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M. Ottobre

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Markovian Approximation of Classical Open Systems

M.Ottobre

Mathematics Department Imperial College London 180 Queen's Gate London SW7 2AZ

Abstract. We discuss exponential convergence to equilibrium for dissipative Markovian systems generated by hypoelliptic non-selfadjoint operators and we present a method to determine the exact rate of convergence to equilibrium. The main example that we will consider is a class of Markovian approximations of the Generalized Langevin equation (GLE).

Keywords: Hypoellipticity, hypocoercivity, singular space theory, ergodicity, dissipative Markovian processes, Markovian approximation.

INTRODUCTION

The Generalized Langevin Equation (GLE),

$$\ddot{q}(t) = -\partial_q V(q) - \int_0^t ds \gamma(t-s) \dot{q}(s) + F(t), \quad (1)$$

is a popular model for a particle immersed in a heat bath and has proven to be a very efficient tool in molecular dynamics. In (1), $q(t)$ represents the position of the distinguished particle (here $q(t) \in \mathbb{R}$ just for simplicity, the equation can be rewritten in \mathbb{R}^n), $V(q)$ is a confining potential, $\gamma(t)$ is a smooth kernel and $F(t)$ is a mean zero stationary Gaussian process. Noise and memory kernel are related through the *fluctuation dissipation principle*

$$E(F(t)F(s)) = \beta^{-1} \gamma(t-s), \quad (2)$$

i.e., the correlation function of the noise is proportional to the memory kernel through a constant β (inverse temperature of the bath). From now on we set $\beta = 1$. For a derivation of the GLE see [14]. The GLE is a stochastic integro-differential equation and, for an arbitrary choice of the kernel $\gamma(t)$, it is in general non-Markovian. Though, for some specific choices of the kernel $\gamma(t)$, it is equivalent to a Markovian dynamics in an extended state space. If, for example, we choose $\gamma(t) = \lambda^2 e^{-|t|}$, then (1) becomes (see [1])

$$\begin{cases} \dot{q} &= p \\ \dot{p} &= -\partial_q V(q) - \lambda^2 \int_0^t ds e^{-(t-s)} p(s) + F(t), \end{cases} \quad (3)$$

and the fluctuation dissipation theorem yields $E(F(t)F(s)) = \lambda^2 e^{-|t-s|}$. If we write $F(t) = \lambda v(t)$, with $v(t)$ satisfying the equation $\dot{v} = -v + \sqrt{2} \dot{W}$, and we define the new process

$$u(t) = -\lambda \int_0^t e^{-(t-s)} p(s) ds + v(t), \quad (4)$$

then (3) becomes

$$\begin{cases} \dot{q} &= p \\ \dot{p} &= -\partial_q V + \lambda u \\ \dot{u} &= -\lambda p - u + \sqrt{2} \dot{W}. \end{cases}$$

As observed in [5], the general form of a Markovian system of ODEs which approximates the dynamics (1) reads as follows :

$$dq = p dt \quad (5a)$$

$$dp = -\partial_q V(q) dt + \Lambda \cdot \mathbf{u} dt \quad (5b)$$

$$d\mathbf{u} = (-p\Lambda - \mathbf{A}\mathbf{u}) dt + C d\mathbf{W}(t), \quad (5c)$$

where $(q, p) \in \mathbb{R}^2$, \mathbf{u} and Λ are column vectors of \mathbb{R}^d , \cdot denotes Euclidean scalar product, $\mathbf{W}(t) = (W_1(t), \dots, W_d(t))$ is a d -dimensional Brownian motion and A and C are constant coefficients $d \times d$ matrices, related through the fluctuation dissipation principle, which in the present case reads

$$A + A^T = CC^T. \quad (6)$$

In (5), q and p are the position and momentum of the distinguished particle and the variables (u_1, \dots, u_d) describe the heat bath. The "Markovianization" of (1) was first done by Mori ([10]) by first approximating the Laplace transform of the memory kernel $\gamma(t)$, $\tilde{\gamma}(\xi)$, by a rational function (if and when this is possible) and then imposing the fluctuation relation, which gives the matrices A and C as well as the vector Λ . If $\gamma(t)$ itself is a sum of exponentials, $\gamma_d(t) = \sum_{i=1}^d \lambda_i^2 e^{-\alpha_i t}$, $t > 0$, then $\tilde{\gamma}_d(\xi) = \sum_{i=1}^d \lambda_i^2 / (\xi + \alpha_i)$, so the procedure indicated by Mori is clearly successful and it corresponds to the case in which $A = \text{diag}\{\alpha_1, \dots, \alpha_d\}$ and $\Lambda = (\lambda_1, \dots, \lambda_d)^T$, i.e. system (5) reduces to

$$dq(t) = q(t)dt \quad (7a)$$

$$dp(t) = -\partial_q V(q(t))dt + \sum_{j=1}^d \lambda_j u_j(t)dt \quad (7b)$$

$$du_j(t) = -\lambda_j p(t)dt - \alpha_j u_j(t)dt + \sqrt{2\alpha_j} dW_j, \quad (7c)$$

for $j = 1, \dots, d$, $\alpha_j > 0$ and $\lambda_j > 0$. The notation for q and p in (5) and (7) should include a subscript d , i.e. q_d, p_d , as the solution will depend on the number of heat bath variables u_j ; we drop the subscript for notational convenience. Another typical situation is when the Laplace transform of γ has a continued fraction representation

$$\tilde{\gamma}(\xi) = \frac{\varepsilon_1^2}{\xi + \theta_1 + \frac{\varepsilon_2^2}{\xi + \theta_2 + \ddots}}, \quad \theta_i > 0.$$

In this case the approximation is done by truncating the fraction at step d and then reading off the corresponding Markovian system of $(d+2)$ SDEs. The matrix A is then tridiagonal,

$$A = \begin{pmatrix} \theta_1 & -\varepsilon_2 & & & \\ \varepsilon_2 & \theta_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & & \theta_d \end{pmatrix}$$

and $\Lambda = (\varepsilon_1, 0, \dots, 0)^T$. It was observed by Eckmann, Pillet and Rey-Bellet (see [15, 2, 3] and references therein) that when the memory kernel $\gamma(t)$ has a rational spectral density, then the GLE is equivalent to a finite dimensional Markovian system. This system is obtained by adding a finite number of additional degrees of freedom which account for the memory in the system.

RATE OF EXPONENTIAL CONVERGENCE

To simplify matters, let us consider system (7) from now on and set $d = 1$ and $\lambda = \alpha = 1$. Several properties of system (7), including ergodicity, exponential decay to equilibrium and homogenization, were studied in [11]. We will use the notation $x(t) = (q(t), p(t), u(t))$. It can be shown that system (7) is ergodic, i.e. it admits a unique invariant measure $\mu(dx) = \rho(x)dx$, with

$$\rho(x) = \frac{1}{Z} \exp \left[- \left(V(q) + \frac{p^2}{2} + \frac{u^2}{2} \right) \right]$$

and Z is a normalization constant. The generator of (7) is then given by

$$\mathcal{L} = p\partial_q - \partial_q V \partial_p + u\partial_p - p\partial_u - u\partial_u + \partial_u^2. \quad (8)$$

\mathcal{L} is hypoelliptic and *hypocoercive* ([16]). We will define a Markov process to be hypoelliptic or hypocoercive when its generator is hypoelliptic or hypocoercive, respectively. We recall that, roughly speaking, an operator \mathcal{L} is said to

be hypoelliptic when, for every distribution f , the sets where f and $\mathcal{L}f$ are C^∞ functions do coincide. By a physical point of view, \mathcal{L} is hypoelliptic because in system (7) noise acts directly only on the heat bath variables, and is then transmitted to the position and momentum variables. The theory of hypocoercivity refers to dissipative (and usually) Markovian evolutions whose generator can be written in the form

$$-\mathcal{L} = \mathcal{B} + \sum_{i=1}^r \mathcal{A}_i^* \mathcal{A}_i,$$

where \mathcal{A}_i^* denotes the adjoint of \mathcal{A}_i in the space $L^2_\rho := \{f \in L^2 : \int f d\mu < \infty\}$ and μ is the invariant measure of the system, with density ρ with respect to the Lebesgue measure. The operator \mathcal{B} is assumed to be antisymmetric in L^2_ρ , whereas $\sum_{i=1}^r \mathcal{A}_i^* \mathcal{A}_i$ is clearly symmetric; hence the dynamics is nicely decomposed into a conservative (deterministic) part, described by \mathcal{B} and a stochastic (dissipative) component, described by $\sum_{i=1}^r \mathcal{A}_i^* \mathcal{A}_i$. Appropriate bounds on the successive commutators between the \mathcal{A}_i 's and \mathcal{B} together with a Poincaré inequality (see [16, Theorem 24]) guarantee hypocoercivity, that is, exponential convergence to equilibrium: there exist $\kappa, c > 0$ such that

$$\| e^{t\mathcal{L}} h \|_{\tilde{H}} \leq \kappa e^{-ct} \| h \|_{\tilde{H}} \quad \forall h \in \tilde{H} \text{ and } t \geq 0, \quad (9)$$

where \tilde{H} is an appropriate Hilbert space, typically the Sobolev space H^1 weighted by the invariant measure (modulo constants). This framework directly applies to the generator \mathcal{L} in (8), when we set

$$\mathcal{A} = -\partial_u \quad \text{and} \quad \mathcal{B} = -(p\partial_q - \partial_q V \partial_p + u\partial_p - p\partial_u).$$

However, the theory of hypocoercivity does not offer a systematic way to calculate the rate of exponential convergence to equilibrium, i.e. the constant c in (9). If \tilde{c} is the (nonzero) eigenvalue of $-\mathcal{L}$ with smallest real part, then c is precisely the real part of \tilde{c} . When $V(q) = q^2/2$, in order to calculate c , we regard the operator \mathcal{L} by the point of view of semiclassical analysis, using in particular the *singular space theory* (SST), [4]. Indeed, \mathcal{L} is a quadratic operator, i.e. a pseudodifferential operator, defined in the Weyl quantization ([6]) by symbols $\mathfrak{l}(x, \xi)$, with $(x, \xi) \in \mathbb{R}^n \times \mathbb{R}^n$, which are complex-valued quadratic forms (in the example at hand, $n = d + 2$). These operators are differential operators with simple and fully explicit expression. Indeed, the Weyl quantization of the quadratic symbol $x^\alpha \xi^\beta$, with $(\alpha, \beta) \in \mathbb{N}^{2n}$, $(\alpha + \beta) = 2$, is the differential operator

$$\frac{x^\alpha D_x^\beta + D_x^\beta x^\alpha}{2}, \quad D_x = i^{-1} \partial_x.$$

(For example, if x_j is the j -th coordinate of x , the operator associated with the symbol $x_j \xi_k$ is $-ix_j \partial_{x_k} + \delta_{\{j=k\}} \frac{1}{2}$.) In this way, the Weyl symbol of \mathcal{L} (more precisely of $-\mathcal{L} - 1/2$) is the quadratic form

$$\mathfrak{l}(q, p, u, \chi, \eta, \zeta) = -i(p\chi - q\eta + u\eta - p\zeta - u\zeta) + \zeta^2.$$

Uniquely associated to the quadratic form \mathfrak{l} there is a matrix, the Hamilton map F , defined through the relation

$$\mathfrak{l}((x, \xi); (y, \eta)) = \theta((x, \xi), F(y, \eta)), \quad (x, \xi) \in \mathbb{R}^{2n}, (y, \eta) \in \mathbb{R}^{2n}, \quad (10)$$

where $\mathfrak{l}(\cdot; \cdot)$ stands for the polarized form associated to the quadratic form \mathfrak{l} and θ is the canonical symplectic form

$$\theta((x, \xi), (y, \eta)) = \xi y - x \eta, \quad (x, \xi) \in \mathbb{R}^{2n}, (y, \eta) \in \mathbb{R}^{2n}. \quad (11)$$

In other words, F is the matrix associated to the quadratic form \mathfrak{l} when we consider the symplectic scalar product instead of the usual Euclidean one. For any quadratic operator whose symbol has a positive real part, $\text{Re } \mathfrak{l} \geq 0$, it was pointed out in [4] the existence of a particular linear vector space S in the phase space \mathbb{R}^{2n} , intrinsically associated to the symbol \mathfrak{l} and called *singular space*, which plays a basic role in the understanding of the properties of non-elliptic quadratic operators,

$$S = \bigcap_{j=0}^{2n-1} \text{Ker} [\text{Re } F(\text{Im } F)^j]. \quad (12)$$

In particular, consider an (in general non-elliptic) quadratic operator \mathcal{G} whose symbol \mathfrak{l} has a non-negative real part, $\text{Re } \mathfrak{l} \geq 0$, and such that $S = 0$. Then \mathcal{G} is hypoelliptic and its spectrum is an integer combination of the eigenvalues of the matrix F ([12], [4]):

$$\sigma(\mathcal{G}) = \left\{ \sum_{\substack{v \in \sigma(F) \\ -iv \in \mathbb{C}_+}} (r_v + 2k_v)(-iv) : k_v \in \mathbb{N} \right\} \quad (13)$$

where r_ν is the algebraic multiplicity of the eigenvalue $\nu \in \sigma(F)$ and $\mathbb{C}_+ = \{z \in \mathbb{C} : \operatorname{Re} z > 0\}$. If H is an operator (bounded or unbounded) we denote by $\sigma(H)$ the spectrum of H . We can apply this machinery to the degenerate Ornstein-Uhlenbeck (O-U) process (14), where $X \in \mathbb{R}^n$ and B and Σ are (nonzero) constant coefficients $n \times n$ matrices with $\det(\Sigma) = 0$. Indeed the generator of (14), say \mathcal{H} , has quadratic Weyl symbol. Employing the SST we can show that the spectrum of the hypoelliptic O-U process (14) depends only on the drift matrix B .

Proposition 1. *Suppose $\sigma(B) \subset \mathbb{C}_+$. Then the singular space S associated with \mathcal{H} is trivial if and only if the process*

$$dX(t) = -BX(t)dt + \Sigma dW \quad (14)$$

is hypoelliptic.

Proposition 2. *Suppose that the singular space associated with \mathcal{H} is zero. Then \mathcal{H} is hypoelliptic and its spectrum depends only on the drift matrix B ; in particular*

$$\sigma(\mathcal{H}) = \left\{ - \sum_{\mu \in \sigma(B)} \mu k_\mu, \quad k_\mu \in \mathbb{N} \right\}. \quad (15)$$

The proof of the above two propositions as well as more detailed information on the hypoellipticity of (14) can be found in [13] and references therein. An analogous result to Proposition 2 had been obtained in [9] using different techniques. Proposition 1 and 2 apply to the Markovian approximations of the GLE, (5), when $V(q)$ is quadratic.

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