#20 Thermodynamics of Strongly Coupled Systems

what if
not ideal?

$$E = E^S + E^B + E^I$$

↑
not small!?

eg
Embedding System
cubic foot of copper

Lake Michigan

?

Jarzynski

$$P_{XY}(x, y \mid \lambda) = \exp(-\beta F_{XY}(\lambda) - \beta E_{XY}(x, y))$$

entropy production

total heat = change in entropy of environment

$$\frac{P_{XY}(\vec{x}, \vec{y} \mid \vec{\lambda}, x_a, y_a)}{P_{XY}(\tilde{x}, \tilde{y} \mid \tilde{\lambda}, x_a, y_a)} = \Sigma = \Delta s_{x,y} - \beta Q_{x,y}$$

$$= \frac{P(x_a, y_a)}{P(x_b, y_b)}$$

<u>Joint FT</u>

total change in F.E

Measure work, $\rightarrow \left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F_{XY}}$

③

Jarzynski 2004
2017

$$P_x(x|\lambda) \propto \exp\left[-\beta \overline{E}(x,\lambda)\right]$$ PMF

$$E = E_x + E_y + E^I_{xy}$$

Marginalize

$$\propto \int dy \; e^{-\beta E} = \int e^{-\beta E_x(x)} + \int dy\, e^{-\beta E_y(y) + E^I(x,y)}$$

$$\overline{E}^{PMF}_x = E_x(x) - \ln \frac{1}{\beta} \int dy\; e^{-\beta E_y(y) + E^I(x,y)}$$

$$\left\langle e^{-\beta W - \alpha} \right\rangle = e^{-\beta \Delta F^s}$$

extra term from <u>interactions</u>

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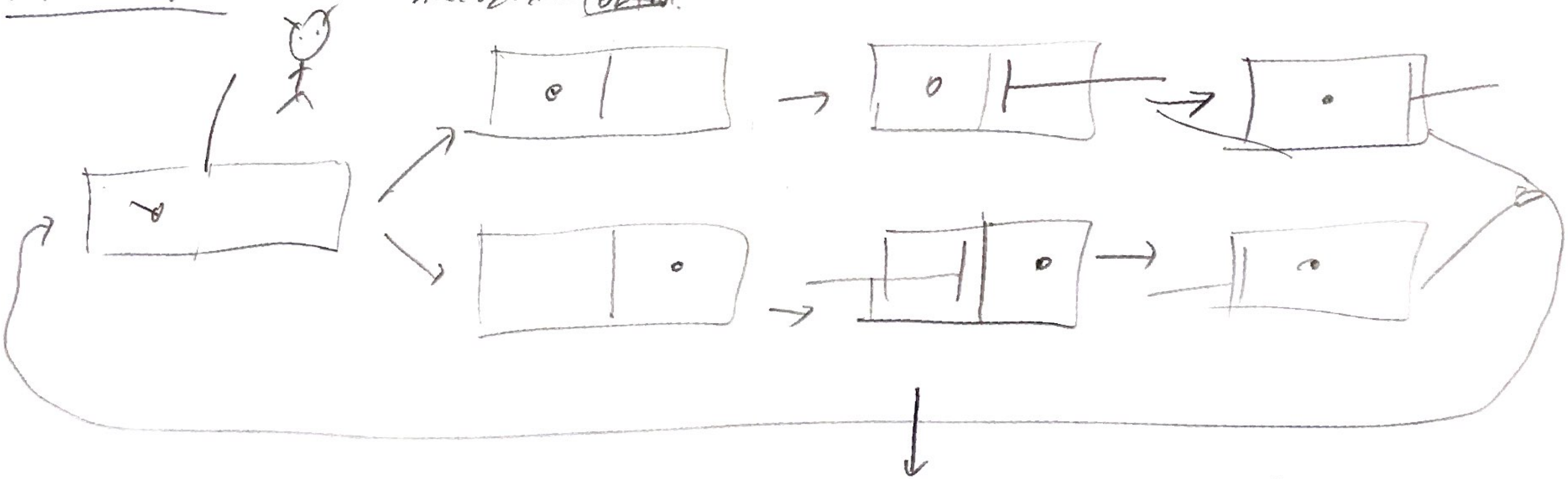
Maxwells demon

~~Feedback Control~~



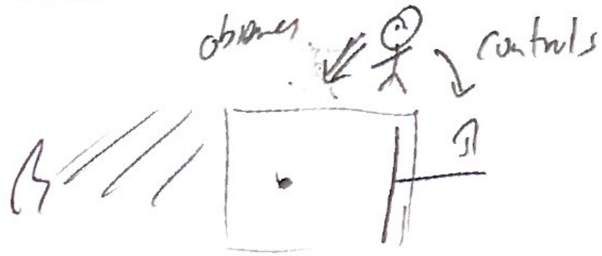
extracts $W^{Rev} = k_B T \ln \frac{V^f}{V_i} = k_B T \ln 2$

$= 0.7$

10 bits ≈ 7 nats ≈ 3 digits.

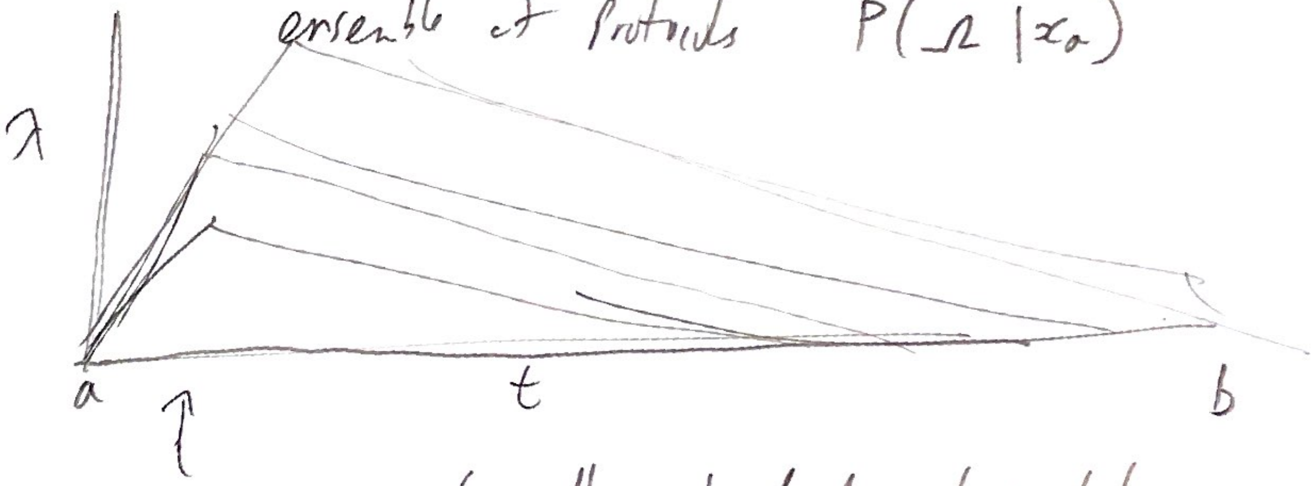
Resolution - Max has a bit of memory

Feedback FT   No energetic coupling - only dynamics change



Simplify → Max observes system once

ensemble of Protocols $P(\Omega \mid x_0)$



e.g. insert rapidly up to location of particle, then slow expansion.

U. Tokyo
Sagawa & Ueda 2010

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Feedback FT

U. Michigan Horowitz & Vaikuntanathan 2010

Jordan U. Chicago

Joint FT

$$\frac{P(X,\Lambda)}{P(\tilde{X},\tilde{\Lambda})} = \frac{P(x_a|\lambda_a)}{P(x_b|\lambda_b)} \frac{P(\Lambda|x_a)}{P(\tilde{\Lambda}|x_b)} \frac{P(X|\Lambda,x_a)}{P(\tilde{X}|\tilde{\Lambda},x_b)}$$

→ No feedback in Reverse Process $\quad P(\tilde{\Lambda}) = \sum_{x_a} P(\Lambda|x_a)P(x_a) = P(\Lambda)$

(general principle. Have freedom in reference)

(Jarzynski style start and end in eq.)

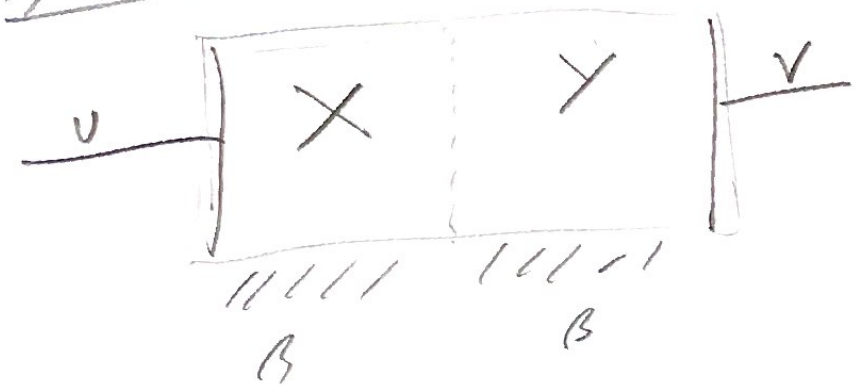
$$= \exp\left\{\beta W - \beta\Delta F + \overbrace{\ln\frac{P(\Lambda|x_a)}{P(\Lambda)}}^{\theta}\right\}$$

IDEAL DEMON

Information term

$$\left\langle e^{-\beta W + \beta\Delta F - \theta}\right\rangle = 1 \qquad \theta = \ln\frac{P(\Lambda,x_a)}{P(\Lambda)P(x_a)} \qquad \langle\theta\rangle = I$$

Symmetric



$$S(X,Y) = -\sum_{x,y} p(x,y) \ln p(x,y)$$

Joint FT

Bipartite System

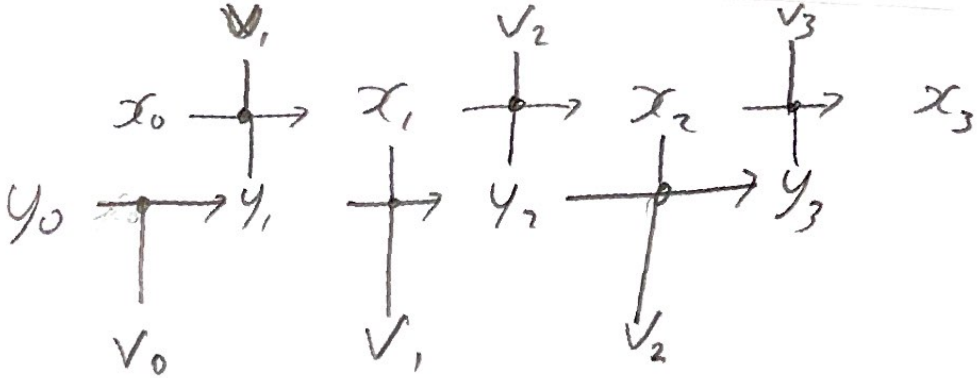
$$\Sigma_{X,Y} = \ln \frac{P(X,Y \mid U,V)}{P(\tilde{X},\tilde{Y} \mid \hat{U},\hat{V})} -$$

Marginal FT $\quad \Sigma_X = \ln \frac{P(X \mid U)}{P(\tilde{X} \mid \hat{U})}$

Crooks & Still 2019

Esposito

DTMC



transition probabilities

$$P(X, Y \mid x_0, y_0) = \underbrace{\prod p(y_{t+1} \mid y_t, x_t)}_{q(Y;\, X,\, x_0)} \; \underbrace{\prod p(x_{t+1} \mid x_t, y_{t+1})}_{q(X;\, Y,\, y_0)}$$

Fixed, no feedback!

$$\langle e^{+\Sigma} \rangle = 1 \quad \langle \Sigma_{XY} \rangle \geq (\Sigma_{X|Y}, \Sigma_{Y|X} ; \Sigma_X, \Sigma_Y) \geq 0$$

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$$\Sigma_X = \frac{\ln P(\vec{x})}{\ln P(\overleftarrow{x})} = \ln \frac{P(\vec{x}, \vec{y})}{P(\overleftarrow{x}, \overleftarrow{y})} \frac{P(\overleftarrow{y} | \overleftarrow{x})}{P(\vec{y} | \vec{x})}$$

$$= \underbrace{\ln \frac{P(x_a)}{P(x_b)}}_{\Delta S_X} + \underbrace{\ln \frac{q(\vec{x}; \vec{y}, x_a)}{q(\overleftarrow{x}; \overleftarrow{y}, x_b)}}_{-\beta Q_X} - \underbrace{\left[\ln \frac{P(\vec{y} | \vec{x}, y_a)}{P(\overleftarrow{y} | \overleftarrow{x}, y_b)} - \ln \frac{q(\vec{y}, \vec{x}, y_a)}{q(\overleftarrow{y}, \overleftarrow{x}, y_b)} \right]}_{-\Sigma_X^{trn}}$$

Effect of feedback!

Feedback dissipation

$$\ln \frac{P(X)}{P(\tilde{X})} = \ln \frac{P(X, Y)}{P(\tilde{X}, Y)} \frac{P(\tilde{Y}|\tilde{X})}{P(Y|X)}$$

$$= \ln \underbrace{\frac{P(X, Y | x_a\, y_a)}{P(\tilde{X}, \tilde{Y} | x_b, y_b)}}_{} \frac{P(\tilde{Y} | \tilde{X}, y_b)}{P(Y | X, y_a)} \frac{P(x_a)}{P(x_b)}$$

$$\frac{q(X; Y, x_a\, y_a)}{q(\tilde{X}; \tilde{Y}, x_b\, y_b)} \frac{q(\cancel{Y}; X, x_a\, y_a)}{q(\cancel{\tilde{Y}}; \tilde{X}, x_b, y_b)} \quad - \bar{\Sigma}_X^{trns}$$

$$= \Delta S_X - \beta Q_X - \overbrace{\left(\ln \frac{P(Y|X, y_a)}{P(\tilde{Y}|\tilde{X}, y_b)} - \ln \frac{q(Y|X, y_a)}{q(\tilde{Y}|\tilde{X}, y_b)} \right)}^{0}$$

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$$\Sigma_{XY} = \Delta s_{XY} - \beta Q_X - \beta Q_Y =$$

$$\langle \Sigma_{X,Y} \rangle \geq 0 \quad \langle e^{-\Sigma_{XY}} \rangle = 1$$

$$\Sigma_Y = \Delta s_X - \beta Q_X - \Sigma_X^{trn} = \frac{P(x)}{P(\tilde{x})}$$

$$\langle \Sigma_X \rangle \geq 0$$

$$\Sigma_{X|Y} = \Delta s_{X|Y} - \beta Q_X + \Sigma_Y^{trn}$$

↑

interactions between systems

~~extent of feedback~~

$$\Delta S_X - \beta \langle Q_Y \rangle - \langle \Sigma_Y^{trn} \rangle \geq 0$$