Fluctuation Relations for Anomalous Stochastic Dynamics

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Outline

- **Transient fluctuation relations** (TFRs): motivation and warm-up

- **Correlated Gaussian dynamics:**
  check TFRs for *generalized Langevin dynamics*

- **Non-Gaussian dynamics:**
  check TFRs for *time-fractional Fokker-Planck equations*

- **Relations to experiments:**
  glassy dynamics and biological cell migration
Motivation: Fluctuation relations

Consider a (classical) particle system evolving from some initial state into a nonequilibrium steady state. Measure the probability distribution $\rho(\xi_t)$ of entropy production $\xi_t$ during time $t$:

$$\ln \frac{\rho(\xi_t)}{\rho(-\xi_t)} = \xi_t$$

Transient Fluctuation Relation (TFR)
Evans, Cohen, Morriss (1993); Gallavotti, Cohen (1995)

**why important?** of *very general validity* and

1. generalizes the **Second Law** to small systems in nonequ.
2. connection with **fluctuation dissipation relations**
3. can be checked in **experiments** (Wang et al., 2002)
Fluctuation relation for Langevin dynamics

**warm-up:** check TFR for the overdamped Langevin equation

\[ \dot{x} = F + \zeta(t) \]  
(set all irrelevant constants to 1)

with constant field \( F \) and Gaussian white noise \( \zeta(t) \).

entropy production \( \xi_t \) is equal to (mechanical) work \( W_t = Fx(t) \)
with \( \rho(W_t) = F^{-1} \rho(x, t) \); remains to solve corresponding Fokker-Planck equation for initial condition \( x(0) = 0 \):

the position pdf is Gaussian,

\[ \rho(x, t) = \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp \left( -\frac{(x-\langle x \rangle)^2}{2\sigma_x^2} \right) \]

straightforward:

(work) TFR holds if \( \langle x \rangle = F\sigma_x^2/2 \)

and \( \exists \) fluctuation-dissipation relation 1 (FDR1) \( \Rightarrow \) TFR

see, e.g., van Zon, Cohen, PRE (2003)
**Goal:** check TFR for Gaussian stochastic processes defined by the (overdamped) generalized Langevin equation

$$\int_0^t dt' \dot{x}(t') K(t-t') = F + \zeta(t)$$

e.g., Kubo (1965)

with Gaussian noise $\zeta(t)$ and memory kernel $K(t)$

This dynamics can generate **anomalous diffusion:**

$$\sigma_x^2 \sim t^\alpha \quad \text{with} \quad \alpha \neq 1 \quad (t \to \infty)$$
consider two generic cases:

1. **internal Gaussian noise** defined by the $\text{FDR}_2$,

\[
< \zeta(t)\zeta(t') > \sim K(t - t'),
\]

with non-Markovian (correlated) noise; e.g., $K(t) \sim t^{-\beta}$

solving the corresponding generalized Langevin equation in Laplace space yields

\[
\text{FDR}_2 \Rightarrow '\text{FDR}_1'
\]

and since $\rho(W_t) \sim \rho(x, t)$ is Gaussian

\[
'\text{FDR}_1' \Rightarrow \text{TFR}
\]

for correlated internal Gaussian noise $\exists \text{TFR}$
Correlated external Gaussian noise

2. **external Gaussian noise** for which there is no FDR2, modeled by the (overdamped) generalized Langevin equation

\[ \dot{x} = F + \zeta(t) \]

consider two types of Gaussian noise correlated by

\[ g(\tau) = \langle \zeta(t)\zeta(t') \rangle_{\tau=t-t'} \sim (\Delta/\tau)^\beta \quad \text{for } \tau > \Delta, \beta > 0: \]

- **persistent**
- **anti-persistent**

it is \( <x> = Ft \) and \( \sigma_x^2 = 2 \int_0^t d\tau (t - \tau) g(\tau) \)
Results: TFRs for correlated external Gaussian noise

\[ \sigma_x^2 \text{ and the fluctuation ratio } R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)} \text{ for } t \gg \Delta \text{ and} \]

\[ g(\tau) = \langle \zeta(t)\zeta(t') \rangle_{\tau=t-t'} \sim (\Delta/\tau)^\beta : \]

<table>
<thead>
<tr>
<th>( \beta )</th>
<th>( \sigma_x^2 )</th>
<th>( R(W_t) )</th>
<th>( \sigma_x^2 )</th>
<th>( R(W_t) )</th>
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</thead>
<tbody>
<tr>
<td>( 0 &lt; \beta &lt; 1 )</td>
<td>( \sim t^{2-\beta} )</td>
<td>( \sim \frac{W_t}{t^{1-\beta}} )</td>
<td>( \sim \frac{W_t}{t^{1-\beta}} )</td>
<td>( \text{regime does not exist} )</td>
</tr>
<tr>
<td>( \beta = 1 )</td>
<td>( \sim t \ln \left( \frac{t}{\Delta} \right) )</td>
<td>( \sim \frac{W_t}{\ln(t/\Delta)} )</td>
<td>( \text{regime does not exist} )</td>
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<tr>
<td>( 1 &lt; \beta &lt; 2 )</td>
<td>( \sim 2Dt )</td>
<td>( \sim \frac{W_t}{D} )</td>
<td>( \sim \ln(t/\Delta) )</td>
<td>( \sim \frac{t}{\ln(t/\Delta)} W_t )</td>
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<tr>
<td>( \beta = 2 )</td>
<td>( \sim 2Dt )</td>
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<tr>
<td>( 2 &lt; \beta &lt; \infty )</td>
<td>( \sim 2Dt )</td>
<td>( \sim \frac{W_t}{D} )</td>
<td>( \sim \ln(t/\Delta) )</td>
<td>( \sim \frac{t}{\ln(t/\Delta)} W_t )</td>
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* antipersistence for \( \int_0^\infty d\tau g(\tau) > 0 \) yields normal diffusion with generalized TFR; above antipersistence for \( \int_0^\infty d\tau g(\tau) = 0 \)
relation between **TFR** and **FDR I,II** for **correlated Gaussian stochastic dynamics**: (‘normal FR’= conventional TFR)

in particular:

\[
\text{FDR2} \Rightarrow \text{FDR1} \Rightarrow \text{TFR} \\
\neg\text{TFR} \Rightarrow \neg\text{FDR2}
\]
Modeling non-Gaussian dynamics

- Start again from overdamped Langevin equation $\dot{x} = F + \zeta(t)$, but here with **non-Gaussian** power law correlated noise:
  
  \[ g(\tau) = \langle \zeta(t)\zeta(t') \rangle_{\tau=t-t'} \sim (K_\alpha/\tau)^{2-\alpha}, \quad 1 < \alpha < 2 \]

- ‘Motivates’ the non-Markovian Fokker-Planck equation

  **type A:**
  \[
  \frac{\partial \rho_A(x, t)}{\partial t} = -\frac{\partial}{\partial x} \left[ F - K_\alpha D_t^{1-\alpha} \frac{\partial}{\partial x} \right] \rho_A(x, t)
  \]

  with Riemann-Liouville fractional derivative $D_t^{1-\alpha}$ (Balescu, 1997)

- Two **formally similar** types derived from CTRW theory, for $0 < \alpha < 1$:

  **type B:**
  \[
  \frac{\partial \rho_B(x, t)}{\partial t} = -\frac{\partial}{\partial x} \left[ F - K_\alpha D_t^{1-\alpha} \frac{\partial}{\partial x} \right] \rho_B(x, t)
  \]

  **type C:**
  \[
  \frac{\partial \rho_C(x, t)}{\partial t} = -\frac{\partial}{\partial x} \left[ FD_t^{1-\alpha} - K_\alpha D_t^{1-\alpha} \frac{\partial}{\partial x} \right] \rho_C(x, t)
  \]

  They model a **very different** class of stochastic process!
Properties of non-Gaussian dynamics

Riemann-Liouville fractional derivative defined by

\[
\frac{\partial^\gamma \varrho}{\partial t^\gamma} := \begin{cases} 
\frac{\partial^m \varrho}{\partial t^m} \\
\frac{\partial^m \varrho}{\partial t^m} \left[ \frac{1}{\Gamma(m-\gamma)} \int_0^t dt' \frac{\varrho(t')}{(t-t')^{\gamma+1-m}} \right]
\end{cases}, \quad \gamma = m, \quad m - 1 < \gamma < m
\]

with \( m \in \mathbb{N} \); power law inherited from correlation decay.

two important properties:

- **FDR1**: exists for type C but not for A and B
- **mean square displacement**:
  - type A: superdiffusive, \( \sigma_x^2 \sim t^\alpha \), \( 1 < \alpha < 2 \)
  - type B: subdiffusive, \( \sigma_x^2 \sim t^\alpha \), \( 0 < \alpha < 1 \)
  - type C: sub- or superdiffusive, \( \sigma_x^2 \sim t^{2\alpha} \), \( 0 < \alpha < 1 \)

- **position pdfs**: can be calculated approx. analytically for A, B, only numerically for C
Probability distributions and fluctuation relations

- **PDFs:**
  - type A
  - type B
  - type C

- **TFRs:**

\[ R(W_t) = \log \frac{\rho(W_t)}{\rho(-W_t)} \sim \begin{cases} 
  c_\alpha W_t, & W_t \to 0 \\
  t(2\alpha-2)/(2-\alpha) W_t^{\alpha/(2-\alpha)}, & W_t \to \infty
\end{cases} \]
Relations to experiments: glassy dynamics

**example 1:** computer simulations for a binary Lennard-Jones mixture below the glass transition

\[
P_t(\Delta S) / P_{\tau w}(-\Delta S) = 10^{2}
\]

\[
\tau_w = 10^2
\]

\[
\tau_w = 10^3
\]

\[
\tau_w = 10^4
\]

Crisanti, Ritort, PRL (2013)

- again: \( R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)} = f_\beta(t) W_t \); cp. with TFR type B
- similar results for other glassy systems (Sellitto, PRE, 2009)
example 2: single MDCKF cell crawling on a substrate; trajectory recorded with a video camera

new experiments on murine neutrophils under chemotaxis:

Dieterich et al. (2013)
**Anomalous fluctuation relation for cell migration**

**experim. results:** position pdfs $\rho(x, t)$ are Gaussian

- $\langle x(t) \rangle \sim t$ and $\sigma_x^2 \sim t^{2-\beta}$ with $0 < \beta < 1$: FDR1 and

$$R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)} = \frac{W_t}{t^{1-\beta}}$$

**fluctuation ratio $R(W_t)$ is time dependent**

- Data matches to analytical results for persistent correlations
Summary

TFR tested for two generic cases of correlated Gaussian stochastic dynamics:

1. **internal noise**: FDR2 implies the validity of the ‘normal’ work TFR
2. **external noise**: FDR2 is broken; sub-classes of persistent and anti-persistent noise yield both anomalous TFRs

TFR tested for three cases of non-Gaussian dynamics: breaking FDR1 implies again anomalous TFRs

Anomalous TFRs appear to be important for glassy aging dynamics: cf. computer simulations on various glassy models and experiments on (‘gelly’) cell migration
RK, A.V. Chechkin, P. Dieterich, *Anomalous fluctuation relations* in: