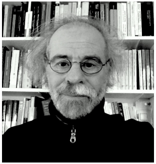
In honour of the 19th :-) birthday of Patrick and Christian

June, 2017



Nonparametric estimation for stochastic damping Hamiltonian systems under partial observation

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Outline of the talk

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Model

We consider a damped hamiltonian system with stochastic noise:
$\left(Z_t := (X_t, Y_t) \in \mathbb{R}^{2d}\,,\ t \geq 0\right)$ given by the s.d.e.

$$\begin{cases} dX_t = Y_t dt \\ dY_t = \sigma(X_t, Y_t) dB_t - (c(X_t, Y_t) Y_t + \nabla V(X_t)) dt \end{cases}$$

where B is a standard Brownian motion.

Particle in contact with a heat bath

Particle in a contact with a heat thermal reservoir:
Consider a particle in a potential V. Its dynamics is described through the Hamiltonian $H(p, q) = \frac{1}{2}p^2 + V(q)$: $\dot{q} = \partial_p H$, $\dot{p} = -\partial_q H$.

This particle is in contact with some heat bath with temperature $T > 0$, modeled by an Ornstein-Uhlenbeck process acting as a noise on the momentum p only:

$$\begin{aligned} dq_t &= p_t dt \\ dp_t &= (-\gamma p_t - \nabla V(q_t))dt + \sqrt{2\gamma T}dB_t. \end{aligned}$$

Chain of oscillators in contact with two heat baths (1/2)

Chain of oscillators in contact with two heat bath reservoirs:
The dynamics is given by the Hamiltoniann

$$H(p,q) = \sum_{1\le i\le d} \frac{p_i^2}{2} + V(q)$$

with $V : \mathbb{R} \to \mathbb{R}$ in the form

$$\sum_{1\le i\le d} U^{(1)}(q_i) + \sum_{1\le i\le d-1} U^{(2)}(q_i - q_{i+1}).$$

$U^{(1)}$ is a trapping potential, $U^{(2)}$ an interaction potential.

Chain of oscillators in contact with two heat baths (2/2)

The two heat baths with temperature T_1 and T_d act on the momenta of particles 1 and d like Ornstein-Uhlenbeck processes:

$$
\begin{aligned}
dq_j(t) &= p_j(t)dt \quad 1 \leq j \leq d \\
dp_1(t) &= (-\gamma p_1(t) - \partial_{q_1} V(q_t))dt + \sqrt{2\gamma T_1} dB_1(t) \\
dp_j(t) &= (-\partial_{q_j} V(q_t))dt \quad 2 \leq j \leq d-1 \\
dp_d(t) &= (-\gamma p_d(t) - \partial_{q_d} V(q_t))dt + \sqrt{2\gamma T_d} dB_d(t).
\end{aligned}
$$

For short:

$$
\begin{cases}
dq(t) = p(t)dt \\
dp(t) = (-\gamma \Lambda p(t) - \nabla_q V(q(t)))dt + \sqrt{2\gamma T} dB(t)
\end{cases}
$$

where $\Lambda : \mathbb{R}^d \to \mathbb{R}^2$ is the projection $\Lambda(x_1, \ldots, x_d) = (x_1, x_d)$, $\sqrt{T} : (x_1, x_d) \to (\sqrt{T_1} x_1, \sqrt{T_d} x_d)$ and $B(t) = (B_1(t), B_d(t))$ is a B.M. in $\mathbb{R}^2$.

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Langevin dynamics

More generally, consider the following system:

$$\begin{cases} dX_t = Y_t dt \\ dY_t = (2\beta^{-1})^{1/2}\sigma(X_t)dW_t - (\sigma^2(X_t)Y_t + \nabla V(X_t))dt. \end{cases}$$

Observe that the diffusion term, $\tilde{\sigma}(x) = (2\beta^{-1})^{1/2}\sigma(x)$, depends only on the x coordinate and on an unknown parameter β. Moreover, the damping force has the form $c(x,y) = \frac{\beta}{2}\tilde{\sigma}^2(x)$.

Since Einstein, this last relationship between the damping force and the diffusion term is known as the fluctuation-dissipation relation and has numerous applications, e.g.,

- it appears as a tool for the simulation of molecular dynamics (see, e.g., Lelièvre *et al.* (2010) [Section 2.2.3]),
- it also appears as limit of the Ehrenfest nuclei dynamics and is called Langevin dynamics (see Szepessy (2011)).

A stochastic neuronal model (1/3)

See, e.g., León and Samson (2017) and references therein.

Data

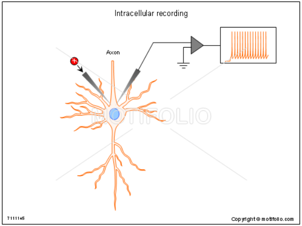
- Membrane potential: difference in voltage between the interior and exterior of the cell
- High frequency records available ($\delta = 0.1$ ms)

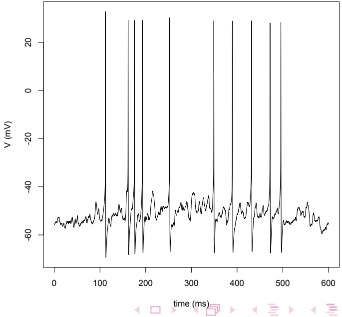
Objective

- Prediction of spike emission

Tools

- Neuronal modeling with stochastic models
- Estimation



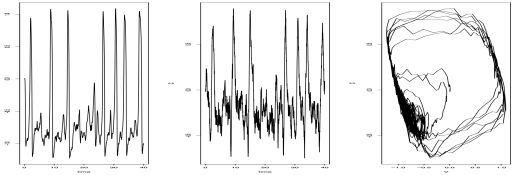


A stochastic neuronal model (2/3)

The stochastic FitzHugh-Nagumo model is defined as follows:

$$\begin{cases} dV_t = \dfrac{1}{\varepsilon}(V_t - V_t^3 - C_t - s)dt \\ dC_t = (\gamma V_t - C_t + \beta)dt + \tilde{\sigma} dB_t \end{cases}$$

- V_t the membrane potential of a single neuron,
- C_t a recovery variable / channel kinetics,
- ε the time scale separation, s the stimulus input,
- β, γ positive constants determining the position of the fixed point and the duration of the excitation,
- B_t a Brownian motion, $\tilde{\sigma} > 0$ the diffusion coefficient.



A stochastic neuronal model (3/3)

Defining $X_t = V_t$ and $Y_t = \frac{1}{\varepsilon}(V_t - V_t^3 - C_t - s)$, we get:

$$\begin{cases} dX_t = Y_t dt \\ dY_t = \dfrac{1}{\varepsilon}(Y_t(1-\varepsilon-3X_t^2) - X_t(\gamma-1) - X_t^3 - (s+\beta))dt + \dfrac{\tilde{\sigma}}{\varepsilon} dB_t. \end{cases}$$

Let $\nabla V(x) = \frac{1}{\varepsilon}(x(\gamma-1) + x^3 + (s+\beta))$ and $c(x) = \frac{1}{\varepsilon}(-1+\varepsilon+3x^2)$.

We recognize the system governing the dynamics of a particle with X_t referring to its position and Y_t to its velocity, whose movement is guided by a potential $V(x)$ and a damping force $c(x)$.

$$\begin{cases} dX_t = Y_t dt \\ dY_t = -(c(X_t)Y_t + \nabla V(X_t))dt + \sigma dB_t \end{cases}$$

with $\sigma = \frac{\tilde{\sigma}}{\varepsilon}$.

Outline of the talk

Assumptions

$Z_t = (X_t, Y_t) \in \mathbb{R}^{2d}$ governed by:

$$\begin{cases} dX_t = Y_t dt \\ dY_t = -(c(X_t, Y_t)Y_t + \nabla V(X_t))dt + \sigma dB_t, \end{cases}$$

with $\sigma > 0$.

$\mathcal{H}_1$ The potential $V(x)$ is smooth over $\mathbb{R}^d$ and lower bounded.

$\mathcal{H}_2$ The damping force $c(x, y)$ is smooth, bounded, and there exist c, $M > 0$ s.t. $c^s(x, y) \geq cId > 0$, $\forall (|x| > M, \ y \in \mathbb{R}^d)$.

From **Wu (2001)**, we know that for every initial state $z = (x, y) \in \mathbb{R}^{2d}$, the system admits a unique weak solution, and that this solution is non-explosive.

The infinitesimal generator writes:

$$L = \frac{\sigma^2}{2}\partial_{yy} + y\partial_x - (c(x, y)y + \nabla_x V(x))\partial_y \, .$$

Local properties, hypoellipticity (1/4)

L can be written in Hörmander's form

$$L = \frac{\sigma^2}{2} \sum_{i=1}^{d} L_i^2 + L_0$$

with vector fields L_i defined by

(1) pour $1 \leq i \leq d$, $L_i = \frac{\partial}{\partial y_i}$,

(2)

$$L_0 = \sum_{k=1}^{d} y_k \frac{\partial}{\partial x_k} - \sum_{k=1}^{d} \left((c(x,y)y)_k + \frac{\partial V}{\partial x_k} \right) \frac{\partial}{\partial y_k} .$$

It holds

$$[L_i, L_0] = L_i L_0 - L_0 L_i = \frac{\partial}{\partial x_i} - \sum_{k=1}^{d} \frac{\partial((c(x,y)y)_k)}{\partial y_i} \frac{\partial}{\partial y_k}$$

so that $\{L_i, 1 \leq i \leq d; [L_i, L_0], 1 \leq i \leq d\}(z)$ span $\mathbb{R}^{2d}$, for all z.

Local properties, hypoellipticity (2/4)

$\Rightarrow$ hypoellipticity (Hörmander sum of squares theorem).

Consequence: $\forall z, \forall t > 0$,
the distribution $P_t(z, \cdot)$ of Z_t starting at z at time 0 admits a C^∞ density $p_t(z, \cdot)$ w.r.t. Lebesgue.

Hence, $\mu(dz) = p_s(z)dz$ with p_s C^∞, and thus the strong Feller property.

Small time behavior of $p_t(z, \cdot)$?

Example: $d = 1$, $c = V = 0$. Then Z_t is a two dimensional gaussian vector, with mean $(x_0 + y_0 t, y_0)$ and covariance matrix

$$\mathrm{Var}(X_t) = \frac{t^3}{3}, \mathrm{Var}(Y_t) = t, \mathrm{Cov}(X_t, Y_t) = \frac{t^2}{2}.$$

So the transition density behaves, for small t, as

$$\frac{\sqrt{3}}{\pi}\frac{1}{t^2}e^{-\frac{y_0^2}{6t}} \quad \text{instead of} \quad \frac{1}{2\pi}\frac{1}{t}$$

which is the classical small time explosion for elliptic diffusions (like the B.M.).

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Local properties, hypoellipticity (3/4)

Theorem (Konakov, Menozzi & Molchanov, 2010)

$$\begin{cases} dX_t &= Y_t dt \\ dY_t &= \sigma\, dW_t + b(X_t, Y_t) dt \,, \end{cases}$$

with b C^∞, bounded as well as all its derivatives. Let $T > 0$. Then $\forall\, z = (x, y)$, $\forall\, t > 0$, the distribution of $Z_t = (X_t, Y_t)$ has a density $q_t(z, .)$ with respect to Lebesgue and $\exists\, C \,,\; C' > 0$ t.q. for $0 < t < T$,

$$q_t(z, z') \;\leq\; C' \, \frac{1}{t^{2d}} \, \exp\left(-\, C \left[\frac{|y - y'|^2}{4t} + \frac{3 \left| x' - x - \frac{t(y+y')}{2} \right|^2}{t^3} \right] \right) .$$

De plus, $\exists\, t_0 > 0 \,,\; \exists\, C'' > 0$ t.q. $\forall\, 0 < t < t_0$,

$$q_t \left((x, y) \,, (x + ty, y) \right) \geq C'' \, \frac{1}{t^{2d}} \,.$$

Local properties, hypoellipticity (4/4)

We can generalize that result to a non bounded drift term.

Corollary (Cattiaux, León & Prieur, 2014)

We do no more assume boundedness.
$\forall\, z$, for any open neighborhood U of z, one can write:

$$\forall\, z' \in U\,,\ \forall\, 0 < t < T\,,\ p_t(z,z') \leq q_t(z,z') + C(U)e^{-\frac{C'(U)}{t}}$$

for constants $C(U)$ and $C'(U) > 0$.
We also prove

$$\forall\, (z,z')\,,\ \exists\, 0 < C(z') \text{ s.t. } \forall\, t \geq 0\,,\ p_t(z,z') \leq D(z') < +\infty\,.$$

Long time behavior, coercivity and mixing (1/2)

We now add the following assumption

$\mathcal{H}_3$ V and ∇V have polynomial growth at infinity with

$$+\infty \geq \liminf_{|x|\to+\infty} \frac{x\cdot\nabla V(x)}{|x|} \geq v > 0 \quad \text{(drift's condition)}.$$

The force $-\nabla V(x)$ is "strong enough" for $|x|$ large to ensure a quick return of the system to compact subsets of $\mathbb{R}^{2d}$.

Under $\mathcal{H}_i$, $i = 1,2,3$, the process $Z_t = (X_t, Y_t)$ is positive recurrent with a unique invariant probability measure μ. Moreover, moments of any order of μ exist: for all k_1, $k_2 \in \mathbb{N}$,

$$\mathbb{E}(X_t^{k_1} Y_t^{k_2}) = \int x^{k_1} y^{k_2} d\mu(x,y) < +\infty\,.$$

Scheme of proof: the proof involves the construction of a Lyapunov function $\Psi(x,y)$, such that there exist a compact $K \in \mathbb{R}^{2d}$ and constants C, $\xi > 0$, such that $-\frac{L\Psi}{\Psi} \geq \xi \mathbb{1}_{K^c} - C\mathbb{1}_K$. The choice of the Lyapounov function is not trivial. See, e.g., Wu (2001) .

Long time behavior, coercivity and mixing (2/2)

For any z, let's $P_t f(z) = \mathbb{E}_z(f(Z_t))$ for bounded f's.

$\psi \in \mathbb{L}^1(\mu)$. *There exist* $D > 0$ *and* $\rho < 1$ *s.t. for all* z*, all* f *s.t.* $\sup_z \frac{|f(z)|}{\psi(z)} < +\infty$,

$$\left| P_t f(z) - \int f d\mu \right| \leq D \sup_a \left(\frac{|f(a) - \int f d\mu]}{\psi(a)} \right) \psi(z) \rho^t.$$

It follows that $(Z_t := (X_t, Y_t)\,,\ t \geq 0)$ is β-mixing.

Outline of the talk

Invariant density estimators

Complete observations: we observe both coordinates X_t and Y_t at discrete times $i\delta$, $i = 1, \dots, n$. Let K be a kernel function, $b = (b_1, b_2)$ a bandwidth.

$$\check{p}_s(x, y) := \frac{1}{n b_1^d b_2^d} \sum_{i=1}^{n} K\left(\frac{x - X_{i\delta}}{b_1}, \frac{y - Y_{i\delta}}{b_2} \right).$$

Now we do not observe y anymore.

Partial observations:

$$\hat{p}_s(x, y) := \frac{1}{n b_1^d b_2^d} \sum_{i=1}^{n-1} K\left(\frac{x - X_{i\delta}}{b_1}, \frac{y - \frac{X_{(i+1)\delta} - X_{i\delta}}{\delta}}{b_2} \right).$$

Main issue: the choice of the bandwidth $b = (b_1, b_2)$.

Invariant density estimators

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Adaptive estimation (1/2)

Data-driven procedure [Comte, Prieur, Samson, 2017]
Our selection criterion is based on Goldenshluger and Lepski (2011).

Let $\check{p}_{b,b'} = K_{b'} \star \check{p}_b(x,y)$, with $K_{b'}(u,v) = \frac{1}{b'_1 b'_2} K(\frac{u}{b'_1}, \frac{v}{b'_2})$. Let $p_b = K_b \star p$. In the following, $d = 1$.

$$\tilde{b} = \arg\min_{b \in \mathcal{B}_n} \left(A(b) + U(b)\right), \quad \textit{with}$$

- $\mathcal{B}_n = \{(b_{1,k}, b_{2,\ell}) = (1/k, 1/\ell), k, \ell = 1, \ldots, B_n\}$,
- $A(b)$ *mimicking the bias* ($= \sup_{b' \in \mathcal{B}_n} (\|\check{p}_{b,b'} - \check{p}_{b'}\|^2 - U(b'))_+$)
- $V(b)$ *mimicking the variance* ($= \kappa \frac{\|K\|_1^2 \|K\|^2}{n b_1 b_2} \sum_{i=0}^{n-1} \beta(i\delta)$)

$$\mathbb{E}\left(\|\check{p}_{\tilde{b}} - p\|^2\right) \leq C \inf_{b \in \mathcal{B}_n} \left(\|p - p_b\|^2 + U(b)\right) + C' \frac{\log(n)}{n\delta}.$$

κ can then be calibrated by the slope heuristic (see Arlot and Massart, 2009, Lacour *et al.*, 2016). Same results in the partial observations case.

Adaptive estimation (2/2)

That procedure is numerically demanding due to the double convolutions $\check{\mathrm{p}}_{b,b'}$, especially in the multidimensional case.

In practice, we implement the selection procedure in Lacour, Massart and Rivoirard (2016):

$$\hat{b} = \arg\min_{b\in\mathcal{B}_n} \left(\|\check{\mathrm{p}}_b - \check{\mathrm{p}}_{b_{min}}\|^2 + U(b)\right) \text{ with}$$

$b_{min} = (\min_{1\leq k\leq B_n} b_{1,k}, \min_{1\leq \ell\leq B_n} b_{2,\ell})$.

Outline of the talk

Numerical results (1/4)

Harmonic Oscillator:

$$\begin{cases} dX_t = Y_t dt \\ dY_t = -(\alpha X_t + \gamma Y_t)dt + \sigma dB_t \end{cases}$$

with $\alpha > 0, \gamma > 0$. In the following, we choose $\alpha = 4, \gamma = 0.5, \sigma = 0.5$. The potential is then $V(x) = \alpha/2x^2$. The stationary distribution is Gaussian, with mean zero and explicit diagonal variance matrix:

$$p(x, y) = \frac{\gamma\sqrt{\alpha}}{\pi\sigma^2} \exp(-\frac{2\gamma}{2\sigma^2} y^2 - \frac{2\gamma\alpha}{2\sigma^2} x^2)$$

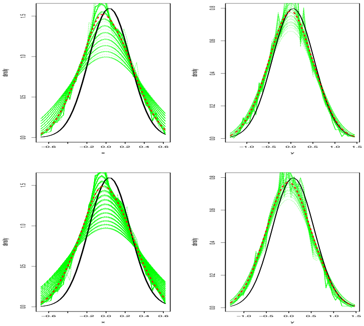
with diagonal variances equal to 1/16 and 1/4, respectively in our case.

Numerical results (2/4)

Kernel estimation of the invariant density:

- complete observations (top)
- partial observations (bottom)

$n = 2000, \delta = 0.2$.
100 trajectories simulated with a Euler scheme with step size $\delta/10$.



$\mathcal{B}_n = \{(b_1, b_2) \in \{1/\sqrt{4n}, 2/\sqrt{4n}, \ldots, 30/\sqrt{4n}\}^2\}$. Anisotropic selected bandwidth $\hat{b} = (8/\sqrt{4n}, 17/\sqrt{4n})$ (complete), $\hat{b} = (9/\sqrt{4n}, 19/\sqrt{4n})$ (partial).

Numerical results (3/4)

Van Der Pol Oscillator:

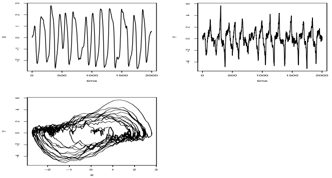
$$\begin{cases} dX_t = Y_t dt \\ dY_t = -\left((c_1 X_t^2 - c_2) Y_t + \omega_0^2 X_t\right) dt + \sigma dB_t \end{cases}$$

with $\sigma, c_1, c_2, \omega_0^2 > 0$. In the following, we choose $\sigma = c_1 = c_2 = \omega_0^2 = 1$. The potential is then $V(x) = \omega_0^2/2x^2$. The invariant density p satisfies Fokker-Planck equation:

$$\frac{1}{2}\frac{\partial^2 p(x,y)}{\partial y^2} - y\frac{\partial p(x,y)}{\partial x} + c(x)p(x,y) + (c(x)y + \nabla D(x))\frac{\partial p(x,y)}{\partial y} = 0$$

solved with finite difference scheme (see Kumar *et al.*, 2006).

Sample $(X_{i\delta})_{i=0,\dots,n}$ (top left), $(Y_{i\delta})_{i=0,\dots,n}$ (top right) and state phase (bottom) for $\delta = 0.5$ and $n = 2000$.

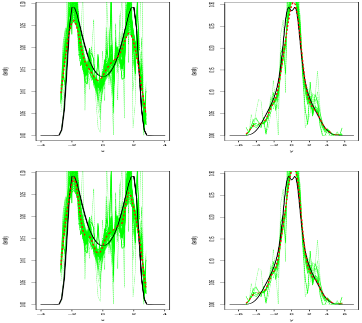


Numerical results (4/4)

Kernel estimation of the invariant density:

- complete observations (top)
- partial observations (bottom)

$n = 2000, \delta = 0.05$.
100 trajectories simulated with a Euler scheme with step size $\delta/10$.



Conclusion, perspectives

Conclusion: we obtained

- non parametric (recursive) estimation for the invariant density (Cattiaux *et al.*, 2014a, 2015),
- a data-driven procedure for the selection of the bandwidth (see Comte *et al.*, 2016),
- see also Cattiaux *et al.* (2014b,2016,2017) for the estimation of the drift and of the diffusion matrix.

We have considered the more realistic non trivial case of partial observations.

Perspectives:

- to consider more complex models which are more realistic for environmental modeling (non linear Fokker-Planck equations, confined models, degenerated variances, . . .),
- adaptive estimation in higher dimension,
- adaptivity with respect to δ,
- . . .

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Thanks for your attention

Happy birthday
Parabéns !