Thermodynamic Uncertainty Relations
Derivation, Interpretation and Generalization

Andreas Dechant

andreas.dechant@outlook.com

Kyoto University, Japan

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京都大学
KYOTO UNIVERSITY

From the second law to the TUR

- second law of thermodynamics: system in contact with thermal environment T

$$\Delta S + \frac{\Delta Q}{T} = \Sigma \geq 0$$

  - ΔS change in entropy of system
  - ΔQ heat transfer system $\rightarrow$ environment
  - $\Sigma \geq 0$ entropy production $\triangleq$ change in entropy of universe

- valid for any macroscopic process
- however: no quantitative statement about Σ

From the second law to the TUR

- in many cases: more information about system
- for example: steady state, overdamped/underdamped diffusion, Markov process ...
- how are measurable properties of system related to Σ?
- thermodynamic uncertainty relation (TUR) [BS15, GHPE16]

$$\Sigma \geq \frac{2\langle J\rangle^2}{\text{Var}(J)}$$

  - J time-integrated current (particle displacement, heat flow, ...)
  - $\langle J\rangle$ average value of J
  - $\text{Var}(J) = \langle J^2\rangle - \langle J\rangle^2$ variance (fluctuations) of J

- non-zero lower bound on $\Sigma \rightarrow$ quantitative second law
- valid in steady state of time-reversal-even, continuous-time Markov process

Different perspectives on the TUR

- fundamental tradeoff between precision and dissipation [PS18, DS18]
  - $\mathcal{P}_J = \frac{\langle J \rangle^2}{\text{Var}(J)}$ dimensionless measure of precision of current
  - TUR: $\mathcal{P}_J \leq \frac{\Sigma}{2}$
  - large precision requires large dissipation
- estimate entropy production from measurable quantities [LHGF19, MGK20, OIDS20, VVVH20]
  - in many cases: difficult to directly measure Σ
  - $\langle J \rangle$ and $\text{Var}(J)$ experimentally accessible
  - lower bound on entropy production $\rightarrow$ can be tight

1. Derivation of the TUR for overdamped Langevin dynamics

Overdamped Langevin equation

- Brownian particle at position $\boldsymbol{x}(t) = (x_1(t), x_2(t), x_3(t))$ in contact with heat bath T: Langevin equation

$$\gamma \dot{\boldsymbol{x}}(t) = \boldsymbol{F}(\boldsymbol{x}(t)) + \sqrt{2\gamma T}\boldsymbol{\xi}(t) \qquad \gamma\text{: friction coefficient} \qquad \boldsymbol{F}(\boldsymbol{x})\text{: force}$$

- $\boldsymbol{\xi}(t)$ Gaussian white noise: random force with $\langle \boldsymbol{\xi}(t) \rangle = 0$, $\langle \xi_i(t)\xi_j(s) \rangle = \delta_{ij}\delta(t-s)$
- equivalent to Langevin equation: Fokker-Planck equation for probability density $p_t(\boldsymbol{x})$

$$\partial_t p_t(\boldsymbol{x}) = -\boldsymbol{\nabla} \cdot \big(\boldsymbol{\nu}_t(\boldsymbol{x}) p_t(\boldsymbol{x})\big) \qquad \boldsymbol{\nu}_t(\boldsymbol{x}) = \frac{1}{\gamma}\big(\boldsymbol{F}(\boldsymbol{x}) - T\boldsymbol{\nabla} \ln p_t(\boldsymbol{x})\big) \text{ local mean velocity}$$

- stochastic equation of motion $\to$ deterministic equation for probability

Path probability for Markovian dynamics

- time evolution is Markovian: independent of the "history"

$$p(\boldsymbol{x},t|\boldsymbol{y},s;\boldsymbol{z},r)=p(\boldsymbol{x},t|\boldsymbol{y},s) \qquad \text{for} \qquad t>s>r$$

- probability density of a path $\hat{\boldsymbol{x}}=((\boldsymbol{x}_0,t_0),(\boldsymbol{x}_1,t_1),(\boldsymbol{x}_2,t_2),\dots,(\boldsymbol{x}_N,t_N))$ factorizes

$$\mathbb{P}(\hat{x})=p(\boldsymbol{x}_N,t_N|\boldsymbol{x}_{N-1},t_{N-1})p(\boldsymbol{x}_{N-1},t_{N-1}|\boldsymbol{x}_{N-2},t_{N-2})\dots p(\boldsymbol{x}_1,t_1|\boldsymbol{x}_0,t_0)p_{t_0}(\boldsymbol{x}_0)$$

- for Langevin equation and short time-difference $dt\ll 1$: explicit expression

$$p(\boldsymbol{x},t+dt|\boldsymbol{y},t)\simeq\frac{1}{(4\pi Ddt)^{\frac{3}{2}}}\exp\left[-\frac{1}{4Ddt}\left\|\boldsymbol{x}-\boldsymbol{y}-\frac{1}{\gamma}\boldsymbol{F}(\boldsymbol{y})dt\right\|^2\right] \qquad D=\frac{T}{\gamma}$$

Time reversal and entropy production

- intuitively: entropy production Σ quantifies irreversibility
- consider time-reversed path $\hat{\boldsymbol{x}} = ((\boldsymbol{x}_0, t_0), \ldots, (\boldsymbol{x}_N, t_N)) \to \hat{\boldsymbol{x}}^\dagger = ((\boldsymbol{x}_N, t_0), \ldots, (\boldsymbol{x}_0, t_N))$
- define entropy production via probability of time-reversed path

$$\Sigma = \sum_{\text{paths}} \mathbb{P}(\hat{\boldsymbol{x}}) \ln\left(\frac{\mathbb{P}(\hat{\boldsymbol{x}})}{\mathbb{P}(\hat{\boldsymbol{x}}^\dagger)}\right) = D_{\mathsf{KL}}\big(\mathbb{P}(\hat{\boldsymbol{x}}) \| \mathbb{P}(\hat{\boldsymbol{x}}^\dagger)\big)$$

- D_{KL} Kullback-Leibler divergence: measures distinguishability of two probability densities
  $D_{\mathsf{KL}}(P\|Q) \geq 0$ with "$=$" only if $P = Q$
- if $\mathbb{P}(\hat{\boldsymbol{x}}^\dagger) \neq \mathbb{P}(\hat{\boldsymbol{x}})$ for some paths: positive entropy production $\Sigma > 0$

Connection to thermodynamic entropy

- for Langevin equation: use short-time transition probability

$$\Sigma = \underbrace{\frac{1}{T} \left\langle \int_0^\tau dt \; \boldsymbol{F}(\boldsymbol{x}(t)) \circ \dot{\boldsymbol{x}}(t) \right\rangle}_{\Delta Q} + \underbrace{S_\tau - S_0}_{\Delta S} \qquad \text{with}$$

$S_t = -\int d\boldsymbol{x} \; p_t(\boldsymbol{x}) \log \big(p_t(\boldsymbol{x})\big)$ Shannon entropy, $\circ$ Stratonovich product

- definition in terms of path probability reproduces second law
- alternative expression: magnitude of local mean velocity

$$\Sigma = \frac{1}{D} \int_0^\tau dt \int d\boldsymbol{x} \; \big\|\boldsymbol{\nu}_t(\boldsymbol{x})\big\|^2 p_t(\boldsymbol{x})$$

Currents

- stochastic heat $\Delta\mathcal{Q}$: example for time-integrated current

$$\Delta\mathcal{Q}_\tau = \int_0^\tau dt\ \boldsymbol{F}(\boldsymbol{x}(t)) \circ \dot{\boldsymbol{x}}(t)$$

- more general: weighting function $\boldsymbol{w}_t(\boldsymbol{x})$, "generalized displacement"

$$J_\tau = \int_0^\tau dt\ \boldsymbol{w}_t(\boldsymbol{x}(t)) \circ \dot{\boldsymbol{x}}(t)$$

$\boldsymbol{w}_t(\boldsymbol{x}) = \hat{\boldsymbol{e}}_1$ displacement in x_1 direction

$\boldsymbol{w}_t(\boldsymbol{x}) = \frac{\boldsymbol{\nu}_t(\boldsymbol{x})}{D}$ stochastic entropy production

- average value given by local mean velocity

$$\langle J_\tau \rangle = \int_0^\tau dt \int d\boldsymbol{x}\ \boldsymbol{w}_t(x) \cdot \boldsymbol{\nu}_t(\boldsymbol{x}) p_t(\boldsymbol{x})$$

- practical relevance: currents are measurable consequence of local flows

Steady-state and invariance under current-rescaling

- from now on: focus on steady state $p_t(\boldsymbol{x}) \underset{t\to\infty}{\longrightarrow} p^{\mathsf{st}}(\boldsymbol{x})$

$$\partial_t p^{\mathsf{st}}(\boldsymbol{x}) = 0 = -\boldsymbol{\nabla}\cdot\big(\boldsymbol{\nu}^{\mathsf{st}}(\boldsymbol{x})p^{\mathsf{st}}(\boldsymbol{x})\big), \qquad \boldsymbol{\nu}^{\mathsf{st}}(\boldsymbol{x}) = \frac{1}{\gamma}\big(\boldsymbol{F}(\boldsymbol{x}) - T\boldsymbol{\nabla}\ln p^{\mathsf{st}}(\boldsymbol{x})\big)$$

- invariant under rescaling of local mean velocity $\boldsymbol{\nu}^{\mathsf{st}}(\boldsymbol{x}) \to \boldsymbol{\nu}^{\mathsf{st},\theta}(\boldsymbol{x}) = \theta\boldsymbol{\nu}^{\mathsf{st}}(\boldsymbol{x})$: same steady state $p^{\mathsf{st}}(\boldsymbol{x})$ for all $\theta \in \mathbb{R}$

- average of time-integrated current

$$\langle J_\tau\rangle^\theta = \tau\int d\boldsymbol{x}\ \boldsymbol{w}(\boldsymbol{x})\cdot\boldsymbol{\nu}^{\mathsf{st},\theta}(\boldsymbol{x})p^{\mathsf{st}}(\boldsymbol{x}) = \theta\langle J_\tau\rangle$$

- same as adding a force $\boldsymbol{G}^\theta(\boldsymbol{x})$

$$\boldsymbol{\nu}^{\mathsf{st},\theta}(\boldsymbol{x}) = \boldsymbol{\nu}^{\mathsf{st}}(\boldsymbol{x}) + (\theta-1)\boldsymbol{\nu}^{\mathsf{st}}(\boldsymbol{x}) = \frac{1}{\gamma}\Big(\boldsymbol{F}(\boldsymbol{x}) + \underbrace{\gamma(\theta-1)\boldsymbol{\nu}^{\mathsf{st}}(\boldsymbol{x})}_{\boldsymbol{G}^\theta(\boldsymbol{x})} - T\boldsymbol{\nabla}\ln p^{\mathsf{st}}(\boldsymbol{x})\Big)$$

Continuous time reversal

- write down Langevin equation with new force

$$\gamma\dot{\boldsymbol{x}}(t) = \boldsymbol{F}(\boldsymbol{x}(t)) + \boldsymbol{G}^{\theta}(\boldsymbol{x}(t)) + \sqrt{2\gamma T}\boldsymbol{\xi}(t)$$

- same steady state, but local mean velocity $\boldsymbol{\nu}^{\mathrm{st},\theta}(\boldsymbol{x}) = \theta\boldsymbol{\nu}^{\mathrm{st}}(\boldsymbol{x})$
  - $\theta = +1$: $\boldsymbol{\nu}^{\mathrm{st},1}(\boldsymbol{x}) = \boldsymbol{\nu}^{\mathrm{st}}(\boldsymbol{x})$ original system
  - $\theta = 0$: $\boldsymbol{\nu}^{\mathrm{st},0}(\boldsymbol{x}) = 0 \Rightarrow \Sigma^0 = 0$ equilibrium system
  - $\theta = -1$: $\boldsymbol{\nu}^{\mathrm{st},-1}(\boldsymbol{x}) = -\boldsymbol{\nu}^{\mathrm{st}}(\boldsymbol{x})$ time-reversed system
- can show $D_{\mathrm{KL}}\left(\mathbb{P}^{\theta=-1}(\hat{\boldsymbol{x}})\|\mathbb{P}(\hat{\boldsymbol{x}}^{\dagger})\right) = 0$
- continuous operation connecting forward and time-reversed process $\Rightarrow$ "continuous time reversal"
- special symmetry of the steady state of a Langevin equation

Intermission: Cramér-Rao inequality

- consider probability density $p^\theta(\omega)$, $\omega \in \Omega$ state space, $\theta \in \mathbb{R}$ parameter

$$\langle Z \rangle^\theta = \int d\omega \; Z(\omega) p^\theta(\omega) \quad \text{average of } Z(\omega) \text{ at parameter value } \theta$$

- Cramér-Rao inequality

$$\frac{\left(\partial_\theta \langle Z \rangle^\theta\right)^2}{\mathrm{Var}^\theta(Z)} \leq I^\theta \equiv \int d\omega \; \left(\partial_\theta \ln p^\theta(\omega)\right)^2 p^\theta(\omega) \quad \text{Fisher information}$$

- interpretation: information about θ from measuring $Z \leq$ information contained in $p^\theta(\omega)$
- proof: Cauchy-Schwarz inequality

$$\begin{aligned}\left(\partial_\theta \langle Z \rangle^\theta\right)^2 &= \left(\int d\omega \; \left(Z(\omega) - \langle Z \rangle^\theta\right) \partial_\theta \ln p^\theta(\omega) p^\theta(\omega) \right)^2 \\ &\leq \int d\omega \; \left(Z(\omega) - \langle Z \rangle^\theta\right)^2 p^\theta(\omega) \int d\omega \; \left(\partial_\theta \ln p^\theta(\omega)\right)^2 p^\theta(\omega) = \mathrm{Var}^\theta(Z) I^\theta\end{aligned}$$

Application to Langevin equation

- need to choose Ω, θ and Z
  - Ω: space of trajectories $\hat{\boldsymbol{x}} \Rightarrow p(\omega) = \mathbb{P}(\hat{\boldsymbol{x}})$ path probability density
  - θ: "continuous time reversal" parameter
  - $Z = J_\tau$ time-integrated current
- let's calculate!
  - $\langle J_\tau \rangle^\theta = \theta \langle J_\tau \rangle \Rightarrow \partial_\theta \langle J_\tau \rangle^\theta = \langle J_\tau \rangle$
  - $I^\theta = \int d\hat{\boldsymbol{x}} \, \left(\partial_\theta \ln \mathbb{P}^\theta(\hat{\boldsymbol{x}})\right)^2 \mathbb{P}^\theta(\hat{\boldsymbol{x}})$
- recall expression for transition probability

$$p^\theta(\boldsymbol{x}, t+dt|\boldsymbol{y}, t) \simeq \frac{1}{(4\pi D dt)^{\frac{3}{2}}} \exp\left[-\frac{1}{4Ddt} \left\| \boldsymbol{x} - \boldsymbol{y} - \frac{1}{\gamma}\left(\boldsymbol{F}(\boldsymbol{y}) + \boldsymbol{G}^\theta(\boldsymbol{y})\right) dt \right\|^2 \right]$$

and $\mathbb{P}^\theta(\hat{x}) = p^\theta(\boldsymbol{x}_N, t_N | \boldsymbol{x}_{N-1}, t_{N-1}) \dots p^\theta(\boldsymbol{x}_1, t_1 | \boldsymbol{x}_0, t_0) p^{\mathrm{st}}(\boldsymbol{x}_0)$

Path Fisher information

$$\left(\partial_\theta \ln \mathbb{P}^\theta(\hat{\boldsymbol{x}})\right)^2 = \left(\sum_{k=0}^{N-1} \frac{1}{2\gamma D}\underbrace{\left(\overbrace{\boldsymbol{x}_{k+1}-\boldsymbol{x}_k}^{\simeq \dot{\boldsymbol{x}}(t)dt} - \frac{1}{\gamma}\left(\boldsymbol{F}(\boldsymbol{x}_k)+\boldsymbol{G}^\theta(\boldsymbol{x}_k)\right)dt\right)}_{\simeq\sqrt{2D}\boldsymbol{\xi}(t)dt} \cdot \partial_\theta \boldsymbol{G}^\theta(\boldsymbol{x}_k)\right)^2$$

$$\Rightarrow \quad \left(\partial_\theta \ln \mathbb{P}^\theta(\hat{\boldsymbol{x}})\right)^2 \simeq \frac{1}{2D\gamma^2}\left(\int_0^\tau dt\ \partial_\theta \boldsymbol{G}^\theta(\boldsymbol{x}(t))\cdot \boldsymbol{\xi}(t)\right)\left(\int_0^\tau ds\ \partial_\theta \boldsymbol{G}^\theta(\boldsymbol{x}(s))\cdot \boldsymbol{\xi}(s)\right)$$

$$\langle \xi_i(t)\xi_j(s)\rangle = \delta_{ij}\delta(t-s) \quad \Rightarrow \quad I_\theta = \left\langle \left(\partial_\theta \ln \mathbb{P}^\theta(\hat{\boldsymbol{x}})\right)^2\right\rangle = \frac{1}{2D\gamma^2}\int_0^\tau dt \left\langle \left\|\partial_\theta \boldsymbol{G}^\theta(\boldsymbol{x}(t))\right\|^2\right\rangle$$

- use definition of $\boldsymbol{G}^\theta(\boldsymbol{x}) = \gamma(\theta-1)\boldsymbol{\nu}^{\mathrm{st}}(\boldsymbol{x})$

$$I_\theta = \frac{\tau}{2D}\int d\boldsymbol{x}\ \left\|\boldsymbol{\nu}^{\mathrm{st}}(\boldsymbol{x})\right\|^2 p^{\mathrm{st}}(\boldsymbol{x}) = \frac{1}{2}\Sigma \quad \text{entropy production!}$$

Thermodynamic uncertainty relation

- use Cramér-Rao inequality

$$\frac{\left(\partial_\theta \langle J_\tau \rangle^\theta\right)^2}{\mathrm{Var}^\theta(J_\tau)} \leq I^\theta \quad \Rightarrow \quad \frac{\langle J_\tau \rangle^2}{\mathrm{Var}^\theta(J_\tau)} \leq \frac{1}{2}\Sigma$$

- true for every $\theta \in \mathbb{R}$, in particular for $\theta = 1$ (original system)

$$\frac{\langle J_\tau \rangle^2}{\mathrm{Var}(J_\tau)} \leq \frac{1}{2}\Sigma \qquad \text{TUR!}$$

- information-theoretic interpretation of TUR [Dec18, HVV19]
  - continuous time-reversal parameter θ changes magnitude of local flows
  - left-hand side: information about flows contained in measurement of J_τ
  - right-hand side: information about flows contained in path probability

Equality condition - finite times

- can we find J_τ that gives an equality?
- in general: no, but why?
- reason: "excess fluctuations" out of equilibrium

$$\mathrm{Var}(J_\tau) > \mathrm{Var}^0(J_\tau) \quad \text{as } t \to \infty \quad \Rightarrow \quad \frac{\langle J_\tau \rangle^2}{\mathrm{Var}(J_\tau)} \leq \frac{\langle J_\tau \rangle^2}{\mathrm{Var}^0(J_\tau)} \leq \frac{1}{2}\Sigma$$

- $\mathrm{Var}^0(J_\tau)$ fluctuations of J_τ in equilibrium system with same steady state
- however: can have equality in the second inequality [DS21a]

$$\frac{\langle J_\tau \rangle^2}{\mathrm{Var}^0(J_\tau)} = \frac{1}{2}\Sigma \qquad \text{for} \quad J_\tau = \hat{\Sigma}_\tau \quad \text{stochastic entropy production}$$

Equality condition - short times

- for short times: explicit expression for variance of J_τ [MGK20, OIDS20]

$$\mathrm{Var}(J_\tau) \simeq 2D\tau \int d\boldsymbol{x} \, \left\|\boldsymbol{w}(\boldsymbol{x})\right\|^2 p^{\mathrm{st}}(\boldsymbol{x}) \simeq \mathrm{Var}^0(J_\tau)$$

- independent of θ $\rightarrow$ same in original system and $(\theta = 0)$-equilibrium system
- can always find J_τ with equality in the TUR at short times
- in this case: just Cauchy-Schwarz inequality

$$\begin{aligned}
\langle J_\tau \rangle^2 &= \left(\tau \int d\boldsymbol{x} \ \boldsymbol{w}(\boldsymbol{x}) \cdot \boldsymbol{\nu}^{\mathrm{st}}(\boldsymbol{x}) p^{\mathrm{st}}(\boldsymbol{x}) \right)^2 \\
&\leq \frac{1}{2} \left(2D\tau \int d\boldsymbol{x} \left\|\boldsymbol{w}(\boldsymbol{x})\right\|^2 p^{\mathrm{st}}(\boldsymbol{x}) \right) \left(\frac{\tau}{D} \int d\boldsymbol{x} \left\|\boldsymbol{\nu}^{\mathrm{st}}(\boldsymbol{x})\right\|^2 p^{\mathrm{st}}(\boldsymbol{x}) \right) \\
&= \frac{1}{2} \mathrm{Var}(J_\tau) \Sigma
\end{aligned}$$

Tightness of TUR

- generally not equality: how tight is inequality?

$$\eta_{J_\tau} = \frac{2\langle J_\tau \rangle^2}{\mathrm{Var}(J_\tau)\Sigma} = \frac{\Sigma^{\text{lower bound}}}{\Sigma} \le 1$$

- biased diffusion: $\eta_{J_\tau} = 1$
- periodic potential with bias F: $\eta_{J_\tau} \simeq 1$ for small and large F, $\eta_{J_\tau} \gtrsim 0.2$
- various molecular motor models: $\eta_{J_\tau} = 0.1 \sim 0.4$
- generally $\eta_{J_\tau} \simeq 1$ requires Gaussian statistics of observable

Markov jump processes

- TUR not only works for Langevin equation, but also for Markov jump process
- discrete state space $i \in \{1, \ldots, N\}$, probability $p_t(i)$ to be in state i at time t
  $W(i,j) \geq 0$ transition rate from state j to state i

$$d_t p_t(i) = \sum_j \big(W(i,j)p_t(j) - W(j,i)p_t(i)\big) \quad \underset{t\to\infty}{\longrightarrow} \quad 0 = \sum_j \big(W(i,j)p^{\text{st}}(j) - W(j,i)p^{\text{st}}(i)\big)$$

- time-integrated current (counting current) defined as

$$J_\tau = \int_0^\tau w(i(t+dt), i(t)) \quad \text{with} \quad w(i,j) = -w(j,i)$$

- steady state average of current

$$\langle J_\tau \rangle = \frac{\tau}{2} \sum_{i,j} w(i,j)\big(W(i,j)p^{\text{st}}(j) - W(j,i)p^{\text{st}}(i)\big)$$

Markov jump processes - continuous time-reversal

- define "local mean velocity"

$$V^{\mathsf{st}}(i,j) = \frac{1}{2}\left(W(i,j) - W(j,i)\frac{p^{\mathsf{st}}(i)}{p^{\mathsf{st}}(j)}\right) \quad \Rightarrow \quad \langle J_\tau \rangle = \tau \sum_{i,j} w(i,j) V^{\mathsf{st}}(i,j) p^{\mathsf{st}}(j)$$

- steady state invariant under rescaling of $V^{\mathsf{st}}(i,j) \to V^{\mathsf{st},\theta}(i,j) = \theta V^{\mathsf{st}}(i,j)$
- rest of proof as for Langevin case, but one difference

$$I^\theta = \frac{\tau}{2}\sum_{i,j} \frac{\big(W(i,j)p^{\mathsf{st}}(j) - W(j,i)p^{\mathsf{st}}(i)\big)^2}{W(i,j)p^{\mathsf{st}}(j) + W(j,i)p^{\mathsf{st}}(i)}$$

"pseudo-entropy production" [Shi21]

$$\leq \frac{\tau}{4}\sum_{i,j}\big(W(i,j)p^{\mathsf{st}}(j) - W(j,i)p^{\mathsf{st}}(i)\big)\ln\left(\frac{W(i,j)p^{\mathsf{st}}(j)}{W(j,i)p^{\mathsf{st}}(i)}\right) = \frac{1}{2}\Sigma$$

Markov jump processes - TUR

- same inequality as for Langevin equation

$$\frac{\left(\partial_\theta \langle J_\tau \rangle^\theta\right)^2}{\mathrm{Var}^\theta(J_\tau)} \leq I^\theta \quad \Rightarrow \quad \frac{\langle J_\tau \rangle^2}{\mathrm{Var}^\theta(J_\tau)} \leq \frac{1}{2}\Sigma \quad \Rightarrow \quad \frac{\langle J_\tau \rangle^2}{\mathrm{Var}(J_\tau)} \leq \frac{1}{2}\Sigma$$

- same interpretation: tradeoff between currents, fluctuations and dissipation
- derivation involves additional inequality $\Rightarrow$ generally less tight

Intermediate summary

- TUR from information-theoretic Cramér-Rao inequality
- required ingredients
  - steady state invariant under uniform rescaling of local flows
  - Fisher information of local flows $\leftrightarrow$ entropy production
- two types of generalization
  - tighter bounds under same conditions
  - extension to systems violating above conditions

2. Some generalizations of the TUR

TUR with higher order cumulants

- TUR only depends on first (average) and second (variance) cumulant of current
- tighter bound using higher-order cumulants?
- cumulant generating function

$$K_{J_\tau}(h) = \ln \left\langle e^{hJ_\tau} \right\rangle \simeq h\langle J_\tau \rangle + \frac{h^2}{2}\mathsf{Var}(J_\tau) + \frac{h^3}{6} \underbrace{\left\langle \left(J_\tau - \langle J_\tau \rangle\right)^3 \right\rangle}_{\mathfrak{K}_3(J_\tau)} + \frac{h^4}{24} \underbrace{\left(\left\langle \left(J_\tau - \langle J_\tau \rangle\right)^4 \right\rangle - 3\mathsf{Var}(J_\tau)^2 \right)}_{\mathfrak{K}_4(J_\tau)} + \dots$$

- higher-order cumulants measure large, rare fluctuations of current
- cumulant generating function closely related to large deviations

Intermission: Kullback inequality

- consider probability densities $p^{\theta_1}(\omega)$ and $p^{\theta_2}(\omega) > 0$

$$K_Z^{\theta_1}(h) = \ln\left(\int d\omega e^{hZ(\omega)} p^{\theta_1}(\omega)\right) = \ln\left(\int d\omega e^{hZ(\omega)} \frac{p^{\theta_1}(\omega)}{p^{\theta_2}(\omega)} p^{\theta_2}(\omega)\right)$$
$$\geq \int d\omega \ln\left(e^{hZ(\omega)} \frac{p^{\theta_1}(\omega)}{p^{\theta_2}(\omega)}\right) p^{\theta_2}(\omega) = h\langle Z\rangle^{\theta_2} - D_{\mathsf{KL}}(p^{\theta_2} \| p^{\theta_1})$$

- Kullback inequality: lower bound on KL divergence

$$D_{\mathsf{KL}}(p^{\theta_2} \| p^{\theta_1}) \geq \sup_h \left(h\langle Z\rangle^{\theta_2} - K_Z^{\theta_1}(h)\right)$$

- includes Cramér-Rao inequality as special case

$$D_{\mathsf{KL}}(p^{\theta+d\theta} \| p^{\theta}) \simeq \frac{d\theta^2}{2} I^{\theta}$$

Application to Langevin equation

- as before: θ continuous time-reversal parameter, $p^\theta(\omega)$ path probability, $Z(\omega)$ current

$$\langle J_\tau \rangle^{\theta_2} = \theta_2 \langle J_\tau \rangle \qquad \text{and} \qquad D_{\mathsf{KL}}\left(\mathbb{P}^{\theta_2} \| \mathbb{P}^{\theta_1}\right) = \frac{(\theta_2 - \theta_1)^2}{4} \Sigma$$

- lower bound on cumulant generating function

$$K_{J_\tau}^{\theta_1}(h) \geq h\theta_2 \langle J_\tau \rangle - \frac{(\theta_2 - \theta_1)^2}{4} \Sigma$$

- maximize with respect to $\theta_2 \to$ quadratic lower bound [BS15, GHPE16]

$$K_{J_\tau}^{\theta_1}(h) \geq h\theta_1 \langle J_\tau \rangle + \frac{h^2 \langle J_\tau \rangle^2}{\Sigma}$$

- define cumulant generating function of fluctuations

$$K_{\delta J_\tau}^{\theta}(h) = \ln \left\langle e^{h(J - \langle J_\tau \rangle^\theta)} \right\rangle^\theta = K_J^\theta(h) - h \langle J_\tau \rangle^\theta \qquad \Rightarrow \qquad \Sigma \geq \langle J_\tau \rangle^2 \sup_h \frac{h^2}{K_{\delta J_\tau}^\theta(h)}$$

Higher-order TUR

- similar to TUR: bound on Σ in terms of average current and fluctuations [DS21a]

$$\Sigma \geq \langle J_\tau \rangle^2 \sup_h \frac{h^2}{K_{\delta J_\tau}(h)} \geq \langle J_\tau \rangle^2 \lim_{h \to 0} \frac{h^2}{K_{\delta J_\tau}(h)} = \frac{2\langle J_\tau \rangle^2}{\mathrm{Var}(J_\tau)}$$

- generally tighter than TUR, same as TUR for Gaussian statistics $P(J_\tau) \sim e^{-\frac{(J_\tau - \langle J_\tau \rangle)^2}{2\mathrm{Var}(J_\tau)}}$

$$K_{\delta J_\tau}(h) = \frac{h^2}{2} \mathrm{Var}(J_\tau)$$

- equality for stochastic entropy production $J_\tau = \hat{\Sigma}_\tau$ and $h = -1$

$$K_{\hat{\Sigma}_\tau}(-1) = \ln \left\langle e^{-\hat{\Sigma}_\tau} \right\rangle = 0 \qquad \Rightarrow \qquad K_{\delta \hat{\Sigma}_\tau}(-1) = \langle \hat{\Sigma}_\tau \rangle = \Sigma$$

- same results for Markov jump process

Multidimensional TUR

- instead of single current J_τ: vector of currents $\boldsymbol{J}_\tau = (J_{1,\tau}, \ldots, J_{K,\tau})$
- Cramér-Rao inequality for vector observables

$$\left(\partial_\theta \langle \boldsymbol{Z} \rangle^\theta\right) \cdot \left(\boldsymbol{\Xi}_Z^\theta\right)^{-1} \left(\partial_\theta \langle \boldsymbol{Z} \rangle^\theta\right) \leq I^\theta$$

$$\left(\boldsymbol{\Xi}_Z^\theta\right)_{ij} = \mathrm{Cov}^\theta(Z_i, Z_j) \qquad \text{covariance matrix}$$

- joint TUR for different currents: always tighter than single current [Dec18]

$$\langle \boldsymbol{J}_\tau \rangle \cdot \left(\boldsymbol{\Xi}_{J_\tau}\right)^{-1} \langle \boldsymbol{J}_\tau \rangle \leq \frac{1}{2}\Sigma$$

- for two currents $J_{1,\tau}$ and $J_{2,\tau}$

$$\frac{\langle J_{1,\tau}\rangle^2 \mathrm{Var}(J_{2,\tau}) - 2\langle J_{1,\tau}\rangle\langle J_{2,\tau}\rangle \mathrm{Cov}(J_{1,\tau}, J_{2,\tau}) + \langle J_{2,\tau}\rangle^2 \mathrm{Var}(J_{1,\tau})}{\mathrm{Var}(J_{1,\tau})\mathrm{Var}(J_{2,\tau}) - \mathrm{Cov}(J_{1,\tau}, J_{2,\tau})^2} \leq \frac{1}{2}\Sigma$$

Correlation TUR

- time-integral of state-dependent observable (not a current)

$$Z_\tau = \int_0^\tau dt\ z(\boldsymbol{x}(t)) \qquad \Rightarrow \qquad \langle Z_\tau \rangle = \tau \int d\boldsymbol{x}\ z(\boldsymbol{x}) p^{\mathsf{st}}(\boldsymbol{x}) = \langle Z_\tau \rangle^\theta$$

- independent of time-reversal parameter θ: $\partial_\theta \langle Z_\tau \rangle^\theta = 0$
- similar result as for two currents [DS21b]

$$\frac{\langle J_\tau \rangle^2}{\mathsf{Var}(J_\tau)} \leq \frac{\langle J_\tau \rangle^2}{\mathsf{Var}(J_\tau) \underbrace{\left(1 - \frac{\mathsf{Cov}(J_\tau, Z_\tau)^2}{\mathsf{Var}(J_\tau)\mathsf{Var}(Z_\tau)}\right)}_{\leq 1}} \leq \frac{1}{2}\Sigma$$

- tighter bound from correlations of current with any state-dependent observable Z_τ

Time-dependent TUR

- so far: generalizations for steady state of Langevin/Markov jump dynamics
- how about time-dependent systems?

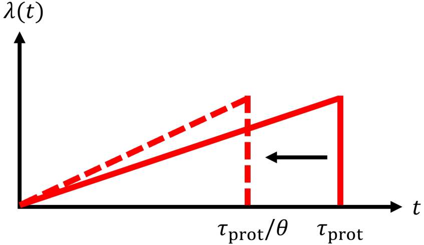
$$\partial_t p_t(\boldsymbol{x}) = -\boldsymbol{\nabla} \cdot \big(\boldsymbol{\nu}_t(\boldsymbol{x}) p_t(\boldsymbol{x})\big)$$

- as before: rescaling of local mean velocity $\boldsymbol{\nu}_t^\theta(\boldsymbol{x}) = \theta \boldsymbol{\nu}_t(\boldsymbol{x}) \Rightarrow I^\theta = \frac{1}{2}\Sigma$
- main challenge: time-dependent state not invariant $p_t^\theta(\boldsymbol{x}) \neq p_t(\boldsymbol{x})$
- intuitively: changing velocity changes speed of time evolution

Time-dependent TUR: time-rescaling

- central idea: overall change in evolution speed $\rightarrow$ change all timescales of system
  - internal time scales $\tau_{\text{int}} \propto 1/\nu_t^\theta \propto 1/\theta$
  - same scaling for external (protocol) time scale $\tau_{\text{prot}} \propto 1/\theta$

  } overall time $\tau \rightarrow \tau/\theta$



- effect on currents: rescaling of overall time τ

$$\partial_\theta \langle J_\tau \rangle = -\tau d_\tau \langle J_\tau \rangle$$

Time-dependent TUR

- use Cramér-Rao inequality: TUR for time-dependent systems [KS19, KS20]

$$\frac{\left(\tau d_\tau \langle J_\tau \rangle\right)^2}{\text{Var}(J_\tau)} \leq \frac{1}{2}\Sigma$$

- in steady state $\langle J_\tau \rangle = \tau \langle \dot{J} \rangle \Rightarrow \tau d_\tau \langle J_\tau \rangle = \langle J_\tau \rangle$: recovers TUR
- also works for non-current observables
- measure response of observable to changing measurement and protocol time

Other generalizations of the TUR

- underdamped Langevin equation (steady state) [LPP19, VVH19b, Dec22]

$$\frac{\langle J_\tau \rangle^2}{\mathrm{Var}(J_\tau)} \leq \frac{1}{2}\Sigma + \text{other terms}$$

  - additional terms: related to frenesy (dynamical activity) or acceleration
  - usual TUR can be violated: coherent oscillations can reduce fluctuations [Pie22]

- discrete-time Markov processes (steady state) [LGU20]

$$\frac{\langle J_\tau \rangle^2}{\mathrm{Var}(J_\tau)} \leq \frac{1}{2P_{\mathrm{stay}}^{\mathrm{min}}}\Sigma$$

  - $P_{\mathrm{stay}}^{\mathrm{min}}$: minimal probability for state not changing in one step
  - continuous time $P_{\mathrm{stay}}^{\mathrm{min}} = 1 - O(dt)$: recovers TUR

Other generalizations of the TUR

- time-delayed systems [VVH19a]
- magnetic systems [CFS19, PP21, Dec22]
- open quantum systems [Has20, Has21, VVS22]
- TURs for excess and housekeeping entropy
- ...

3. Summary and references

Summary: Thermodynamic Uncertainty Relations

- TUR: tradeoff between dissipation and precision in steady state Markovian dynamics
- quantitative version of the second law: positive lower bound on entropy production
- estimate entropy production from measurable quantities (currents)
- derivation relies on
    - entropy production characterizes rescaling of local flows $I^\theta \leftrightarrow \Sigma$
    - steady state invariant under rescaling
- generally no equality condition $\rightarrow$ various tighter inequalities
- relax above conditions $\rightarrow$ generalizations

Beyond the TUR

- TUR one example of thermodynamic inequalities
- other types of lower bounds on Σ
  - speed limits $\Sigma \geq \frac{d(p_{\text{initial}}, p_{\text{final}})^2}{\tau}$; d Wasserstein distance, total variation distance, ... [AMMMG11, SFS18, FE20, VVH21, NI21]
  - lower bounds from waiting time statistics of transitions [SD21]
- inequalities not related to Σ
  - kinetic uncertainty relation: dynamical activity [DTB18]
  - speed limits $\tau_{\text{initial}\to\text{final}} \geq ?$ [Ito18, ID20, YI21]
  - tradeoff relations between response and fluctuations [DS20, FED22]
- why study inequalities?
  - fundamental constraints on what can and cannot happen
  - establish relations between different physical quantities

References I

[AMMMG11] E. Aurell, C. Mejía-Monasterio, and P. Muratore-Ginanneschi.
Optimal protocols and optimal transport in stochastic thermodynamics.
Phys. Rev. Lett., 106:250601, 2011.

[BS15] A. C. Barato and U. Seifert.
Thermodynamic uncertainty relation for biomolecular processes.
Phys. Rev. Lett., 114:158101, 2015.

[CFS19] H.-M. Chun, L. P. Fischer, and U. Seifert.
Effect of a magnetic field on the thermodynamic uncertainty relation.
Phys. Rev. E, 99:042128, 2019.

[Dec18] A. Dechant.
Multidimensional thermodynamic uncertainty relations.
J. Phys. A Math. Theor., 52(3):035001, dec 2018.

[Dec22] A. Dechant.
Bounds on the precision of currents in underdamped langevin dynamics, 2022.

[DS18] A. Dechant and S.-i. Sasa.
Current fluctuations and transport efficiency for general Langevin systems.
J. Stat. Mech. Theory E., 2018(6):063209, 2018.

[DS20] A. Dechant and S.-i. Sasa.
Fluctuation–response inequality out of equilibrium.
Proc. Natl. Acad. Sci., 117(12):6430–6436, 2020.

[DS21a] A. Dechant and S.-i. Sasa.
Continuous time reversal and equality in the thermodynamic uncertainty relation.
Phys. Rev. Research, 3:L042012, 2021.

[DS21b] A. Dechant and S.-i. Sasa.
Improving thermodynamic bounds using correlations.
Phys. Rev. X, 11:041061, 2021.

References II

[DTB18] I. Di Terlizzi and M. Baiesi.
Kinetic uncertainty relation.
J. Phys. A Math. Theor., 52(2):02LT03, 2018.

[FE20] G. Falasco and M. Esposito.
Dissipation-time uncertainty relation.
Phys. Rev. Lett., 125:120604, 2020.

[FED22] G. Falasco, M. Esposito, and J.-C. Delvenne.
Beyond thermodynamic uncertainty relations: nonlinear response, error-dissipation trade-offs, and speed limits.
J. Phys. A Math. Theor., 55(12):124002, 2022.

[GHPE16] T. R. Gingrich, J. M. Horowitz, N. Perunov, and J. L. England.
Dissipation bounds all steady-state current fluctuations.
Phys. Rev. Lett., 116:120601, 2016.

[Has20] Y. Hasegawa.
Quantum thermodynamic uncertainty relation for continuous measurement.
Phys. Rev. Lett., 125:050601, 2020.

[Has21] Y. Hasegawa.
Thermodynamic uncertainty relation for general open quantum systems.
Phys. Rev. Lett., 126:010602, 2021.

[HVV19] Y. Hasegawa and T. Van Vu.
Uncertainty relations in stochastic processes: An information inequality approach.
Phys. Rev. E, 99(6):062126, 2019.

[ID20] S. Ito and A. Dechant.
Stochastic time evolution, information geometry, and the Cramér-Rao bound.
Phys. Rev. X, 10:021056, 2020.

References III

[Ito18] S. Ito.
Stochastic thermodynamic interpretation of information geometry.
Phys. Rev. Lett., 121(3):030605, 2018.

[KS19] T. Koyuk and U. Seifert.
Operationally accessible bounds on fluctuations and entropy production in periodically driven systems.
Phys. Rev. Lett., 122:230601, 2019.

[KS20] T. Koyuk and U. Seifert.
Thermodynamic uncertainty relation for time-dependent driving.
Phys. Rev. Lett., 125:260604, 2020.

[LGU20] K. Liu, Z. Gong, and M. Ueda.
Thermodynamic uncertainty relation for arbitrary initial states.
Phys. Rev. Lett., 125:140602, 2020.

[LHGF19] J. Li, J. M. Horowitz, T. R. Gingrich, and N. Fakhri.
Quantifying dissipation using fluctuating currents.
Nature Comm., 10:1–9, 2019.

[LPP19] J. S. Lee, J.-M. Park, and H. Park.
Thermodynamic uncertainty relation for underdamped Langevin systems driven by a velocity-dependent force.
Phys. Rev. E, 100:062132, 2019.

[MGK20] S. K. Manikandan, D. Gupta, and S. Krishnamurthy.
Inferring entropy production from short experiments.
Phys. Rev. Lett., 124:120603, 2020.

[NI21] M. Nakazato and S. Ito.
Geometrical aspects of entropy production in stochastic thermodynamics based on wasserstein distance.
Phys. Rev. Research, 3:043093, 2021.

References IV

[OIDS20] S. Otsubo, S. Ito, A. Dechant, and T. Sagawa.
Estimating entropy production by machine learning of short-time fluctuating currents.
Phys. Rev. E, 101:062106, 2020.

[Pie22] P. Pietzonka.
Classical pendulum clocks break the thermodynamic uncertainty relation.
Phys. Rev. Lett., 128:130606, 2022.

[PP21] J.-M. Park and H. Park.
Thermodynamic uncertainty relation in the overdamped limit with a magnetic lorentz force.
Phys. Rev. Research, 3:043005, 2021.

[PS18] P. Pietzonka and U. Seifert.
Universal trade-off between power, efficiency, and constancy in steady-state heat engines.
Phys. Rev. Lett., 120:190602, 2018.

[SD21] D. J. Skinner and J. Dunkel.
Estimating entropy production from waiting time distributions.
Phys. Rev. Lett., 127:198101, 2021.

[SFS18] N. Shiraishi, K. Funo, and K. Saito.
Speed limit for classical stochastic processes.
Phys. Rev. Lett., 121:070601, 2018.

[Shi21] N. Shiraishi.
Optimal thermodynamic uncertainty relation in markov jump processes.
J. Stat. Phys., 185(3):1–15, 2021.

[VVH19a] T. Van Vu and Y. Hasegawa.
Uncertainty relations for time-delayed langevin systems.
Phys. Rev. E, 100(1):012134, 2019.

References V

[VVH19b] T. Van Vu and Y. Hasegawa.
Uncertainty relations for underdamped Langevin dynamics.
Phys. Rev. E, 100:032130, 2019.

[VVH21] T. Van Vu and Y. Hasegawa.
Geometrical bounds of the irreversibility in markovian systems.
Phys. Rev. Lett., 126(1):010601, 2021.

[VVS22] T. Van Vu and K. Saito.
Thermodynamics of precision in markovian open quantum dynamics.
Phys. Rev. Lett., 128:140602, 2022.

[VVVH20] T. Van Vu, V. T. Vo, and Y. Hasegawa.
Entropy production estimation with optimal current.
Phys. Rev. E, 101:042138, 2020.

[YI21] K. Yoshimura and S. Ito.
Information geometric inequalities of chemical thermodynamics.
Phys. Rev. Research, 3:013175, 2021.