Anomalous Langevin Dynamics, Fluctuation-Dissipation Relations and Fluctuation Relations

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Non-equilibrium Dynamics of Climate: linking models to data

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Outline

- **Normal Langevin dynamics:**

  brief review and cross-link to stochastic climate dynamics

- **Anomalous Langevin dynamics:**

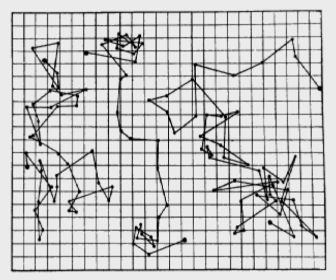
  anomalous diffusion, fluctuation-dissipation relations and relation to long-range memory for modeling earth's temperature

- **Fluctuation relations:**

  motivation by 2nd law of thermodynamics and check them for Langevin dynamics

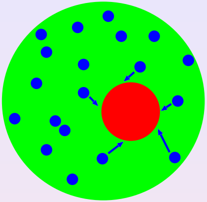
Theoretical modeling of Brownian motion

Brownian motion



Perrin (1913)

three colloidal particles, positions joined by straight lines



'Newton's law of stochastic physics':

$$m\dot{\mathbf{v}} = -\kappa\mathbf{v} + k\,\zeta(t)$$

Langevin equation (1908)

for a tracer particle of velocity **v** immersed in a fluid

force on rhs decomposed into:

- viscous damping as Stokes friction
- random kicks of surrounding particles

modeled by Gaussian white noise

Langevin dynamics

Langevin dynamics characterized by **solutions** of the Langevin equation; here focus on (in 1dim):

- mean square displacement (msd)

$$\sigma_x^2 = \langle (x(t) - \langle x(t) \rangle)^2 \rangle \sim t \quad (t \to \infty) \,,$$

  where $\langle \ldots \rangle$ denotes an ensemble average

- position probability distribution function (pdf)

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

  (from solving the corresponding diffusion equation) reflects the Gaussianity of the noise

A stochastic energy balance equation

model the dynamics of the **earth's surface temperature** T by combining two ideas:

1. use a linearized energy-balance equation derived as
$$C\dot{T} = -\frac{1}{S_{eq}}T + F$$ (e.g., Ghil, 1984)
with heat capacity C, equilibrium climate sensitivity S_{eq} and (solar) radiative influx F

2. model randomness in forcing of ocean-land heat content from atmosphere by adding stochasticity (Hasselmann, 1981),
$$C\dot{T} = -\frac{1}{S_{eq}}T + F + k\,\zeta(t)$$ (Padilla, 2011)
with Gaussian white noise ζ of strength k

Langevin dynamics for surface temperature

compare:

stochastic EB eq. $$C\dot{T} = -\frac{1}{S_{eq}}T + F + k\,\zeta(t)$$

Langevin eq. with field $$m\dot{v} = -\kappa v + F + k\,\zeta(t)$$

mathematically identical

Generalized Langevin equation

Mori, Kubo (1965/66): generalize ordinary Langevin equation to

$$m\dot{v} = -\int_0^t dt'\, \kappa(t-t')v(t') + k\,\zeta(t)$$

by using a time-dependent friction coefficient $\kappa(t) \sim t^{-\beta}$; applications to polymer dynamics (Panja, 2010) and biological cell migration (Dieterich, RK et al., 2008)

solutions of this Langevin equation:

- position pdf is Gaussian (as the noise is still Gaussian)
- but for msd $\sigma_x^2 \sim t^{\alpha(\beta)}$ $(t \to \infty)$ with anomalous diffusion for $\alpha \neq 1$; $\alpha < 1$: subdiffusion; $\alpha > 1$: superdiffusion

(nb: the 1st term on the rhs defines a fractional derivative)

Fluctuation-dissipation relations

Kubo (1966): two fundamental relations characterizing Langevin dynamics

1. fluctuation-dissipation relation of the 2nd kind (FDR2),

$$< \zeta(t)\zeta(t') > \sim \kappa(t-t')$$

defines **internal noise**, which is correlated in the same way as the friction; if broken: **external noise**

2. fluctuation-dissipation relation of the 1st kind (FDR1),

$$< x > \sim \sigma_x^2$$

implies that current and msd have the same time dependence (linear response)

(nb: some technical subtleties neglected)

Implications of fluctuation-dissipation relations

- for generalized Langevin dynamics with power-law correlated internal (FDR2) Gaussian noise, $\kappa(t) \sim t^{-\beta}$, **FDR2 implies FDR1** (Chechkin, Lenz, RK, 2012)
- Rypdal, Rypdal (2014): similar generalized Langevin dynamics used to model long-range memory effects in the earth's temperature dynamics (i.e., previous stochastic energy-balance eq. with memory kernel); fit to data
- but: modeling implies breaking of FDR2; meaningful? whether or not $\exists$ FDR1/FDR2 has crucial consequences!

last part of this talk: illustrate consequences of FDR for a relation generalizing the 2nd law of thermodynamics

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)

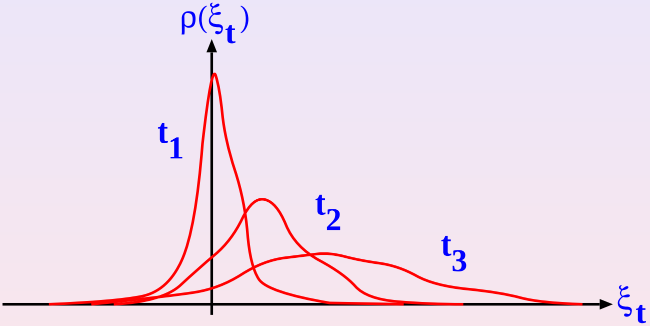
Evans, Cohen, Morriss (1993); Gallavotti, Cohen (1995)

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 and the Second Law

meaning of TFR in terms of the Second Law:



$t_1 < t_2 < t_3$

$$\boxed{\rho(\xi_t) = \rho(-\xi_t)\exp(\xi_t)} \geq \rho(-\xi_t)\ (\xi_t \geq 0) \ \Rightarrow \ <\xi_t> \geq 0$$

Fluctuation relation for normal Langevin dynamics

check TFR for the overdamped Langevin equation

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

for a particle at position x with constant field F and noise ζ.

entropy production ξ_t is equal to (mechanical) work $W_t = Fx(t)$
with $\rho(W_t) = F^{-1}\varrho(x,t)$; choose initial condition $x(0) = 0$

the position pdf is Gaussian which implies straightforwardly

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

hence **FDR1 $\Rightarrow$ TFR**

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

Fluctuation relation for anomalous Langevin dynamics

check TFR for overdamped generalized Langevin equation

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

both for internal and external power-law correlated Gaussian noise $\kappa(t) \sim t^{-\beta}$

1. internal Gaussian noise:

• as FDR2 implies FDR1 and $\rho(W_t) \sim \varrho(x,t)$ is Gaussian, it straightforwardly follows the existence of the transient fluctuation relation

for correlated **internal Gaussian noise** $\exists$ TFR

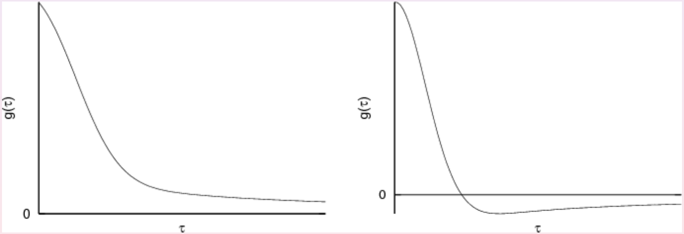
• diffusion and current may both be normal or anomalous depending on the memory kernel

Correlated external Gaussian noise

2. external Gaussian noise: break FDR2, modelled 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 $\sigma_x^2 = 2 \int_0^t d\tau (t-\tau) g(\tau)$

TFRs for correlated external Gaussian noise

results in a nutshell:
(for details see Chechkin, Lenz, RK, JStat, 2012)

• depending on the type of correlation and β the Langevin dynamics exhibits a whole (complicated) spectrum of normal and **anomalous diffusion**

• the **TFR is always anomalous**:

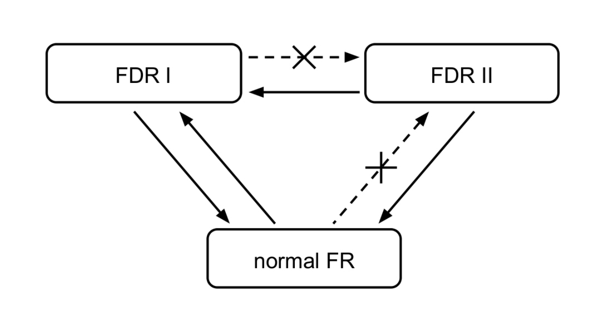
$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = f_\beta(t) W_t$$

where $f_\beta(t)$ depends on the type of diffusive dynamics

$\Rightarrow$ breaking of FDR yields a different type of generalized 2nd law-like relation

Summary: FDR and TFR

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



in particular:

FDR2 $\Rightarrow$ FDR1 $\Rightarrow$ TFR

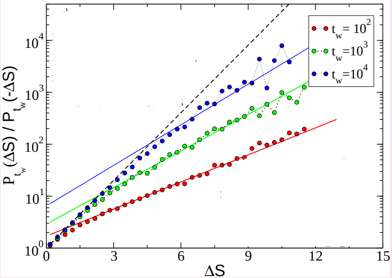
$\nexists$ **TFR** $\Rightarrow$ $\nexists$ **FDR2**

Checking TFR in experiments

$$R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)} = \mathbf{f}_\beta(\mathbf{t}) W_t$$

means by plotting R for different t the slope might change.

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



Crisanti, Ritort, PRL (2013)

similar results for other glassy systems (Sellitto, PRE, 2009)

Summary

- linearized stochastic energy-balance equation for the earth's surface temperature corresponds to Langevin dynamics
- long-range memory effects for stochastic climate dynamics suggest studying generalized Langevin equations
- be careful of how you define your Langevin model with respect to fluctuation-dissipation relations:
  - is the physics modelled correctly in view of internal/external noise?
  - important consequences for (transient) fluctuation relation and the 2nd law

open questions:

- Langevin modeling for stochastic climate dynamics?
- Fluctuation Relations for climate dynamics?

References

- **A.V.Chechkin, F.Lenz, RK, J. Stat. Mech. L11001 (2012)**
- N.Watkins, R.Klages, D.Stainforth, S.Chapman, A.V.Chechkin (in preparation)