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

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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]
Why studying rare events?

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

$\Delta T(t) > 2^\circ C$
Why studying rare events?

Questions for physicists and mathematicians:

- Probability and **dynamics** of rare events?
- How to **sample** these in numerical modelisations?
- Numerical **tools and methods** to understand their formation?
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Questions for physicists and mathematicians:
- Probability and **dynamics** of rare events?
- How to **sample** these in numerical modelisations?
- Numerical **tools and methods** to understand their formation?

Evolution of the return time of the monthly averaged temperature

\[
\frac{1}{t_{\text{max}}} \int_0^{t_{\text{max}}} dt \, T(t)
\]

Due anthropogenic impact on climate?

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

$$\frac{1}{t} \log \text{Prob}(K/t)$$

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

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

Markov processes:

$$\partial_t P(C, t) = \sum_{C'} \left\{ \underbrace{W(C' \rightarrow C) P(C', t)}_{\text{gain term}} - \underbrace{W(C \rightarrow C') P(C, t)}_{\text{loss term}} \right\}$$
s-modified dynamics

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

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

- More detailed dynamics for \( P(C, K, t) \):
  \[
  \frac{\partial}{\partial t} P(C, K, t) = \sum_{C'} \left\{ W(C' \rightarrow C) P(C', K-1, t) - W(C \rightarrow C') P(C, K, t) \right\}
  \]
s-modified dynamics

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  \[ \text{gain term} \quad \text{loss term} \]

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- Canonical description: \( s \) conjugated to \( K \)
  \[ \hat{P}(C, s, t) = \sum_K e^{-s^K} P(C, K, t) \]
s-modified dynamics \( K = \text{activity} = \#\text{events} \)

- Markov processes:
  \[
  \partial_t P(C, t) = \sum_{C'} \left\{ W(C' \rightarrow C) P(C', t) - W(C \rightarrow C') P(C, t) \right\}
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  \hat{P}(C, s, t) = \sum_{K} e^{-sK} P(C, K, t)
  \]

- s-modified dynamics [probability non-conserving]
  \[
  \partial_t \hat{P}(C, s, t) = \sum_{C'} \left\{ e^{-s} W(C' \rightarrow C) \hat{P}(C', s, t) - W(C \rightarrow C') \hat{P}(C, s, t) \right\}
  \]
s-modified dynamics

\[ K = k_{C_0} C_1 + k_{C_1} C_2 + \ldots \]

- 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\}
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- More detailed dynamics for \( P(C, K, t) \):
  \[
  \partial_t P(C, K, t) = \sum_{C'} \left\{ W(C' \to C) P(C', K - k_{C'C}, t) - W(C \to C') P(C, K, t) \right\}
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  \]
Evaluation of large deviation functions \[ à la "Diffusion Monte-Carlo" \]

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

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

Cloning dynamics

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

- \( W_s(\mathcal{C}' \to \mathcal{C}) = e^{-sW(\mathcal{C}' \to \mathcal{C})} \)
- \( r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C} \to \mathcal{C}') \)
- \( \delta r_s(\mathcal{C}) = r_s(\mathcal{C}) - r(\mathcal{C}) \)
Evaluation of large deviation functions

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- modified dynamics
- cloning term

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

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

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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)
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- 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
- optionally: keep population constant by non-biased pruning/cloning

\( \psi(s) \) = the rate of exponential growth/decay of the total population
Explicit construction

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

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- handle a large number of copies of the system
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Explicit construction

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\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

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\( s = \) the rate of exponential growth/decay of the total population

Vivien Lecomte (LPMA & LIPhy)
Population dynamics

Explicit construction

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\]

**Biological interpretation**

- copy in configuration \( C \equiv \text{organism of genome } C \)
- dynamics of rates \( W_s \equiv \text{mutations} \)
- cloning at rates \( \delta r_s \equiv \text{selection} \) rendering atypical histories typical
An example: 4 copies, 1 degree of freedom $C = x \in \mathbb{R}$
Final-time distribution: *proportion* of copies in $C$ at $t$

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

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

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

$[N_{nc}$ = number in non-constant population dynamics]
**Final-time distribution:** proportion of copies in $C$ at $t$

$$\langle N_{nc}(C, t) \rangle_s = \langle N_{nc}(t) \rangle_s \langle C|R \rangle \langle L_j P_i |N_0 \rangle$$

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

[$N_{nc}$ = number in non-constant population dynamics]
How to perform averages? (i) [with R Jack, F Bouchet, T Nemoto]

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

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

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

\[ [ \langle L | = \langle - | @ s = 0 ] \]

Final-time distribution: \textit{proportion} of copies in \textit{C} at \textit{t}

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

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

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

\[ \left[ \langle L| = \langle -| \quad @ s = 0 \right] \]

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

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Population dynamics

Questions

How to perform averages? (i)

[with R Jack, F Bouchet, T Nemoto]

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

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

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

\[ \left[ \langle L| = \langle -| \quad @ \quad s = 0 \right] \]

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

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

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

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

Final-time distribution governed by right eigenvector.

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

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

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

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

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

\[ \left[ \begin{array}{c}
\langle L| = \langle - | \quad @ s = 0 \\
\end{array} \right. \]

\begin{align*}
\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}
\end{align*}

Mid-time distribution: proportion of copies in $C$ at $t_1 \ll t$
How to perform averages? (ii) Intermediate times

\[
\partial_t \hat{P} = \mathbb{W}_s \hat{P} \\
\lim_{t \to \infty} e^{t \mathbb{W}_s} = e^{t \psi(s)} |R\rangle \langle L|
\]

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

\[ \langle L | = (-| @ s = 0 \]

\[ \left[ \begin{array}{c}
\langle N_{nc}(t) \rangle_s = \langle - | e^{t \mathbb{W}_s} | P_i \rangle N_0 \\
\langle N_{nc}(t|C, t_1) \rangle_s = \langle - | e^{(t-t_1) \mathbb{W}_s} | C \rangle \langle C| e^{t_1 \mathbb{W}_s} | P_i \rangle N_0 \sim e^{t \psi(s)} \langle L|C\rangle \langle C|R\rangle \langle L|P_i\rangle N_0
\end{array} \right]
\]

\[
p(t|C, t_1) = \frac{\langle N_{nc}(t|C, t_1) \rangle_s}{\langle N_{nc}(t) \rangle_s} \quad t \to \infty \quad \langle L|C\rangle \langle C|R\rangle \equiv p_{\text{ave}}(C)
\]

\[
\text{Mid-time distribution: proportion of copies in } C \text{ at } t_1 \ll t
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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 \( \mathcal{C} \) 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 \text{ } \underset{t \to \infty}{\sim} \text{ } e^{t\psi(s)} \langle L|P_i\rangle N_0 \\
\langle N_{nc}(t|\mathcal{C}, t_1) \rangle_s = \langle - | e^{(t-t_1)\mathbb{W}_s} |\mathcal{C}\rangle \langle \mathcal{C}| e^{t_1\mathbb{W}_s} |P_i\rangle N_0 \sim e^{t\psi(s)} \langle L|\mathcal{C}\rangle \langle \mathcal{C}|R\rangle \langle L|P_i\rangle N_0 \\
p(t|\mathcal{C}, t_1) = \langle N_{nc}(t|\mathcal{C}, t_1) \rangle_s \text{ } \underset{t \to \infty}{\sim} \text{ } \langle L|\mathcal{C}\rangle \langle \mathcal{C}|R\rangle \equiv p_{\text{ave}}(\mathcal{C})
\]

Mid-time distribution governed by **left** and **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 $t_f$:

$$p_{\text{anc}}(C, t_1; C_f, t_f) = \frac{\langle N_{nc}(C_f, t_f|C, t_1) \rangle_s}{\sum_{C'} \langle N_{nc}(C_f, t_f|C', t_1) \rangle_s} \quad \text{as} \quad t_{f,1} \to \infty$$

The “ancestor statistics” of a configuration $C_f$ is thus independent (far enough in the past) of the configuration $C_f$. 

$$\langle L|C\rangle \langle C|R \rangle = p_{\text{ave}}(C)$$
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: [Maes, Jack & Sollich, Touchette & Chetrite]

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

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

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

Whichever $L_{\text{test}}$, the simulation is still correct.

Iterate

Similar in spirit to multi-canonical (e.g. Wang-Landau) approach in static thermodynamics
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    \[ W_s^{\text{aux}} = L W_s L^{-1} - \psi(s) 1 \]
  - Issue: determining $L$ is difficult
  - Solution: evaluate $L$ as $L_{\text{test}}$ on the fly and simulate
    \[ W_s^{\text{test}} = L_{\text{test}} W_s L_{\text{test}}^{-1} \]
  - Whichever $L_{\text{test}}$, the simulation is still correct. Iterate
How to make mid- and final-time distribution closer?

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- Issue: determining $L$ is difficult
- Solution: evaluate $L$ as $L_{\text{test}}$ on the fly and simulate

$$W_{s}^{\text{test}} = L_{\text{test}}W_{s}L_{\text{test}}^{-1}$$

- Whichever $L_{\text{test}}$, the simulation is still correct. **Iterate**

Similar in spirit to **multi-canonical** (e.g. Wang-Landau) approach in static thermodynamics
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 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
Summary and questions (1)

Multicanonical approach [with F Bouchet, R Jack, T Nemoto]
- Sampling problem (depletion of ancestors)
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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?
Questions (2): why is it working?

Improvement of the depletion-of-ancestors problem:

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

\[ \text{Prob}[K] \sim e^{t \varphi(K/t)} \]
\[
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\]
$\frac{1}{t} \log \text{Prob}(K/t) \sim e^{t \varphi(K/t)}$
$\text{Prob}[K] \sim e^{t\varphi(K/t)}$

Finite-time & -size scalings matter.
[Merrolle, Garrahan and Chandler, 2005]
Conclusion

Exponential divergence of the susceptibility
Explicit construction (1/3)

Conclusion

Explicit construction

Probability-preserving contribution

\[ \partial_t \hat{P}(C, t) = \sum_{C'} \left\{ W_s(C' \rightarrow C) \hat{P}(C', t) - W_s(C \rightarrow C') \hat{P}(C, t) \right\} \]

\[ \text{gain term} \quad \text{loss term} \]

Vivien Lecomte (LPMA & LIPhy)
Explicit construction (1/3)

Which configurations will be visited?

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

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

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 $t_n - t_{n-1}$

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Explicit construction (2/3)

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  \]

- 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)

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

- **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 \( e^{\Delta t \delta r_s(C)} \) copies
- \( \psi(s) \) = the rate of exponential growth/decay of the total population
- **optionally:** keep population constant by non-biased pruning/cloning
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modified dynamics

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**How to take into account loss/gain of probability?**

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Vivien Lecomte (LPMA & LIPhy)
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Where the terms are:
- Modified dynamics
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How to take into account loss/gain of probability?
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- 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, $\epsilon \sim [0, 1]$
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Vivien Lecomte (LPMA & LIPhy)
**Conclusion**

**Explicit construction (3/3)**

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

- **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