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Small eigenvalues and mean transition times for irreversible diffusions

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Motivation: Two coupled oscillators

Synchronization of two coupled oscillators

First observed by Huygens; see e.g. [Pikovsky, Rosenblum, Kurths 2001]

Motion of pendulums $x_i = (\theta_i, \dot{\theta}_i)$

$$\begin{cases} \dot{x}_1 = f_1(x_1) \\ \dot{x}_2 = f_2(x_2) \end{cases}$$

For a good parametrisation ϕ_i of the limit cycles

$$\begin{cases} \dot{\phi}_1 = \omega_1 \\ \dot{\phi}_2 = \omega_2 \end{cases}$$

where ω_i denotes the natural frequencies

Synchronization of two coupled oscillators

First observed by Huygens; see e.g. [Pikovsky, Rosenblum, Kurths 2001]

Motion of pendulums $x_i = (\theta_i, \dot{\theta}_i)$ with coupling

$$\begin{cases} \dot{x}_1 = f_1(x_1) + \varepsilon h_1(x_1, x_2) \\ \dot{x}_2 = f_2(x_2) + \varepsilon h_2(x_1, x_2) \end{cases}$$

For a good parametrisation ϕ_i of the limit cycles

$$\begin{cases} \dot{\phi}_1 = \omega_1 + \varepsilon g_1(x_1, x_2) \\ \dot{\phi}_2 = \omega_2 + \varepsilon g_2(x_1, x_2) \end{cases}$$

where ω_i denotes the natural frequencies

Coupled oscillators with slightly different frequencies

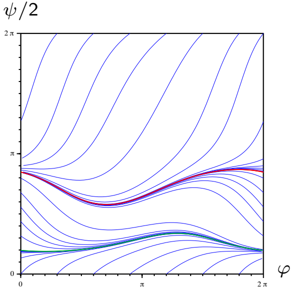
$$\begin{cases}\psi = \phi_1 - \phi_2 \\ \varphi = \frac{\phi_1+\phi_2}{2}\end{cases} \implies \begin{cases}\dot\psi = -\nu + \varepsilon \boldsymbol{q}(\psi,\varphi) & \text{with } \nu = \omega_2 - \omega_1 \\ \dot\varphi = \omega + \mathcal{O}(\varepsilon) & \text{with } \omega = \frac{\omega_1+\omega_2}{2}\end{cases}$$

Assume

- Detuning $\nu = \omega_2 - \omega_1$ small
- Coupling strength $\varepsilon \geqslant \varepsilon_0$

Observation

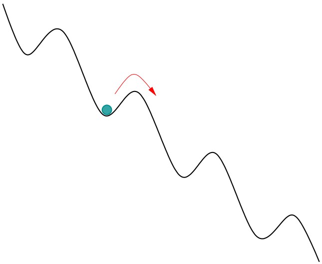
- Synchronization



Coupled oscillators subject to noise

Averaging

$$\omega \frac{d\psi}{d\varphi} \simeq -\nu + \varepsilon \bar{q}(\psi)$$



Adler equation (special choice of coupling)

$$\bar{q}(\psi) = \sin \psi$$

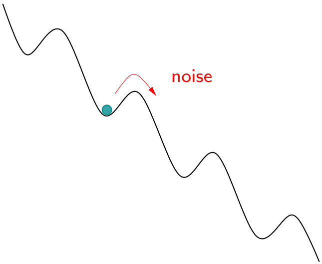
Observations

- Fixed points at $\sin \psi = \frac{\nu}{\varepsilon}$
- Synchronization

Coupled oscillators subject to noise

Averaging

$$\omega \frac{\mathrm{d}\psi}{\mathrm{d}\varphi} \simeq -\nu + \varepsilon \bar{q}(\psi) + \text{noise}$$



Adler equation (special choice of coupling)

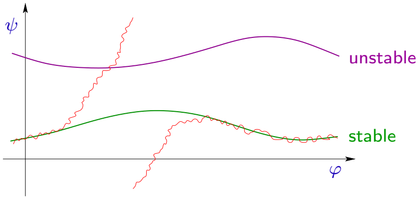
$$\bar{q}(\psi) = \sin\psi$$

Observations

- Fixed points at $\sin\psi = \frac{\nu}{\varepsilon}$
- Synchronization
- In the presence of noise: occasional transitions ($\rightarrow$ phase slips)

Without averaging

$$\begin{cases} \dot{\psi} = -\nu + \varepsilon \boldsymbol{q}(\psi, \varphi) + \text{noise} \\ \dot{\varphi} = \omega + \mathcal{O}(\varepsilon) + \text{noise} \end{cases}$$



Observations

- Synchronization
- In the presence of noise: occasional transitions ($\rightarrow$ phase slips)
- Phase slips correspond to passage through unstable orbit

Question

- Distribution of phase φ when crossing unstable periodic orbit?

To tackle

- Stochastic exit problem

Exit problem:
Wentzell–Freidlin theory and beyond

Transition probabilities and generators

$$\mathrm{d}x_t = f(x_t)\,\mathrm{d}t + \sigma g(x_t)\,\mathrm{d}W_t\;, \qquad x \in \mathbb{R}^n$$

- Transition probability density $p_t(x,y)$
- Markov semigroup T_t: For measurable $\varphi \in L^\infty$,

$$(T_t\varphi)(x) = \mathbb{E}^x\{\varphi(x_t)\} = \int p_t(x,y)\varphi(y)\,\mathrm{d}y$$

- Infinitesimal generator $L\varphi = \frac{\mathrm{d}}{\mathrm{d}t} T_t\varphi|_{t=0}$ of the diffusion:

$$(L\varphi)(x) = \sum_i f_i(x)\frac{\partial\varphi}{\partial x_i} + \frac{\sigma^2}{2}\sum_{i,j}(gg^T)_{ij}(x)\frac{\partial^2\varphi}{\partial x_i \partial x_j}$$

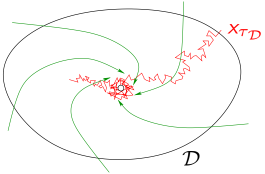
- Adjoint semigroup: For probability measures μ

$$(\mu T_t)(y) = \mathbb{P}^\mu\{x_t = \mathrm{d}y\} = \int p_t(x,y)\,\mu(\mathrm{d}x)$$

with generator L^*

Stochastic exit problem

- $\mathcal{D} \subset \mathbb{R}^n$ bounded domain
- First-exit time $\tau_{\mathcal{D}} = \inf\{t > 0 \colon x_t \notin \mathcal{D}\}$
- First-exit location $x_{\tau_{\mathcal{D}}} \in \partial\mathcal{D}$
- Harmonic measure $\mu(A) = \mathbb{P}^x\{x_{\tau_{\mathcal{D}}} \in A\}$



Facts (following from Dynkin's formula – see textbooks on stochastic analysis)

- $u(x) = \mathbb{E}^x\{\tau_{\mathcal{D}}\}$ satisfies

$$\begin{cases} Lu(x) = -1 & \text{for } x \in \mathcal{D} \\ u(x) = 0 & \text{for } x \in \partial\mathcal{D} \end{cases}$$

- For $\varphi \in L^\infty(\partial\mathcal{D}, \mathbb{R})$, $h(x) = \mathbb{E}^x\{\varphi(x_{\tau_{\mathcal{D}}})\}$ satisfies

$$\begin{cases} Lh(x) = 0 & \text{for } x \in \mathcal{D} \\ h(x) = \varphi(x) & \text{for } x \in \partial\mathcal{D} \end{cases}$$

Wentzell–Freidlin theory

$$\mathrm{d}x_t = f(x_t)\,\mathrm{d}t + \sigma g(x_t)\,\mathrm{d}W_t \;, \qquad x \in \mathbb{R}^n$$

▷ Large-deviation rate function / action funtional

$$I(\gamma) = \frac{1}{2}\int_0^T [\dot\gamma_t - f(\gamma_t)]^T D(\gamma_t)^{-1}[\dot\gamma_t - f(\gamma_t)]\,\mathrm{d}t \;, \qquad \text{where } D = gg^T$$

▷ Large-deviation principle: For a set Γ of paths $\gamma : [0, T] \to \mathbb{R}^n$

$$\mathbb{P}\{(x_t)_{0\leqslant t\leqslant T} \in \Gamma\} \simeq \mathrm{e}^{-\inf_\Gamma I/\sigma^2}$$

Consider first exit from $\mathcal{D}$ contained in basin of attraction of an attractor $\mathcal{A}$

▷ Quasipotential

$$V(y) = \inf\{I(\gamma) \colon \gamma \text{ connects } \mathcal{A} \text{ to } y \text{ in arbitrary time}\} \;, \qquad y \in \partial\mathcal{D}$$

Wentzell–Freidlin theory

$$V(y) = \inf\{I(\gamma)\colon \gamma \text{ connects } \mathcal{A} \text{ to } y \text{ in arbitrary time}\}\,, \qquad y \in \partial\mathcal{D}$$

Facts

- $\lim_{\sigma\to 0} \sigma^2 \log \mathbb{E}\{\tau_{\mathcal{D}}\} = \overline{V} = \inf_{y\in\partial\mathcal{D}} V(y)$ [Wentzell, Freidlin 1969]
- If infimum is attained in a single point $y^* \in \mathcal{D}$ then
  $\lim_{\sigma\to 0} \mathbb{P}\{\|x_{\tau_{\mathcal{D}}} - y^*\| > \delta\} = 0 \quad \forall\delta > 0$ [Wentzell, Freidlin 1969]
- Minimizers of I are optimal transition paths; found from Hamilton equations
- Limiting distribution of $\tau_{\mathcal{D}}$ is exponential
  $\lim_{\sigma\to 0} \mathbb{P}\{\tau_{\mathcal{D}} > s\,\mathbb{E}\{\tau_{\mathcal{D}}\}\} = \mathrm{e}^{-s}$ [Day 1983; Bovier *et al* 2005]

The reversible case

$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sigma\,\mathrm{d}W_t\,, \qquad x \in \mathbb{R}^n$$

- $L = \frac{\sigma^2}{2}\Delta - \nabla V(x)\cdot\nabla = \frac{\sigma^2}{2}\,\mathrm{e}^{2V/\sigma^2}\,\nabla\cdot\mathrm{e}^{-2V/\sigma^2}\,\nabla$ is self-adjoint in $L^2(\mathbb{R}^n, \mathrm{e}^{-2V/\sigma^2}\,\mathrm{d}x)$
- Reversibility (detailed balance): $\mathrm{e}^{-2V(x)/\sigma^2}\,p_t(x,y) = \mathrm{e}^{-2V(y)/\sigma^2}\,p_t(y,x)$

Facts

Assume V has N local minima

- $-L$ has N exponentially small ev's $0 = \lambda_0 < \dots < \lambda_{N-1}$ + spectral gap
- Precise expressions for the λ_i (Kramers' law)
- λ_i^{-1} are the expected transition times between neighbourhoods of minima, $i = 1, \dots, N-1$ (in specific order)

Methods

Large deviations [Wentzell, Freidlin, Sugiura, . . .]; Semiclassical analysis [Mathieu, Miclo, Kolokoltsov, . . .]; Potential theory [Bovier, Gayrard, Eckhoff, Klein]; Witten Laplacian [Helffer, Nier, Le Peutrec, Viterbo]; Two-scale approach, using transport techniques [Menz, Schlichting 2012]

The irreversible case

Irreversible case

If f is *not* of the form $-\nabla V$

- Large-deviation techniques still work, but ...
- L not self-adjoint, analytical approaches harder
- not reversible, standard potential theory does not work

Nevertheless,

- Results exist on the Kramers–Fokker–Planck operator

$$L = \frac{\sigma^2}{2} y \frac{\partial}{\partial x} - \frac{\sigma^2}{2} V'(x) \frac{\partial}{\partial y} + \frac{\gamma}{2} \Big(y - \frac{\sigma^2}{2} \frac{\partial}{\partial y} \Big) \Big(y + \frac{\sigma^2}{2} \frac{\partial}{\partial y} \Big)$$

  [Hérau, Hitrik, Sjöstrand, ...]
- Question

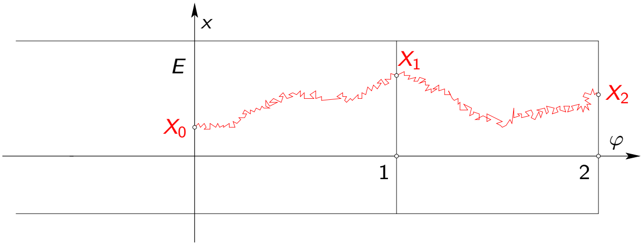
  What is the harmonic measure for the exit through an unstable periodic orbit?

Random Poincaré maps

Near a periodic orbit, in appropriate coordinates

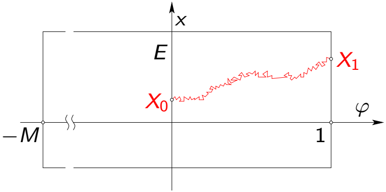
$$\begin{aligned} d\varphi_t &= f(\varphi_t, x_t)\,dt + \sigma F(\varphi_t, x_t)\,dW_t & \varphi &\in \mathbb{R} \\ dx_t &= g(\varphi_t, x_t)\,dt + \sigma G(\varphi_t, x_t)\,dW_t & x &\in E \subset \mathbb{R}^{n-1} \end{aligned}$$

- All functions periodic in φ (e.g. period 1)
- $f \geqslant c > 0$ and σ small $\Rightarrow \varphi_t$ likely to increase
- Process may be killed when x leaves E



Random variables $X_0, X_1, \dots$ form (substochastic) Markov chain

Random Poincaré map and harmonic measures



- First-exit time τ of $z_t = (\varphi_t, x_t)$ from $\mathcal{D} = (-M, 1) \times E$
- $\mu_z(A) = \mathbb{P}^z\{z_\tau \in A\}$ is harmonic measure (w.r.t. generator L)
- μ_z admits (smooth) density $h(z, y)$ w.r.t. arclength on $\partial\mathcal{D}$ (under hypoellipticity condition) [Ben Arous, Kusuoka, Stroock 1984]
- Remark: $Lh(\cdot, y) = 0$ (kernel is harmonic)
- For Borel sets $B \subset E$

$$\mathbb{P}^{X_0}\{X_1 \in B\} = K(X_0, B) := \int_B K(X_0, \mathrm{d}y)$$

where $K(x, \mathrm{d}y) = h((0, x), (1, y))\,\mathrm{d}y =: k(x, y)\,\mathrm{d}y$

Fredholm theory

Consider integral operator K acting

- on L^∞ via $f \mapsto (Kf)(x) = \int_E k(x,y) f(y) \, dy = \mathbb{E}^x\{f(X_1)\}$
- on L^1 via $m \mapsto (mK)(\cdot) = \int_E m(x) k(x,\cdot) \, dx = \mathbb{P}^\mu\{X_1 \in \cdot\}$

[Fredholm 1903]

- If $k \in L^2$, then K has eigenvalues λ_n of finite multiplicity
- Eigenfunctions $Kh_n = \lambda_n h_n$, $h_n^* K = \lambda_n h_n^*$ form a complete ONS

[Perron; Frobenius; Jentzsch 1912; Krein–Rutman 1950; Birkhoff 1957]

- Principal eigenvalue λ_0 is real, simple, $|\lambda_n| < \lambda_0 \quad \forall n \geqslant 1$ and $h_0 > 0$

Spectral decomposition: $k\ (x,y) = \lambda_0 h_0(x) h_0^*(y) + \lambda_1 h_1(x) h_1^*(y) + \dots$

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Spectral decomposition: $\quad k^n(x,y) = \lambda_0^n h_0(x)h_0^*(y) + \lambda_1^n h_1(x)h_1^*(y) + \dots$

Fredholm theory

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Spectral decomposition: $\quad k^n(x,y) = \lambda_0^n h_0(x) h_0^*(y) + \lambda_1^n h_1(x) h_1^*(y) + \dots$

$$\Rightarrow \quad \mathbb{P}^x\{X_n \in \mathrm{d}y | X_n \in E\} = \pi_0(\mathrm{d}y) + \mathcal{O}((|\lambda_1|/\lambda_0)^n)$$

where $\pi_0 = h_0^* \,/ \int_E h_0^*$ is the quasistationary distribution (QSD)

How to estimate the principal eigenvalue ?

- Trivial bounds: $\forall A \subset E$ with Lebesgue$(A) > 0$,

$$\inf_{x \in A} K(x, A) \leqslant \lambda_0 \leqslant \sup_{x \in E} K(x, E)$$

Proof

$$x^* = \text{argmax}\ h_0 \Rightarrow \lambda_0 = \int_E k(x^*, y) \frac{h_0(y)}{h_0(x^*)} \,\mathrm{d}y \leqslant K(x^*, E)$$

$$\lambda_0 \int_A h_0^*(y) \,\mathrm{d}y = \int_E h_0^*(x) K(x, A) \,\mathrm{d}x \geqslant \inf_{x \in A} K(x, A) \int_A h_0^*(y) \,\mathrm{d}y$$

- Donsker–Varadhan-type bound:

$$\lambda_0 \leqslant 1 - \frac{1}{\sup_{x \in E} \mathbb{E}^x\{\tau_\Delta\}} \qquad \text{where} \quad \tau_\Delta = \inf\{n > 0 \colon X_n \notin E\}$$

- Bounds using Laplace transforms (see below)

How to estimate λ_1 ?

Theorem [Birkhoff 1957]
Uniform positivity condition

$$s(x)\nu(A) \leq K(x,A) \leq Ls(x)\nu(A) \qquad \forall x \in E \; \forall A \subset E$$

implies spectral-gap-type estimate

$$|\lambda_1|/\lambda_0 \leq 1 - L^{-2}$$

Localized version
Assume $\exists\, A \subset E$ and $\exists\, m : A \to (0,\infty)$ such that

$$m(y) \leq k(x,y) \leq Lm(y) \qquad \forall x,y \in A$$

Then

$$|\lambda_1| \leq L - 1 + \mathcal{O}\Big(\sup_{x\in E} K(x, E\setminus A)\Big) + \mathcal{O}\Big(\sup_{x\in A}[1 - K(x,E)]\Big)$$

To apply localized version

- For initial conditions $x, y \in A$: $X_n^x - X_n^y$ decreases exponentially fast
- Use Harnack inequality once $X_n^x - X_n^y = \mathcal{O}(\sigma^2)$

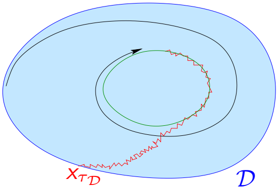
Application:
Exit through an unstable periodic orbit

Exit through an unstable periodic orbit

- Planar SDE

  $$dx_t = f(x_t)\,dt + \sigma g(x_t)\,dW_t$$

- $\mathcal{D} \subset \mathbb{R}^2$: interior of unstable periodic orbit
- First-exit time $\tau_{\mathcal{D}} = \inf\{t > 0 \colon x_t \notin \mathcal{D}\}$



Law of first-exit location $x_{\tau_{\mathcal{D}}} \in \partial\mathcal{D}$?

- Large-deviation principle with rate function

  $$I(\gamma) = \frac{1}{2}\int_0^T [\dot\gamma_t - f(\gamma_t)]^T D(\gamma_t)^{-1}[\dot\gamma_t - f(\gamma_t)]\,dt\,, \qquad \text{where } D = gg^T$$

- Quasipotential

  $$V(y) = \inf\{I(\gamma) \colon \gamma \text{ connects } \mathcal{A} \text{ to } y \text{ in arbitrary time}\}$$

Theorem [Freidlin, Wentzell 1969]
If V attains its min at a unique $y^* \in \partial\mathcal{D}$, then $x_{\tau_{\mathcal{D}}}$ concentrates in y^* as $\sigma \to 0$

Problem: V is constant on $\partial\mathcal{D}$!

Most probable exit paths

Minimizers of I obey Hamilton equations with Hamiltonian

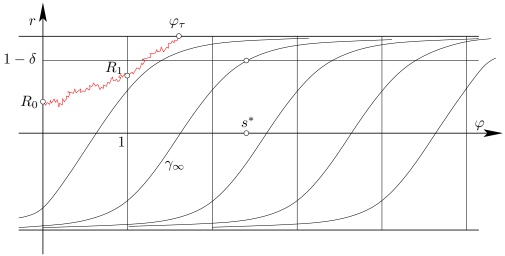
$$H(\gamma,\psi) = \frac{1}{2}\psi^T D(\gamma)\psi + f(\gamma)^T\psi$$

where $\psi = D(\gamma)^{-1}(\dot{\gamma} - f(\gamma))$

Generically optimal path (for infinite time) is isolated

Random Poincaré map

In polar-type coordinates (r, φ)



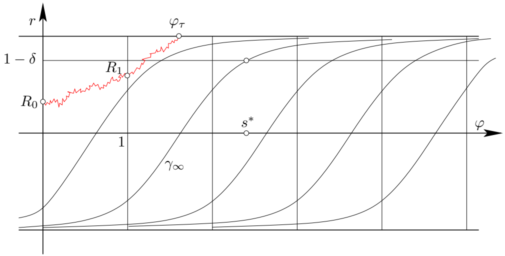
$$\mathbb{P}^{R_0}\{R_n \in A\} = \lambda_0^n h_0(R_0) \int_A h_0^*(y)\,\mathrm{d}y \big[1 + \mathcal{O}((|\lambda_1|/\lambda_0)^n)\big]$$

If $t = n + s$,

$$\mathbb{P}^{R_0}\{\varphi_\tau \in \mathrm{d}t\} = \lambda_0^n h_0(R_0) \int h_0^*(y) \mathbb{P}^y\{\varphi_\tau \in \mathrm{d}s\}\,\mathrm{d}y \big[1 + \mathcal{O}((|\lambda_1|/\lambda_0)^n)\big]$$

Periodically modulated exponential distribution

Computing the exit distribution



Split into two Markov chains:

- First chain killed upon r reaching $1-\delta$ in $\varphi = \varphi_{\tau_-}$

$$\mathbb{P}^0\{\varphi_{\tau_-} \in [\varphi_1, \varphi_1 + \Delta]\} \simeq (\lambda_0^{\mathsf{s}})^{\varphi_1} \, \mathrm{e}^{-J(\varphi_1)/\sigma^2}$$

- Second chain killed at $r = 1 - 2\delta$ and on unstable orbit $r = 1$
  - Principal eigenvalue: $\lambda_0^{\mathsf{u}} = \mathrm{e}^{-2\lambda_+ T_+}(1 + \mathcal{O}(\delta))$
    $\lambda_+ =$ Lyapunov exponent, $T_+ =$ period of unstable orbit
  - Using LDP

$$\mathbb{P}^{\varphi_1}\{\varphi_\tau \in [\varphi, \varphi + \Delta]\} \simeq (\lambda_0^{\mathsf{u}})^{\varphi - \varphi_1} \, \mathrm{e}^{-[I_\infty + c(\mathrm{e}^{-2\lambda_+ T_+(\varphi - \varphi_1)})]/\sigma^2}$$

Main result: Cycling

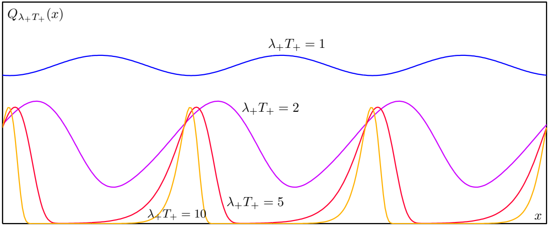
Theorem [Berglund & G 2014]

$\forall\,\Delta > 0\ \forall\,\delta > 0\ \exists\,\sigma_0 > 0\ \forall\,0 < \sigma < \sigma_0$

$$\mathbb{P}^{r_0,0}\{\varphi_\tau \in [\varphi, \varphi+\Delta]\} = C(\sigma)(\lambda_0)^{\varphi}\theta'(\varphi)\Delta Q_{\lambda_+ T_+}\left(\frac{|\log\sigma| - \theta(\varphi) + \mathcal{O}(\delta)}{\lambda_+ T_+}\right) \times \left[1 + \mathcal{O}(\mathrm{e}^{-c\varphi/|\log\sigma|}) + \mathcal{O}(\delta|\log\delta|)\right]$$

- Cycling profile, periodicized Gumbel distribution

$$Q_{\lambda T}(x) = \sum_{n=-\infty}^{\infty} A(\lambda T(n-x)) \quad \text{with} \quad A(x) = \tfrac{1}{2}\exp\{-2x - \tfrac{1}{2}\,\mathrm{e}^{-2x}\}$$



Main result: Cycling

Theorem [Berglund & G 2014]

$\forall\,\Delta > 0\;\forall\,\delta > 0\;\exists\,\sigma_0 > 0\;\forall\,0 < \sigma < \sigma_0$

$$\mathbb{P}^{r_0,0}\{\varphi_\tau \in [\varphi, \varphi+\Delta]\} = C(\sigma)(\lambda_0)^{\varphi}\theta'(\varphi)\Delta\, Q_{\lambda_+ T_+}\biggl(\frac{|\log\sigma| - \theta(\varphi) + \mathcal{O}(\delta)}{\lambda_+ T_+}\biggr) \times \bigl[1 + \mathcal{O}(\mathrm{e}^{-c\varphi/|\log\sigma|}) + \mathcal{O}(\delta|\log\delta|)\bigr]$$

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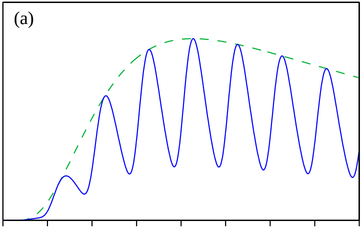
$$Q_{\lambda T}(x) = \sum_{n=-\infty}^{\infty} A(\lambda T(n-x)) \quad \text{with} \quad A(x) = \tfrac{1}{2}\exp\{-2x - \tfrac{1}{2}\,\mathrm{e}^{-2x}\}$$

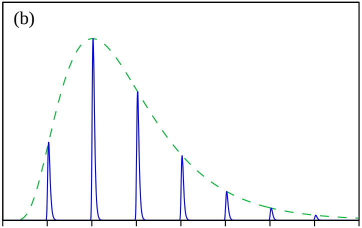
- $\theta(\varphi)$ explicit function of $D_{rr}(1,\varphi)$, $\theta(\varphi+1) = \theta(\varphi) + \lambda_+ T_+$
  (λ_+ = Lyapunov exponent, T_+ = period of unstable orbit)
- λ_0 principal eigenvalue, $\lambda_0 = 1 - \mathrm{e}^{-\tilde{V}/\sigma^2}$
- $C(\sigma) = \mathcal{O}(\mathrm{e}^{-\tilde{V}/\sigma^2})$
- $\mathbb{P}^{\pi_0^u}\{\varphi_\tau \in [\varphi, \varphi+\Delta]\} \sim \theta'(\varphi)\Delta$

Periodic in $|\log\sigma|$: [Day 1990, Maier & Stein 1996, Getfert & Reimann 2009]

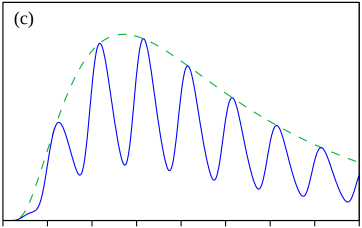
Density of the first-passage time (for $V = 0.5,\ \lambda_+ = 1$)



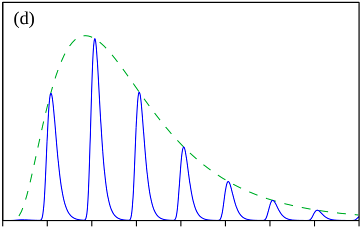
$\sigma^2 = 0.4,\ T_+ = 2$



$\sigma^2 = 0.4,\ T_+ = 20$



$\sigma^2 = 0.5,\ T_+ = 2$



$\sigma^2 = 0.5,\ T_+ = 5$

Dependence of exit distribution on the noise intensity

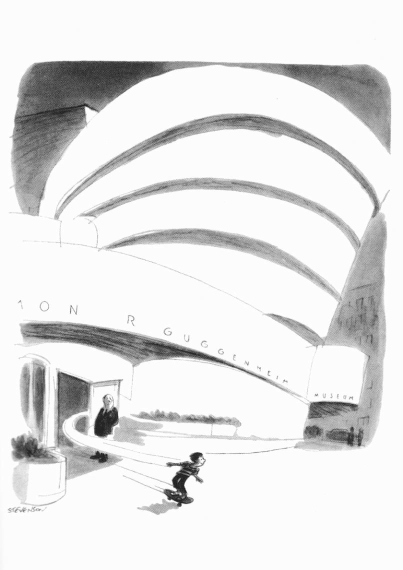
Author: Nils Berglund

- ▷ σ decreasing from 1 to 0.0001
- ▷ Parameter values: $\lambda_+ = 1$, $T_+ = 4$, $\overline{V} = 1$

Modifications

- ▷ System starting in quasistationary distribution (no transitional phase)
- ▷ Maximum is chosen to be constant (area under the curve *not* constant)

Why $|\log \sigma|$-periodic oscillations?



Concluding remarks

Warning

Naive WKB expansion may suggest absence of cycling, despite of $|\log \sigma|$-dependence of the exit distribution

Origin of Gumbel distribution

- Extreme-value distribution
- Connection with residual lifetimes [Bakhtin 2013]
- Connection with transition-paths theory [Cerou, Guyader, Lelièvre & Malrieu 2013]

(see also [Berglund 2014])

Open questions

- Proof involving only spectral theory, without using large-deviation principle
- More precise estimates on spectrum and eigenfunctions of K
- Link between spectra of K and of L (with Dirichlet b.c.)

Thank you for your attention!