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 ξ_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

$$\dot{x} = F + \zeta(t) \quad \text{(set all irrelevant constants to 1)}$$

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

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

the position pdf is Gaussian,

$$\varrho(x,t) = \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp\left(-\frac{(x-<x>)^2}{2\sigma_x^2}\right)$$

straightforward:

(work) TFR holds if $< x >= F\sigma_x^2/2$

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

see, e.g., van Zon, Cohen, PRE (2003)

Gaussian stochastic dynamics

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**:

$$\sigma_x^2 \sim t^\alpha \text{ with } \alpha \neq 1 \ (t \to \infty)$$

TFR for correlated internal Gaussian noise

consider two generic cases:

1. **internal Gaussian noise** defined by the **FDR2**,

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

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

solving the corresponding generalized Langevin equation in Laplace space yields

FDR2 ⇒ 'FDR1'

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

'FDR1' ⇒ TFR

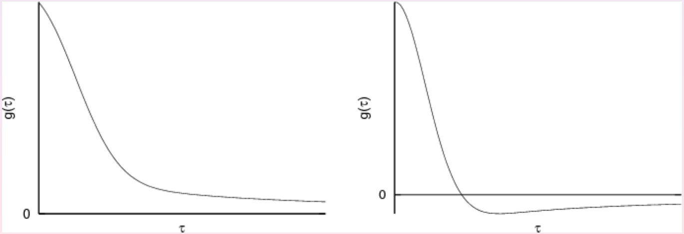
for correlated **internal Gaussian noise** ∃ TFR

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
$g(\tau) =< \zeta(t)\zeta(t') >_{\tau=t-t'} \sim (\Delta/\tau)^\beta$ 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

σ_x^2 and the fluctuation ratio $R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)}$ for $t \gg \Delta$ and

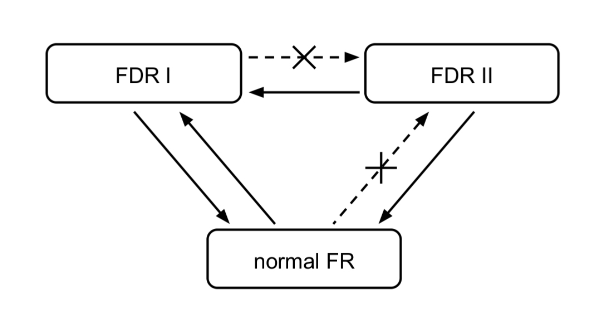
$g(\tau) = < \zeta(t)\zeta(t') >_{\tau=t-t'} \sim (\Delta/\tau)^{\beta}$:

	persistent		antipersistent *	
β	σ_x^2	$R(W_t)$	σ_x^2	$R(W_t)$
$0 < \beta < 1$	$\sim t^{2-\beta}$	$\sim \frac{W_t}{t^{1-\beta}}$	*regime*	
$\beta = 1$	$\sim t \ln\left(\frac{t}{\Delta}\right)$	$\sim \frac{W_t}{\ln\left(\frac{t}{\Delta}\right)}$	*does not exist*	
$1 < \beta < 2$			$\sim t^{2-\beta}$	$\sim t^{\beta-1} W_t$
$\beta = 2$	$\sim 2Dt$	$\sim \frac{W_t}{D}$	$\sim \ln(t/\Delta)$	$\sim \frac{t}{\ln\left(\frac{t}{\Delta}\right)} W_t$
$2 < \beta < \infty$			$= const.$	$\sim t W_t$

* antipersistence for $\int_0^\infty d\tau g(\tau) > 0$ yields normal diffusion with generalized TFR; above antipersistence for $\int_0^\infty d\tau g(\tau) = 0$

FDR and TFR

relation between TFR and FDR I,II for **correlated Gaussian stochastic dynamics**: ('normal FR'= conventional TFR)



in particular:

$$\textbf{FDR2} \Rightarrow \textbf{FDR1} \Rightarrow \textbf{TFR}$$

$$\nexists\ \textbf{TFR} \Rightarrow \nexists\ \textbf{FDR2}$$

Modeling non-Gaussian dynamics

- start again from overdamped Langevin equation $\dot{x} = F + \zeta(t)$, but here with **non-Gaussian** power law correlated noise

$$g(\tau) = < \zeta(t)\zeta(t') >_{\tau=t-t'} \sim (K_\alpha/\tau)^{2-\alpha} \ , \ 1 < \alpha < 2$$

- 'motivates' the non-Markovian Fokker-Planck equation

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

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: $\frac{\partial \varrho_B(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[F - K_\alpha D_t^{1-\alpha}\frac{\partial}{\partial x}\right]\varrho_B(x,t)$

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

They model a *very different* class of stochastic process!

Properties of non-Gaussian dynamics

Riemann-Liouville fractional derivative defined by

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

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, $\sigma_x^2 \sim t^\alpha$, $0 < \alpha < 1$

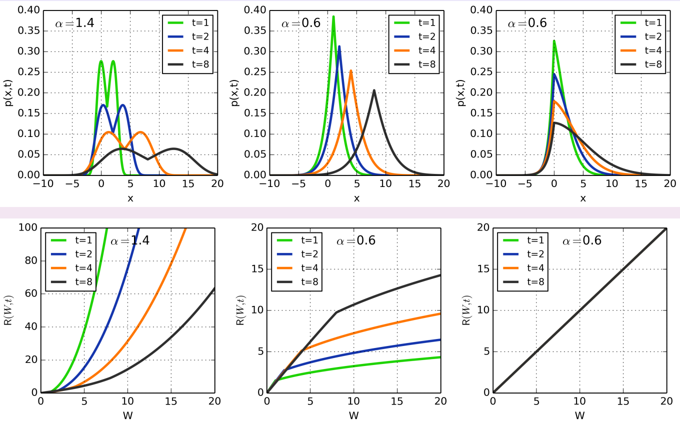
- type C: sub- or superdiffusive, $\sigma_x^2 \sim t^{2\alpha}$, $0 < \alpha < 1$

- **position pdfs:** can be calculated approx. analytically for A, B, only numerically for C

Probability distributions and fluctuation relations

type A type B type C

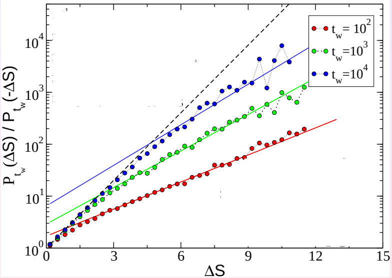
- **PDFs:**
- **TFRs:**



$$R(W_t) = \log \frac{\rho(W_t)}{\rho(-W_t)} \sim \begin{cases} c_\alpha W_t \,, & W_t \to 0 \\ t^{(2\alpha-2)/(2-\alpha)} W_t^{\alpha/(2-\alpha)} \,, & W_t \to \infty \end{cases}$$

Relations to experiments: glassy dynamics

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

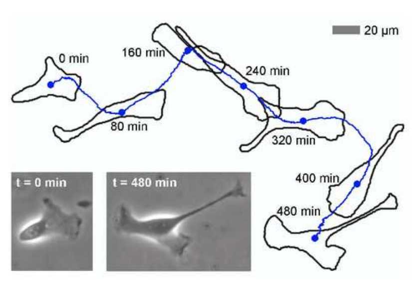


Crisanti, Ritort, PRL (2013)

- again: $R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)} = \mathbf{f}_\beta(\mathbf{t}) W_t$; cp. with TFR type B
- similar results for other glassy systems (Sellitto, PRE, 2009)

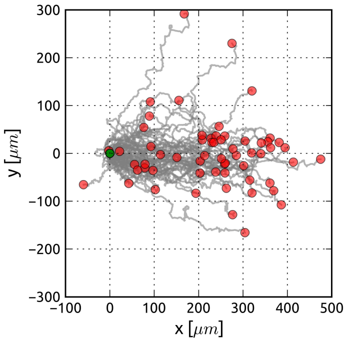
Cell migration without and with chemotaxis

example 2: single MDCKF cell crawling on a substrate; trajectory recorded with a video camera



Dieterich et al., PNAS, 2008

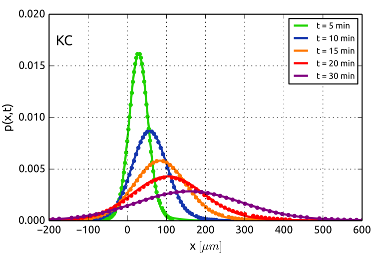
new experiments on murine neutrophils under chemotaxis:



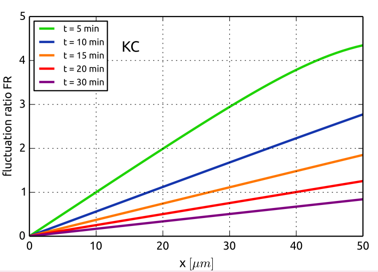
Dieterich et al. (2013)

Anomalous fluctuation relation for cell migration

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



fluctuation ratio $R(W_t)$ is time dependent



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

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

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

References

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