Population dynamics method for rare events: systematic errors & feedback control

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ICTS Bangalore — 5 September 2017
Why studying rare events?

2003 heat wave, Europe [Terra MODIS]
Why studying rare events?

[Anomaly for 1-month average] 2003 heat wave, Europe [Terra MODIS]
Why studying rare events?

2010 heat wave in Western Russia [Dole et al., 2011]
Introduction

Motivations

Why studying rare events?

\[ t_{\text{max}} = 40 \text{ days} \]

\[ \frac{1}{t_{\text{max}}} \int_0^{t_{\text{max}}} dt \Delta T(t) > 2^{\circ}C \Rightarrow \text{« Teleconnection patterns »} \quad [\text{Bouchet et al.}] \]
Why studying rare events?

Questions for physicists and mathematicians:
- Probability and \textit{dynamics} of rare events?
- How to \textit{sample} these in numerical modelisation?
- Numerical \textit{tools and methods} to understand their formation?

Evolution of the return time of the monthly averaged temperature

\[
\int_{t_{\text{max}}}^{\infty} T(t) \, dt
\]

\cite{Otto et al., 2012}
Why studying rare events?

Questions for physicists and mathematicians:

- Probability and **dynamics** of rare events?
- How to **sample** these in numerical modelisation?
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Evolution of the return time of the monthly averaged temperature

\[
\frac{1}{t_{\text{max}}} \int_{0}^{t_{\text{max}}} dt \ T(t)
\]

\[\leftrightarrow \] anthropogenic impact on climate?

[Otto et al., 2012]
Distribution of a time-extensive observable $K$ on $[0, t]$.

$\text{Prob}[K, t] \sim e^{t \varphi(K/t)}$
Distribution of a time-extensive observable $K$ on $[0, t]$

$$\text{Prob}[K, t] \sim e^{t \varphi(K/t)}$$
s-modified dynamics

- Markov processes:

\[ \partial_t P(C, t) = \sum_{C'} \left\{ \underbrace{W(C' \to C) P(C', t)}_{\text{gain term}} - \underbrace{W(C \to C') P(C, t)}_{\text{loss term}} \right\} \]

Configs. \( C \), jump rates \( W(C \to C') \)
s-modified dynamics \[ K = \text{activity} = \#\text{events} \]

- Markov processes: 
  \[
  \partial_t P(C, t) = \sum_{C'} \left\{ W(C' \rightarrow C) P(C', t) - W(C \rightarrow C') P(C, t) \right\}
  \]
  \[\text{gain term}\]
  \[\text{loss term}\]

- More detailed dynamics for \( P(C, K, t) \): 
  \[
  \partial_t P(C, K, t) = \sum_{C'} \left\{ W(C' \rightarrow C) P(C', K-1, t) - W(C \rightarrow C') P(C, K, t) \right\}
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\[ K = \text{activity} = \#\text{events} \]

- **Markov processes:**

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\frac{\partial}{\partial t} P(C, t) = \sum_{C'} \left\{ W(C' \rightarrow C) P(C', t) - W(C \rightarrow C') P(C, t) \right\}
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  - Gain term
  - Loss term

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\]

- **Canonical description:** \( s \) conjugated to \( K \)

\[
\hat{P}(C, s, t) = \sum_{K} e^{-sK} P(C, K, t)
\]
\[ s \text{-modified dynamics} \]

\[ K = \text{activity} = \# \text{events} \]

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- \( s \)-modified dynamics [probability non-conserving]
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**s-modified dynamics**

\[ \mathbf{K} = k_{C_0}c_{-1} + k_{C_1}c_2 + \ldots \]

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  \]
Evaluation of large deviation functions \[ \text{[à la “Diffusion Monte-Carlo”]} \]

\[
\sum_C \hat{P}(C, s, t) = \langle e^{-sK} \rangle \sim e^{t\psi(s)}
\]

- discrete time: Giardinà, Kurchan, Peliti [PRL 96, 120603 (2006)]
- continuous time: VL, Tailleur [JSTAT P03004 (2007)]

Cloning dynamics

\[
\partial_t \hat{P}(C, s) = \sum_{C'} W_s(C' \rightarrow C) \hat{P}(C', s) - r_s(C) \hat{P}(C, s) + \delta r_s(C) \hat{P}(C, s)
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- modified dynamics
- cloning term

\[
W_s(C' \rightarrow C) = e^{-s}W(C' \rightarrow C)
\]

\[
r_s(C) = \sum_{C'} W_s(C \rightarrow C')
\]

\[
r(C) = \sum_{C'} W(C \rightarrow C')
\]

\[
\delta r_s(C) = r_s(C) - r(C)
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Evaluation of large deviation functions \([\text{à la “Diffusion Monte-Carlo”}]\]

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Explicit construction

\[ \partial_t \hat{P}(C, s) = \sum_{C'} W_{s}(C' \rightarrow C) \hat{P}(C', s) - r_s(C) \hat{P}(C, s) + \delta r_s(C) \hat{P}(C, s) \]

How to take into account loss/gain of probability?

- handle a large number of copies of the system
- implement a selection rule: on a time interval \( \Delta t \) a copy in config \( C \) is replaced by \( e^{\Delta t \delta r_s(C)} \) copies
- \( \psi(s) = \) the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning
Explicit construction

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- **modified dynamics**
- **cloning term**

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**Biological interpretation**

- Copy in configuration $C \equiv$ organism of genome $C$
- Dynamics of rates $W_s \equiv$ mutations
- Cloning at rates $\delta r_s \equiv$ selection rendering typical the rare histories
An example: 4 copies, 1 degree of freedom $\mathcal{C} = x \in \mathbb{R}$
How to perform averages? (i) [spectral analysis]

☆ Final-time distribution: *proportion* of copies in $C$ at $t$

\[
\langle N_{nc}(t) \rangle_s
\]
\[
\langle N_{nc}(C, t) \rangle_s
\]
\[
p_{\text{end}}(C, t) = \frac{\langle N_{nc}(C, t) \rangle_s}{\langle N_{nc}(t) \rangle_s}
\]

$[N_{nc} = \text{number in non-constant population dynamics}]$
How to perform averages? (i) [spectral analysis]

\[ \partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle \]

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\([N_{nc} = \text{number in non-constant population dynamics}]\)
How to perform averages? (i) \[ \partial_t \hat{P} = \mathcal{W}_s \hat{P} \]  
\[ \mathcal{W}_s |R\rangle = \psi(s) |R\rangle \]
\[ \langle L | \mathcal{W}_s = \psi(s) \langle L | \]
\[ [ \langle L | = \langle - | \quad @ s = 0 \quad ] \]

* Final-time distribution: *proportion* of copies in \( C \) at \( t \)

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\[ \langle N_{nc}(C, t) \rangle_s \]

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[\( N_{nc} = \) number in non-constant population dynamics]
How to perform averages? (i) [spectral analysis]

$$\partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle$$

$$\mathbb{W}_s |\mathbf{R}\rangle = \psi(s) |\mathbf{R}\rangle$$

$$e^{t\mathbb{W}_s} \sim e^{t\psi(s)} |\mathbf{R}\rangle \langle \mathbf{L}|$$

$$\langle \mathbf{L}| \mathbb{W}_s = \psi(s) \langle \mathbf{L}|$$

$$[ \langle \mathbf{L}| = \langle -| \text{ @ } s = 0 ]$$

**Final-time distribution:** *proportion* of copies in $\mathcal{C}$ at $t$

$$\langle N_{nc}(t) \rangle_s$$

$$\langle N_{nc}(\mathcal{C}, t) \rangle_s$$

$$p_{\text{end}}(\mathcal{C}, t) = \frac{\langle N_{nc}(\mathcal{C}, t) \rangle_s}{\langle N_{nc}(t) \rangle_s}$$

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\[ \partial_t \hat{P} = \mathbb{W}_s \hat{P} \]

\[ \mathbb{W}_s | R \rangle = \psi(s) | R \rangle \]

\[ e^{t\mathbb{W}_s} \sim e^{t\psi(s)} | R \rangle \langle L | \]

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★ Final-time distribution: proportion of copies in \( C \) at \( t \)

\[ \langle N_{nc} (t) \rangle_s = \langle - | e^{t\mathbb{W}_s} | P_i \rangle N_0 \sim e^{t\psi(s)} \langle L | P_i \rangle N_0 \]

\[ \langle N_{nc} (C, t) \rangle_s = \langle C | e^{t\mathbb{W}_s} | P_i \rangle N_0 \sim e^{t\psi(s)} \langle C | R \rangle \langle L | P_i \rangle N_0 \]

\[ p_{\text{end}} (C, t) = \frac{\langle N_{nc} (C, t) \rangle_s}{\langle N_{nc} (t) \rangle_s} \sim \langle C | R \rangle \equiv p_{\text{end}} (C) \]

[\( N_{nc} = \) number in non-constant population dynamics]

Final-time distribution governed by right eigenvector.
An example: 4 copies, 1 degree of freedom $C = x \in \mathbb{R}$
How to perform averages? (ii) Intermediate times

\[ \partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle \]

\[ e^{t\mathbb{W}_s} \sim e^{t\psi(s)} |R\rangle \langle L| \]

\[ \langle L | \mathbb{W}_s = \psi(s) \langle L | \]

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★ Mid-time distribution: proportion of copies in \( C \) at \( t_1 \ll t \)

\[ \langle N_{nc}(t) \rangle_s \]

\[ \langle N_{nc}(t|C, t_1) \rangle_s \]

\[ p(t|C, t_1) = \frac{\langle N_{nc}(t|C, t_1) \rangle_s}{\langle N_{nc}(t) \rangle_s} \]
How to perform averages? (ii) Intermediate times

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\partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle
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★ Mid-time distribution: proportion of copies in \(C\) at \(t_1 \ll t\)

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\langle N_{nc}(t) \rangle_s = \langle - | e^{t\mathbb{W}_s} |P_i\rangle N_0 \sim e^{t\psi(s)} \langle L |P_i\rangle N_0
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\[
\langle N_{nc}(t|C, t_1) \rangle_s = \langle - | e^{(t-t_1)\mathbb{W}_s} |C\rangle \langle C| e^{t_1\mathbb{W}_s} |P_i\rangle N_0 \sim e^{t\psi(s)} \langle L|C\rangle \langle C|R\rangle \langle L |P_i\rangle N_0
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\[
p(t|C, t_1) = \frac{\langle N_{nc}(t|C, t_1) \rangle_s}{\langle N_{nc}(t) \rangle_s} \sim \langle L|C\rangle \langle C|R\rangle \equiv p_{ave}(C)
\]
How to perform averages? (ii) Intermediate times

\[
\begin{align*}
\partial_t \langle \hat{P} \rangle &= \mathbb{W}_s \langle \hat{P} \rangle \\
\mathbb{W}_s | R \rangle &= \psi(s) | R \rangle \\
e^{t \mathbb{W}_s} &\sim e^{t \psi(s)} | R \rangle \langle L | \\
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\begin{align*}
\langle N_{nc}(t) \rangle &= \langle - | e^{t \mathbb{W}_s} | P_i \rangle N_0 \\
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\end{align*}
\]

Mid-time distribution governed by \textit{left} and \textit{right} eigenvectors.
An example: 4 copies, 1 degree of freedom $C = x \in \mathbb{R}$
How to perform averages?

- Mid-time ancestor distribution:
  
  fraction of copies (at time $t_1$) which were in configuration $C$, knowing that there are in configuration $C_f$ at final time $t_f$:
  
  $$p_{anc}(C, t_1; C_f, t_f) = \frac{\langle N_{nc}(C_f, t_f|C, t_1) \rangle_s}{\sum_{C'} \langle N_{nc}(C_f, t_f|C', t_1) \rangle_s} \sim_{t_{f,1} \to \infty} \langle L|C\rangle \langle C|R \rangle = p_{ave}(C)$$

  The “ancestor statistics” of a configuration $C_f$ is thus independent (far enough in the past) of the configuration $C_f$. 
Example distributions for a simple Langevin dynamics

final-time: \( p_{\text{end}}(x) \)

intermediate-time: \( p_{\text{ave}}(x) \)
The small-noise crisis: systematic errors grow as $\epsilon \to 0$

Cause: as $\epsilon \to 0$, $p_{\text{ave}}(x)$ & $p_{\text{end}}(x)$ → sharply peaked at different points i.e. the clones do not attack sample correctly the phase space
How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics:  
- Probability preserving
- No mismatch between $p_{\text{ave}}$ and $p_{\text{end}}$
- Constructed as

$$W_s^{\text{aux}} = LW_sL^{-1} - \psi(s)1$$
How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics: [Maes, Jack&Sollich, Touchette&Chetrite]

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- No mismatch between $p_{\text{ave}}$ and $p_{\text{end}}$
- Constructed as

$$W_s^{\text{aux}} = LW_sL^{-1} - \psi(s)1$$

Issue: determining $L$ is difficult
Solution: evaluate $L$ as $L_{\text{test}}$ on the fly and simulate $W_{\text{test}}s = L_{\text{test}}W_sL_{\text{test}}^{-1}$.

Iterate. [For any $L_{\text{test}}$, the simulation is in principle correct.]

Similar in spirit to multi-canonical (e.g. Wang-Landau) approaches in static thermodynamics. [Here, one flattens the left-eigenvector of $W_{\text{test}}s$.]
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Similar in spirit to **multi-canonical** (e.g. Wang-Landau) approaches in static thermodynamics. [Here, one flattens the left-eigenvector of $W^\text{test}_s$.]
Improvement of the small-noise crisis (i.i)

Physical insight: probability loss transformed into *effective forces*. 
Improvement of the small-noise crisis (i.ii)

Much more efficient evaluation of the biased distribution.
Even for a very crude (polynomial) approximation of the effective force.
Improvement of the small-noise crisis (ii)

Interacting system in 1D.
Effective force: 1-, 2-, 3- body interactions only [also crude approx.].
## Summary and open questions (1)

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Summary and open questions (1)

Multicanonical approach [with F Bouchet, R Jack, T Nemoto]
- Sampling problem (depletion of ancestors)
- On-the-fly evaluated auxiliary dynamics
- Solution to the small-noise crisis
- Systems with large number of degrees of freedom

Finite-population effects [with E Guevara, T Nemoto]
- Quantitative finite-$N_{\text{clones}}$ scaling $\rightarrow$ interpolation method
- Initial transient regime due to small population
- Analogy with biology: many small islands vs. few large islands?
- Question: effective forces $\leftrightarrow$ selection?
Open question (2): why is it working?

Improvement of the depletion-of-ancestors problem:

Dashed line: lower noise  Continuous line: higher noise
Thanks for your attention!

References:

- *Population dynamics method with a multi-canonical feedback control*
  Takahiro Nemoto, Freddy Bouchet, Robert L. Jack and Vivien Lecomte
  PRE 93 062123 (2016)

- *Finite-time and finite-size scalings in the evaluation of large deviation functions: Analytical study using a birth-death process*
  Takahiro Nemoto, Esteban Guevara Hidalgo and Vivien Lecomte
  PRE 95 012102 (2017)

- *Finite-size scaling of a first-order dynamical phase transition: adaptive population dynamics and effective model*
  Takahiro Nemoto, Robert L. Jack and Vivien Lecomte
  PRL 118 115702 (2017)
Supplementary material
\[ \text{Prob}[K] \sim e^{t \varphi(K/t)} \]
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Finite-time & -size scalings matter.

\[ \text{Prob}[K] \sim e^{t \varphi(K/t)} \]
[Merolle, Garrahan and Chandler, 2005]
Exponential divergence of the susceptibility
Explicit construction (1/3)

Supplementary material

Vivien Lecomte (LPMA & LIPhy)

Explicit construction

Probability-preserving contribution

$$\partial_t \hat{P}(C, t) = \sum_{C'} \left\{ W_s(C' \to C) \hat{P}(C', t) - W_s(C \to C') \hat{P}(C, t) \right\}$$

- gain term
- loss term
Explicit construction (1/3)

Which configurations will be visited?

Configurational part of the trajectory: $C_0 \rightarrow \ldots \rightarrow C_K$

$$\text{Prob}\{\text{hist}\} = \prod_{n=0}^{K-1} \frac{W_s(C_n \rightarrow C_{n+1})}{r_s(C_n)}$$

where

$$r_s(C) = \sum_{C'} W_s(C \rightarrow C')$$
When shall the system jump from one configuration to the next one?

- Probability density for the time interval $t_n - t_{n-1}$

$$r_s(C_{n-1})e^{-(t_n-t_{n-1})r_s(C_{n-1})}$$
Explicit construction (2/3)

When shall the system jump from one configuration to the next one?

- probability density for the time interval $t_n - t_{n-1}$
  
  $$r_s(C_{n-1})e^{-(t_n-t_{n-1})r_s(C_{n-1})}$$

- probability not to leave $C_K$ during the time interval $t - t_K$
  
  $$e^{-(t-t_K)r_s(C_K)}$$
Explicit construction (3/3)

\[
\partial_t \hat{P}(C, s) = \sum_{C'} W_s(C' \to C) \hat{P}(C', s) - r_s(C) \hat{P}(C, s) + \delta r_s(C) \hat{P}(C, s)
\]

- **modified dynamics**
- **cloning term**

How to take into account loss/gain of probability?

- handle a large number of copies of the system
- implement a **selection** rule: on a time interval \(\Delta t\) a copy in config \(C\) is replaced by \(e^{\Delta t \delta r_s(C)}\) copies
- \(\psi(s)\) = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning
 Explicit construction (3/3)

\[ \partial_t \hat{P}(C, s) = \sum_{C'} W_{s}(C' \rightarrow C) \hat{P}(C', s) - r_s(C) \hat{P}(C, s) + \delta r_s(C) \hat{P}(C, s) \]

- modified dynamics
- cloning term

How to take into account loss/gain of probability?

- handle a large number of copies of the system
- implement a selection rule: on a time interval \( \Delta t \) a copy in config \( C \) is replaced by \( \lfloor e^{\Delta t \delta r_s(C)} + \epsilon \rfloor \) copies, \( \epsilon \sim [0, 1] \)
- \( \psi(s) \) = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning
Explicit construction (3/3)

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\frac{\partial_t \hat{P}(C, s)}{\partial t} = \sum_{C'} W_s(C' \to C) \hat{P}(C', s) - r_s(C) \hat{P}(C, s) + \delta r_s(C) \hat{P}(C, s)
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- modified dynamics
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Biological interpretation

- copy in configuration \( C \equiv \) organism of genome \( C \)
- dynamics of rates \( W_s \equiv \) mutations
- cloning at rates \( \delta r_s \equiv \) selection rendering atypical histories typical