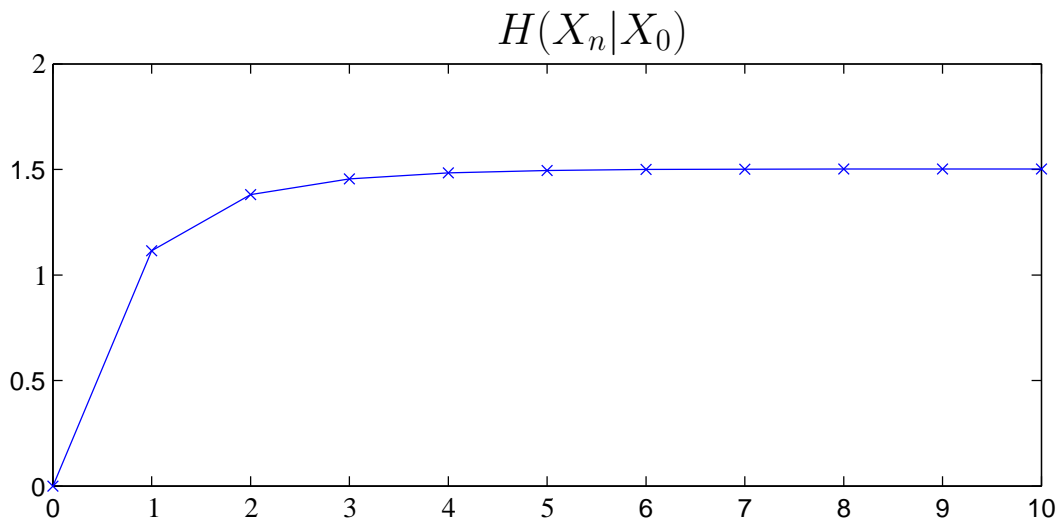
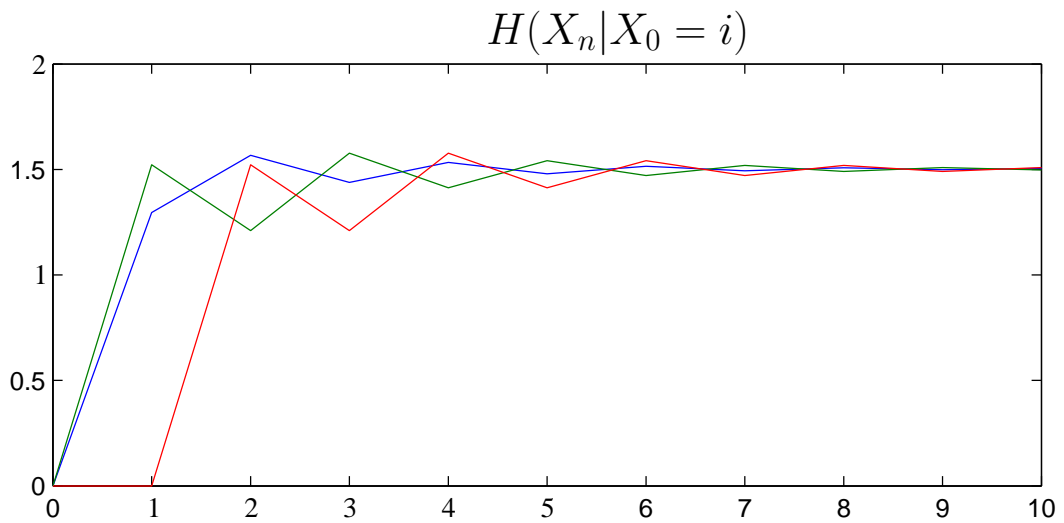
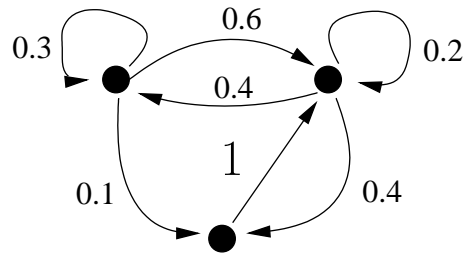
Entropy curves

$$P = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{3} \end{bmatrix}$$



Entropy curves

$$P = \begin{bmatrix} .3 & .6 & .1 \\ .4 & .2 & .4 \\ 0 & 1 & 0 \end{bmatrix}$$



Entropy of present given infinite past

No conditions:

Theorem (Entropy increases):

$H(X_0|X_{-\infty}^{-n}) \nearrow$ (is increasing in n)
for *all stochastic processes*.

Proof:

$$\begin{aligned} H(X_0|X_{-\infty}^{-n}) &= H\left(X_0|X_{-n}, X_{-\infty}^{-(n+1)}\right) \\ &\leq H\left(X_0|X_{-\infty}^{-(n+1)}\right). \end{aligned}$$

What about entropy $H(X_n|X_{-\infty}^0)$ of the future, given history through the present?

Entropy of future given infinite past

Stationarity only.

Need stationarity assumption for the entropy of future given the present-past.

Theorem (Stationarity):

$H(X_n | X_{-\infty}^0) \nearrow$
for *all* stationary processes.

Proof:

$$\begin{aligned} H(X_{n+1} | X_{-\infty}^0) &= H(X_n | X_{-\infty}^{-1}) \\ &\geq H(X_n | X_{-\infty}^0). \end{aligned}$$

Proof that conditional entropy increases

Stationary, Markov.

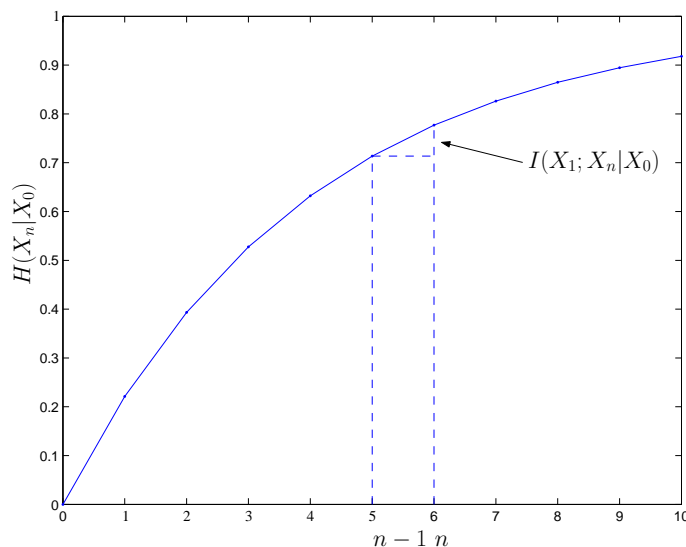
$$H_n = H(X_n|X_0), \quad \Delta_n = H_n - H_{n-1}$$

Theorem (Entropy increases): For stationary Markov processes,

$$\Delta_n \geq 0$$

Proof:

$$\begin{aligned} \Delta_n &= H_n - H_{n-1} \\ &= H(X_n|X_0) - H(X_{n-1}|X_0) \\ &= H(X_n|X_0) - H(X_{n-1}|X_0, X_{-1}) && \text{(Markovity)} \\ &= H(X_n|X_0) - H(X_n|X_1, X_0) && \text{(Stationarity)} \\ &= I(X_1; X_n|X_0) \\ &\geq 0. \end{aligned}$$



Concavity of $H(X_n|X_0)$ in n

Let $\{X_n\}_{-\infty}^{\infty}$ be a stationary Markov chain.

Let $H_n = H(X_n|X_0)$.

Define:

$$\Delta_n = H_n - H_{n-1}$$

$$\Delta_n^{(2)} = \Delta_n - \Delta_{n-1}$$

Theorem: For stationary Markov processes,

$$\Delta_n \geq 0$$

$$\Delta_n^{(2)} \leq 0$$

Thus H_n is *concave* and *increasing*.

Proof of concavity

Recall $\Delta_n^{(2)} = (H_n - H_{n-1}) - (H_{n-1} - H_{n-2})$.

Theorem (Concavity): For stationary Markov processes,

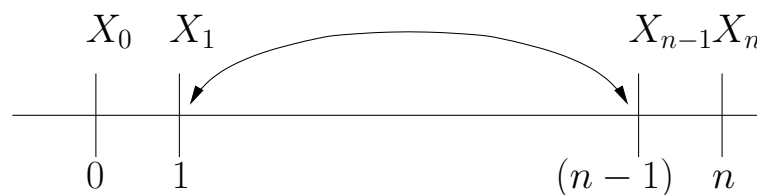
$$\Delta_n^{(2)} \leq 0$$

Proof:

$$\begin{aligned}\Delta_n &= I(X_1; X_n | X_0) \\ &= H(X_1 | X_0) - H(X_1 | X_n, X_0)\end{aligned}$$

$$\begin{aligned}\Delta_{n-1} &= I(X_1; X_{n-1} | X_0) \\ &= H(X_1 | X_0) - H(X_1 | X_{n-1}, X_0)\end{aligned}$$

$$\begin{aligned}\Delta_n^{(2)} &= \Delta_n - \Delta_{n-1} = H(X_1 | X_{n-1}, X_0) - H(X_1 | X_n, X_0) \\ &= H(X_1 | X_n, X_{n-1}, X_0) - H(X_1 | X_n, X_0) \\ &= -I(X_1; X_{n-1} | X_0, X_n) \\ &\leq 0.\end{aligned}$$

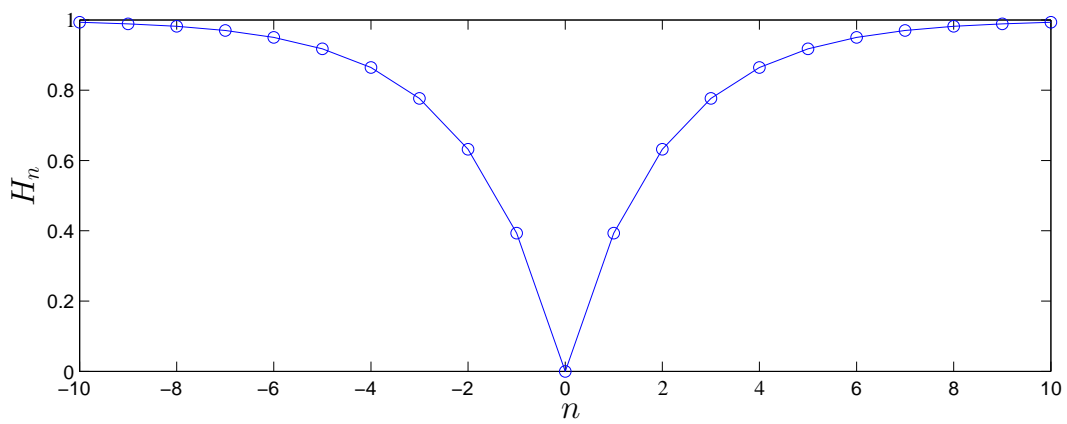


Symmetry

Stationarity only. $H_n = H(X_n|X_0)$

Theorem(Time symmetry): Stationarity implies

$$H_{-n} = H_n$$



H_n is symmetric in n .

Proof:

$$\begin{aligned} H(X_0, X_n) &= H(X_0) + H(X_n|X_0) = H(X_0) + H_n \\ &= H(X_n) + H(X_0|X_n) = H(X_n) + H(X_{-n}|X_0) \\ &= H(X_n) + H_{-n} \end{aligned}$$

But $H(X_n) = H(X_0)$ by stationarity. Thus, $H_n = H_{-n}$.

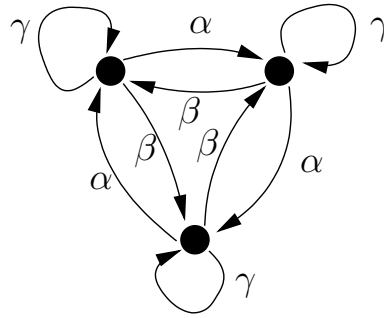
“Isotropic” Markov chains

When does initial state not matter?

Informally: Each state sees the other states the same.

Example:

$$P = \begin{bmatrix} c & & & \\ Tc & & & \\ \vdots & & & \\ T^{m-1}c & & & \end{bmatrix}$$



$T =$ cyclic rotation.

Consequences:

1. $\mu = (\frac{1}{m}, \frac{1}{m}, \dots, \frac{1}{m})$.

2. $H(X_n|x_0)$ increasing and concave.

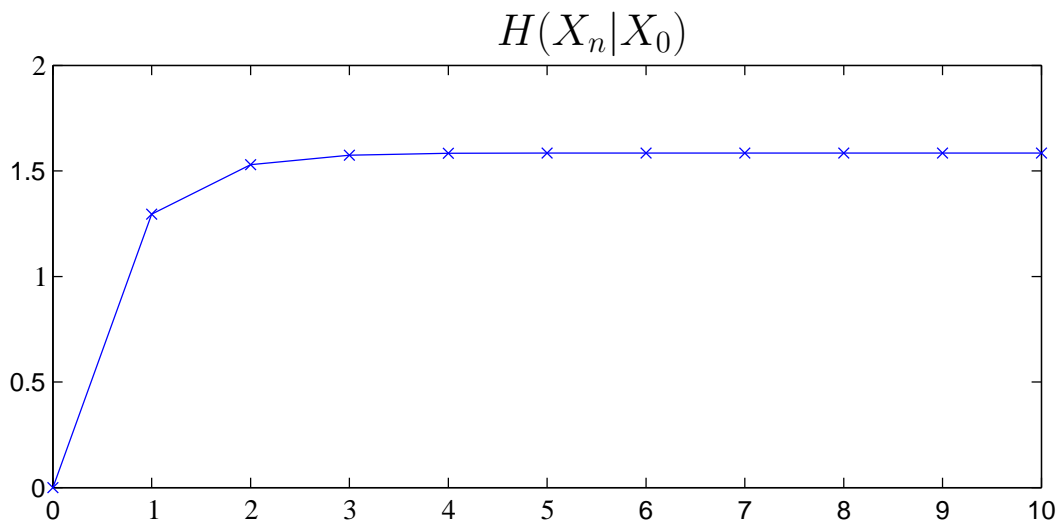
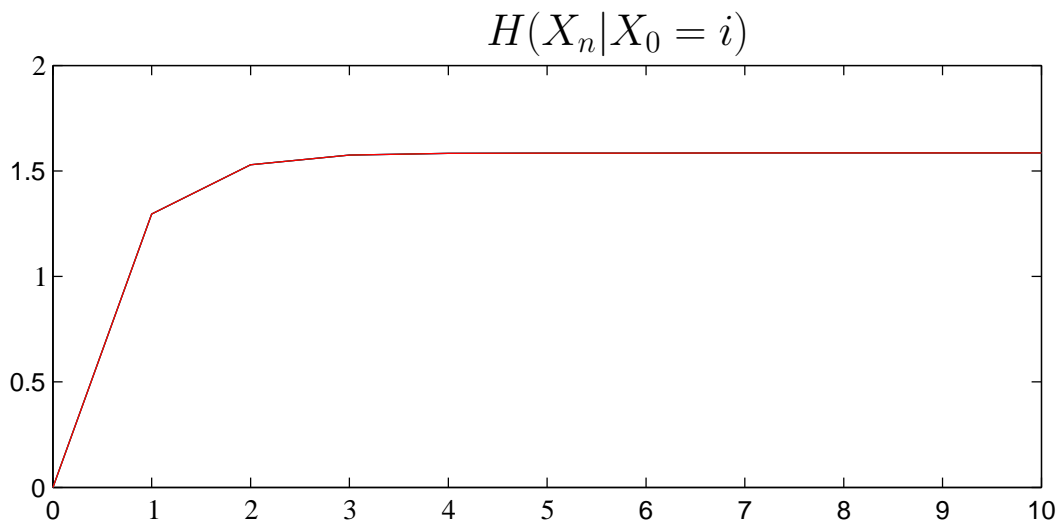
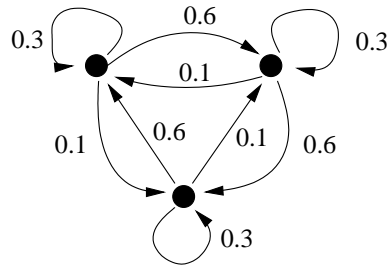
3. $H(X_n|x_0) \nearrow \log m$.

4. Do not need stationarity for concavity of second law.

Thus $H(X_n|x_0)$ increasing and concave, for all x_0 .

Isotropic entropy curves

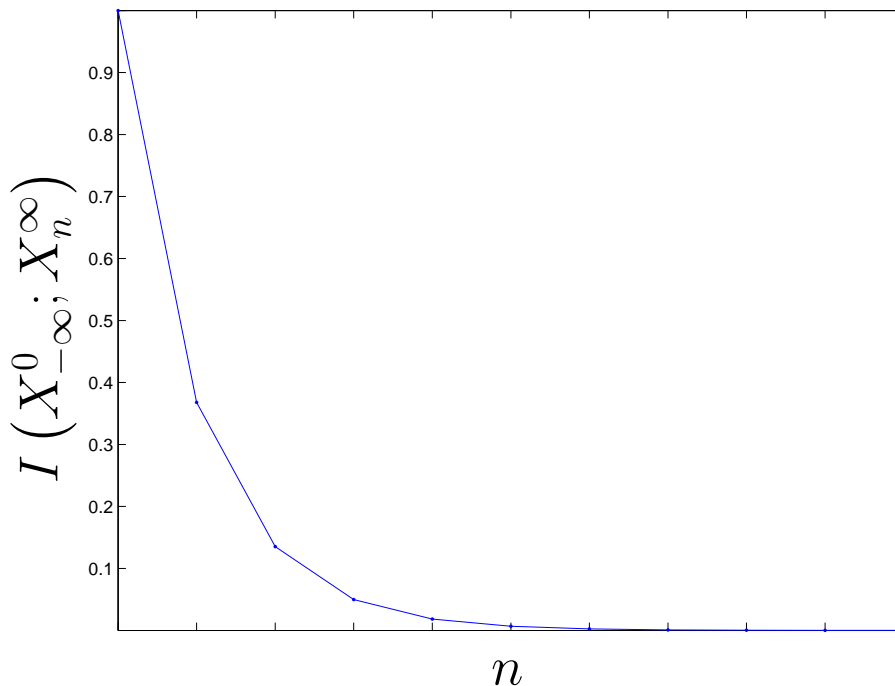
$$P = \begin{bmatrix} .3 & .6 & .1 \\ .1 & .3 & .6 \\ .6 & .1 & .3 \end{bmatrix}$$



Generalizations for Second Law

Can we remove Markovity?

We can show $I(X_{-\infty}^0; X_n^\infty)$ is *decreasing* and *convex* for any *stationary* process.



Note: $I(X_{-\infty}^0; X_n^\infty) = H(X_n^\infty) - H(X_n^\infty | X_{-\infty}^0)$.

So this suggests that $H(X_n^\infty | X_{-\infty}^0)$ is increasing and concave. (Although this entropy is actually infinite for all n .)

Entropy of Future Given the Past

$\dots, X_{-3}, X_{-2}, X_{-1}, X_0, X_1, X_2, \dots, X_{n-1}, X_n, X_{n+1}, X_{n+2}, \dots$

P_0

F_n

Let

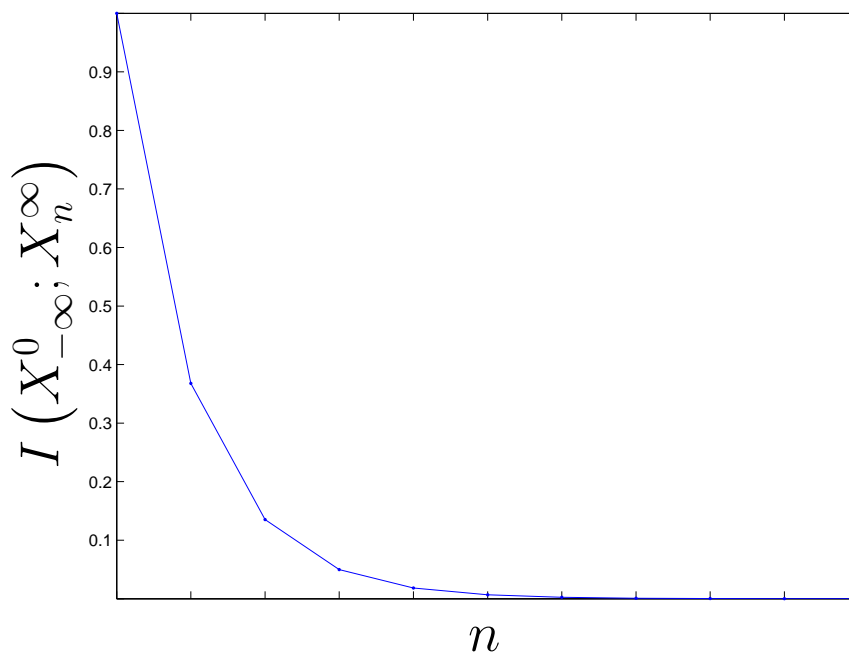
$$I_n = I(X_{-\infty}^0; X_n^\infty) = I(P_0; F_n)$$

$$\Delta_n = I_n - I_{n-1}$$

$$\Delta_n^{(2)} = \Delta_n - \Delta_{n-1}$$

Theorem For any stationary process with $I(P_0; F_1) < \infty$, we have $I(P_0; F_n)$ decreasing and convex:

$$\begin{aligned} \Delta_n &\leq 0, \\ \Delta_n^{(2)} &\geq 0. \end{aligned}$$



Proof of Convexity of $I(\text{Past}; \text{Future})$

Proof:

1)

$$\begin{aligned}\Delta_n &= I(P_0; F_n) - I(P_0; F_{n-1}) \\ &\quad I(P_0; X_{n-1}, F_n) \\ &\quad I(P_0; F_n) + I(P_0; X_{n-1}|F_n) \\ &= -I(P_0; X_{n-1}|F_n) \leq 0\end{aligned}$$

Thus $I(P_0; F_n)$ is decreasing.

2)

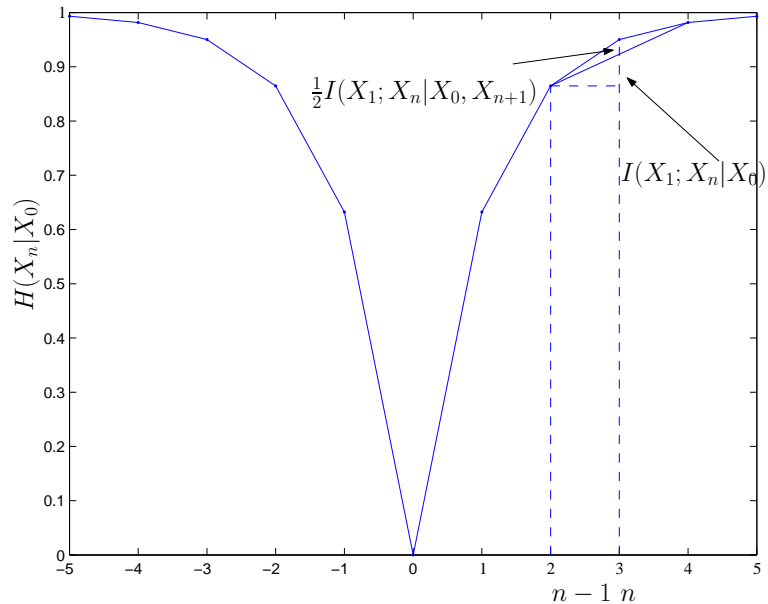
$$\begin{aligned}\Delta_n^{(2)} &= -I(P_0; X_{n-1}|F_n) + I(P_0; X_{n-2}|F_{n-1}) \\ &= -[H(X_{n-1}|F_n) - H(X_{n-1}|P_0, F_n)] \\ &\quad + H(X_{n-2}|F_{n-1}) - H(X_{n-2}|P_0, F_{n-1}) \\ &= H(X_{n-1}|P_0, F_n) - H(X_{n-2}|P_0, F_{n-1}) \\ &\quad H(X_{n-1}|P_1, F_n) \\ &\quad H(X_{n-1}|P_0, X_1, F_n) \\ &= I(X_1; X_{n-1}|P_0, F_n) \\ &\geq 0\end{aligned}$$

Thus $I(P_0; F_n)$ is convex.

$$P_0, X_1, \dots, X_{n-1}, F_n$$

Concluding remarks

- For a stationary Markov chain, the entropy looks like this:



Increasing, symmetric, and concave.

- Is this true of the second law of thermodynamics?
- Drum-beat of time?