Theoretical analysis and numerical methods for conservation laws, metastability and uncertainty propagation

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HABILITATION À DIRIGER DES RECHERCHES

Discipline : Mathématiques

Présentée par

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Theoretical analysis and numerical methods for conservation laws, metastability and uncertainty propagation

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Soutenue le 15 septembre 2021 devant le jury composé de

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Remerciements

Mes premiers remerciements sont adressés à Sofiane Martel, Mouad Ramil et Adrien Touboul, au côté desquels j'ai appris à faire des maths autrement et dont les travaux de thèse constituent une part importante de ce manuscrit. Je remercie également Sébastien Boyaval, Tony Lelièvre, Bernard Lapeyre, Fabien Mangeant, Pierre Benjamin et Mouadh Yagoubi, qui m'ont accompagné dans l'encadrement de ces thèses. Je remercie enfin les stagiaires, de césure ou de M2, avec lesquels j'ai eu le plaisir de travailler, ainsi que les collègues, du CERMICS ou d'ailleurs, avec lesquels j'ai partagé l'encadrement de ces stages.

Parmi les collègues déjà cités, une mention spéciale doit être décernée à Tony Lelièvre, pour sa bienveillance à mon égard depuis mon arrivée au CERMICS et ses multiples invitations à travailler ensemble, dans l'enseignement, l'encadrement de stagiaires et doctorants, et plus généralement pour les nombreuses discussions scientifiques que nous avons eues. Son rôle de coordinateur officieux de cette habilitation rend un bien modeste honneur à ses qualités humaines et professionnelles.

Je remercie Anne de Bouard, José Carrillo et Paul Dupuis pour leur lecture attentive de ce manuscrit. Je suis très honoré de l'intérêt qu'ils ont porté à mes travaux. Je suis également très honoré de la participation d'Annie Millet et Josselin Garnier à mon jury. Sept ans après la soutenance de ma thèse, rares sont les jours où je ne mets pas à profit les conseils et enseignements que j'ai reçus de Benjamin Jourdain et Lorenzo Zambotti pendant ma thèse. Je me réjouis donc de leur présence dans mon jury.

Je remercie l'ensemble des membres du CERMICS pour l'ambiance conviviale et dynamique qui y règne, même en temps de Covid. En lisant les remerciements des thèses et habilitations qui y sont soutenues, on pourrait croire qu'adresser une acclamation particulière à Stéphanie Bonnel et Isabelle Simunic est une figure imposée par le règlement du laboratoire ; c'est au contraire une évidence pour tous, tant leur présence nous est précieuse.

Je remercie l'ensemble des collègues avec lesquels j'ai eu la chance d'échanger, au travers de simples discussions, de bons moments passés en conférence, de collaborations scientifiques plus ou moins avancées, de coaching pour le dépôt de projets, d'enseignements communs ou de co-organisation d'événements — chacun se reconnaîtra. J'adresse un remerciement particulier à Freddy Bouchet, dont l'influence sur mes thèmes de recherche va bien au-delà de nos travaux communs présentés dans ce manuscrit.

Je remercie enfin mes amis et ma famille. Merci à Sara de ne jamais hésiter à prendre le relais lorsque j'ai besoin d'un petit moment pour faire des maths, et à Raphaël et Théophile de faire que ce moment ne dure jamais trop longtemps. Ce manuscrit vous est dédié, à tous les trois.

Contents

List of publications and organisation of the manuscript

This manuscript summarises the works that I have carried out since the end of my PhD thesis, first as a postdoc at Laboratoire de Physique in ENS de Lyon, and then as a researcher at CERMICS in École des Ponts ParisTech. It is divided into several chapters which present various projects and collaborations in which I have been involved. The chapters are written in order to be read independently one from each other. In particular, they all start with a short introduction to the general context, and most of them contain sketches of perspectives for future research.

In the present brief introduction, chapters are grouped into three thematic parts: conservation laws, metastability and uncertainty propagation. They are shortly described, and the corresponding publications are listed. The articles which are indicated with an asterisk are not reviewed in the body of the manuscript.

Approximation and long-time behaviour of conservation laws

Chapters 1 and 2 present results on the study of the probabilistic interpretation, and the approximation by particle systems, of one-dimensional scalar conservation laws. They are continuations of works from my PhD thesis [JR13, JR14, JR15, Rey15, JR16, Rey17], most of which were written in collaboration with my advisor Benjamin Jourdain (CERMICS, École des Ponts ParisTech).

[A1] J. Reygner.
Equilibrium large deviations for mean-field systems with translation invariance.
Annals of Applied Probability, 28(5):2922-2965, 2018.
Complement available at *hal-01546442v2*.

[A2] B. Jourdain, J. Reygner.
Optimal convergence rate of the multitype sticky particle approximation of one-dimensional diagonal hyperbolic systems with monotonic initial data.
Discrete and Continuous Dynamical Systems - Series A, 36(9):4963-4996, 2016.

Chapter 3 is dedicated to a collaboration with Sébastien Boyaval (Laboratoire d'Hydraulique Saint-Venant, École des Ponts ParisTech) on the Finite-Volume approximation of the invariant measure of stochastic scalar conservation laws. Together, we supervised the PhD thesis of Sofiane Martel (defended in 2019), who studied viscous conservation laws.

[A3] S. Martel, J. Reygner.
Viscous scalar conservation law with stochastic forcing: strong solution and invariant measure.
Nonlinear Differential Equations and Applications NoDEA, 27(3):34, 2020.

[A4] S. Boyaval, S. Martel, J. Reygner.
Finite-Volume approximation of the invariant measure of a viscous stochastic scalar conservation law.
Preprint arXiv:1909.08899, accepted in *IMA Journal of Numerical Analysis*.

Metastability and nonreversibility: theoretical and numerical issues

Chapter 4 presents works in collaboration with Freddy Bouchet (Laboratoire de Physique, ENS de Lyon) which started during my postdoc, on a formal approach to the metastability of nonreversible diffusion processes.

[A5] F. Bouchet, J. Reygner.
Generalisation of the Eyring–Kramers transition rate formula to irreversible diffusion processes.
Annales Henri Poincaré, 17(12):3499-3532, 2016.

[A6] F. Bouchet, J. Reygner.
Path integral derivation and numerical computation of large deviation prefactors for non-equilibrium dynamics through matrix Riccati equations.
Preprint arXiv:2108.06916.

Chapter 5 is dedicated to my collaboration with Tony Lelièvre (CERMICS, École des Ponts ParisTech) on the theoretical analysis of algorithms of molecular dynamics. Together, we supervised the masters' internship of Loucas Pillaud-Vivien (2016) on Fleming–Viot particle systems, and then the PhD thesis of Mouad Ramil (defended in 2020) on various aspects of Langevin processes.

[A7] T. Lelièvre, L. Pillaud-Vivien, J. Reygner.
Central Limit Theorem for stationary Fleming–Viot particle systems in finite spaces.
ALEA Latin American Journal of Probability and Mathematical Statistics, 15:1163-1182, 2018.

[A8] T. Lelièvre, M. Ramil, J. Reygner.
A probabilistic study of the kinetic Fokker-Planck equation in cylindrical domains.
Preprint arXiv:2010.10157.

[A9] T. Lelièvre, M. Ramil, J. Reygner.
Quasi-stationary distribution for the Langevin process in cylindrical domains, part I: existence, uniqueness and long-time convergence.
Preprint arXiv:2101.11999.

Uncertainty quantification in industrial problems

With Bernard Lapeyre (CERMICS, École des Ponts ParisTech), we have supervised the PhD thesis of Adrien Touboul (defended in 2021), in collaboration with Mouadh Yagoubi (IRT SystemX), Fabien Mangeant (Renault) and Pierre Benjamin (Airbus). The thesis is divided into two parts: the first part is dedicated to the formalisation of the concept of design margin in engineering processes and is not reviewed in the present manuscript; the second part is presented in Chapter 6 and is dedicated to numerical methods for uncertainty propagation in a graph of models.

[*A10] A. Touboul, J. Reygner, F. Mangeant, P. Benjamin.
A formal framework to define margins in industrial processes.
Preprint hal-02156493.

[A11] J. Reygner, A. Touboul.
Reweighting samples under covariate shift using a Wasserstein distance criterion.
Preprint arXiv:2010.09267, in revision for *Electronic Journal of Statistics*.

[A12] J. Reygner, A. Touboul.
Nonparametric regression reweighting and Bayesian network interpretation for decomposition-based uncertainty propagation in graphs of numerical models.
In progress.

Other industrial collaborations

As a conclusion to this introduction, I shall briefly present two more 'applied' projects on which I have worked but which are not reviewed in the manuscript.

First, as the teacher in charge of the course of *Statistics and Data Analysis* at École des Ponts ParisTech, I took part in a research project carried out by Matthieu Toulemont, a student in the engineering curriculum, in collaboration with cardiologists Serge Cazeau (Hôpital Saint-Joseph and Microport CRM) and Philippe Ritter (CHU Bordeaux).

[*A13] S. Cazeau, M. Toulemont, P. Ritter, J. Reygner.
Statistical ranking of electromechanical dyssynchrony parameters for CRT.
Open Heart, 6:e000933, 2019.
Complement available at *hal-01990215*.

Second, together with Frédéric Legoll (Laboratoire Navier, École des Ponts ParisTech), we have started a collaboration with OSMOS Group on the simulation and estimation of rare events in civil engineering. This project already hosted two six-month internships under our supervision and now supports the PhD thesis of Ales Libal (started in September 2020).

Chapter 1

Viscous scalar conservation laws and free energy

This chapter presents the results of the article [A1] and discusses research perspectives related to the works [JR13, Rey15, Rey17] from my PhD thesis.

1.1 Introduction

1.1.1 Rank-based interacting diffusions

Systems of one-dimensional *rank-based interacting diffusions* are defined by the system of stochastic differential equations (SDEs)

$$\mathrm{d}X_t^i = \sum_{k=1}^{n} \mathbb{1}_{\{X_t^i = X_t^{(k)}\}} \left(b_n(k)\mathrm{d}t + \sigma_n(k)\mathrm{d}B_t^i \right), \qquad i = 1, \dots, n, \tag{1.1}$$

where $b_n(1), \dots, b_n(n) \in \mathbb{R}$, $\sigma_n(1), \dots, \sigma_n(n) > 0$, $B^1, \dots, B^n$ are independent Brownian motions and, for any $t \geq 0$, the notation $X_t^{(1)} \leq \cdots \leq X_t^{(n)}$ denotes the order statistics of $X_t^1, \dots, X_t^n$. In this system, each process $(X_t^i)_{t\geq 0}$ describes the position of a particle on the real line; the particle with rank k has a constant drift coefficient $b_n(k)$ and diffusion coefficient $\sigma_n(k)$; and particles exchange their drift and diffusion coefficients when they cross each other. Such systems appear in particular in mathematical finance [Fer02, BFK05]. The fact that both the order statistics $(X_t^{(1)}, \dots, X_t^{(n)})_{t\geq 0}$ and the *gap process* $(X_t^{(2)} - X_t^{(1)}, \dots, X_t^{(n)} - X_t^{(n-1)})_{t\geq 0}$ write as multidimensional reflected Brownian motions [Tan79, Wil87] also makes them connected with the study of spin glasses models [RA05, AA09] or queuing systems [HW87a, HW87b, Wil95]. More references on applications and extensions of (1.1) may be found in the review paper [Rey17].

The *mean-field scaling*, under which the coefficients $b_n(1), \dots, b_n(n)$ and $\sigma_n(1), \dots, \sigma_n(n)$ are given by

$$b_n(k) = b\left(\frac{k}{n}\right), \qquad \sigma_n(k) = \sigma\left(\frac{k}{n}\right), \tag{1.2}$$

for some continuous functions $b : [0,1] \to \mathbb{R}$, $\sigma : [0,1] \to (0, +\infty)$, has the peculiarity to allow the study of the $n \to +\infty$ limit using the notion of *propagation of chaos* originating from statistical mechanics and kinetic theory [Kac56, Szn91]. Indeed, the system of SDEs (1.1) then rewrites

$$\mathrm{d}X_t^i = b\left(H * \mu_t^n(X_t^i)\right)\mathrm{d}t + \sigma\left(H * \mu_t^n(X_t^i)\right)\mathrm{d}B_t^i, \qquad i = 1, \dots, n,$$

where $H(x) = \mathbb{1}_{\{x\geq 0\}}$ denotes the Heaviside function and

$$\mu_t^n = \frac{1}{n}\sum_{i=1}^{n} \delta_{X_t^i}$$

is the empirical measure of $X_t^1, \dots, X_t^n$. Therefore, it may be expected that when $n \to +\infty$, any finite collection of particles behaves as independent copies of the diffusion process X solution to the SDE

$$\mathrm{d}X_t = b\left(H * \mu_t(X_t)\right)\mathrm{d}t + \sigma\left(H * \mu_t(X_t)\right)\mathrm{d}B_t, \qquad \mu_t := \mathrm{Law}(X_t). \tag{1.3}$$

Such a process is usually called *nonlinear* in McKean's sense [McK66, McK67] because the evolution of its time-marginal distribution μ_t is given by the nonlinear Fokker–Planck equation

$$\partial_t \mu_t = \frac{1}{2}\partial_{xx}\left(\sigma^2(H * \mu_t)\mu_t\right) - \partial_x\left(b(H * \mu_t)\mu_t\right). \tag{1.4}$$

Remarkably, the fact that the interaction kernel H be the Heaviside function allows one to integrate both sides of (1.4) on $(-\infty, x]$ and deduce that the Cumulative Distribution Function (CDF)

$$u(t,x) := H * \mu_t(x)$$

of X_t satisfies the local, nonlinear PDE

$$\partial_t u = \partial_{xx} A(u) - \partial_x B(u), \tag{1.5}$$

where

$$A(u) := \int_{v=0}^{u} \frac{\sigma^2(v)}{2}\mathrm{d}v, \qquad B(u) := \int_{v=0}^{u} b(v)\mathrm{d}v.$$

The equation (1.5) is a one-dimensional, scalar *conservation law* with *nonlinear viscosity* A and *flux* function B. Convergence results of the empirical CDF $u^n(t,x) = H * \mu_t^n(x)$ to $u(t,x)$ were obtained, under various assumptions on A, B and the initial condition u_0, by Bossy and Talay [BT96, BT97], Jourdain and coauthors [Jou97, Jou00b, Jou00a, Jou02b, JM08, JR13], Shkolnikov [Shk12]. These results were also complemented with Central Limit Theorems [Jou00a, KS18] and a Large Deviation Principle [DSVZ16], and rates of convergence for numerical methods were studied in [Bos04, BJb].

1.1.2 Link with McKean–Vlasov equation and free energy

Another well-studied class of particle systems with mean-field interaction is the so-called *McKean–Vlasov* particle system

$$\mathrm{d}X_t^i = -\nabla V(X_t^i)\mathrm{d}t - \frac{1}{n}\sum_{j=1}^{n}\nabla W(X_t^i - X_t^j)\mathrm{d}t + \sigma\mathrm{d}B_t^i, \qquad i = 1, \dots, n, \tag{1.6}$$

in $\mathbb{R}^d$, where $\sigma > 0$ and $V, W : \mathbb{R}^d \to \mathbb{R}$ are respectively called the *external* and *interaction* potentials. Their mean-field limit is described by the nonlinear Fokker–Planck equation

$$\partial_t \mu_t = \frac{\sigma^2}{2}\Delta\mu_t + \mathrm{div}\left(\mu_t\left(\nabla V + \nabla W * \mu_t\right)\right), \tag{1.7}$$

which we shall call the *McKean–Vlasov equation*[1] — it is also known as the *granular media equation* [BCP97, BCCP98, Mal03, CGM08].

Dawson and Gärtner [DG89] observed that the large deviations of the empirical measure μ_t^n of the particle system (1.6) around μ_t are described with a formalism similar to the Freidlin–Wentzell theory of finite-dimensional SDEs [FW12], where the role of the quasipotential is played by the *free energy function*. The latter is defined on the space $\mathcal{P}(\mathbb{R}^d)$ of probability measures on $\mathbb{R}^d$ by

$$\mathcal{F}[\mu] := \mathcal{S}[\mu] + \left(\mathcal{V}[\mu] + \mathcal{W}[\mu]\right), \tag{1.8}$$

[1] In this chapter, we take the convention to reserve the denomination 'McKean–Vlasov equation' for (1.7), while in the litterature this denomination sometimes refers to more general nonlinear Fokker–Planck equations.

where

$$\mathcal{S}[\mu] := \frac{\sigma^2}{2} \int_{x\in\mathbb{R}^d} (\log \mu(x))\, \mu(\mathrm{d}x) \tag{1.9}$$

is *Boltzmann's entropy*, and

$$\mathcal{V}[\mu] := \int_{x\in\mathbb{R}^d} V(x)\mu(\mathrm{d}x), \qquad \mathcal{W}[\mu] := \frac{1}{2}\int_{x,y\in\mathbb{R}^d} W(x-y)\mu(\mathrm{d}x)\mu(\mathrm{d}y), \tag{1.10}$$

respectively denote the *potential energy* and the *interaction energy*. Notice that in the definition of $\mathcal{S}[\mu]$, we implicitly assume that μ is absolutely continuous with respect to the Lebesgue measure and we keep the notation $\mu(x)$ to refer to its density — otherwise, we set $\mathcal{S}[\mu] = +\infty$. The free energy function is also central in the study of the long time behaviour of μ_t, since the McKean–Vlasov equation (1.7) is known to be the *gradient flow*, with respect to the metric structure induced on $\mathcal{P}(\mathbb{R}^d)$ by the quadratic Wasserstein distance, of this function [JKO98, Ott01, CMV03, CMV06, AGS08].

The purpose of Section 1.2 is to discuss the derivation of a similar free energy function for the system of rank-based interacting particles (1.1). We first do so from a large deviation perspective, presenting the results of [A1]. In Section 1.3, we then sketch perspectives for the application of the gradient flow approach to study the long time behaviour of (1.4).

1.2 The free energy of viscous conservation laws

1.2.1 Free energy for the McKean–Vlasov equation

In the Freidlin–Wentzell theory, the quasipotential associated with a small noise SDE is known to be closely related with the large deviation rate function of its stationary distribution, see [FW12, Theorem 4.3, p. 111 and Chapter 6]. We do not enter into the details of this theory here but take as a starting point of our study the equivalent question for the empirical measure of the particle system (1.6): if $(X^1_\infty, \dots, X^n_\infty)$ is a random vector in $(\mathbb{R}^d)^n$, distributed according to the stationary distribution[2] of the McKean–Vlasov particle system (1.6), how to describe the asymptotic (in the $n \to +\infty$ regime) distribution of the empirical measure

$$\mu^n_\infty := \frac{1}{n}\sum_{i=1}^n \delta_{X^i_\infty}, \tag{1.11}$$

which is a random variable in the space $\mathcal{P}(\mathbb{R}^d)$?

Formal derivation

Let us first assume that the interaction potential W in (1.6) vanishes, so that $X^1, \dots, X^n$ are independent diffusion processes, with drift $-\nabla V$. Then it is known that these processes have a unique stationary probability distribution if and only if

$$z := \int_{x\in\mathbb{R}^d} \exp\left(-\frac{2}{\sigma^2}V(x)\right) \mathrm{d}x < +\infty, \tag{1.12}$$

and that this distribution ν has density

$$q(x) := \frac{1}{z}\exp\left(-\frac{2}{\sigma^2}V(x)\right)$$

with respect to the Lebesgue measure $\mathrm{d}x$ on $\mathbb{R}^d$. Under this condition, let us denote by $Q_n := \nu^{\otimes n}$ the stationary distribution of the process $(X^1_t, \dots, X^n_t)_{t\geq 0}$ and by $\mathbb{Q}_n := Q_n \circ \pi_n^{-1}$ the pushfoward of Q_n

[2] The existence and uniqueness of which is discussed below, see (1.14).

by the mapping

$$\pi_n : \begin{cases} (\mathbb{R}^d)^n & \to & \mathcal{P}(\mathbb{R}^d) \\ (x_1, \dots, x_n) & \mapsto & \dfrac{1}{n}\displaystyle\sum_{i=1}^n \delta_{x_i}. \end{cases} \tag{1.13}$$

In other words, $\mathbb{Q}_n$ is the law of the random probability measure μ_∞^n defined in (1.11) when $W \equiv 0$. The classical Sanov theorem then states that the sequence $(\mathbb{Q}_n)_{n\geq 1}$ satisfies a large deviation principle (LDP) on the space $\mathcal{P}(\mathbb{R}^d)$, endowed with the topology of weak convergence, with rate function the relative entropy with respect to ν, defined by

$$\mathcal{R}(\mu|\nu) := \begin{cases} \displaystyle\int_{\mathbb{R}^d} \frac{\mathrm{d}\mu}{\mathrm{d}\nu} \log\left(\frac{\mathrm{d}\mu}{\mathrm{d}\nu}\right) \mathrm{d}\nu & \text{if } \mu \ll \nu, \\ +\infty & \text{otherwise.} \end{cases}$$

Let us now come back to the general case where W does not vanish. We assume that W is smooth on $\mathbb{R}^d$, bounded from below, and even. Then it is easily observed that the system of SDEs (1.6) rewrites under the form

$$\mathrm{d}\mathbf{X}_t = -n\boldsymbol{\nabla} U_n(\mathbf{X}_t)\mathrm{d}t + \sigma \mathrm{d}\mathbf{B}_t$$

in $(\mathbb{R}^d)^n$, with $\mathbf{X}_t = (X_t^1, \dots, X_t^n)$, $\mathbf{B}_t = (B_t^1, \dots, B_t^n)$, $\boldsymbol{\nabla} = (\nabla_{x_1}, \dots, \nabla_{x_n})$ and, for $\mathbf{x} = (x_1, \dots, x_n) \in (\mathbb{R}^d)^n$,

$$U_n(\mathbf{x}) := V_n(\mathbf{x}) + W_n(\mathbf{x}), \quad V_n(\mathbf{x}) := \frac{1}{n}\sum_{i=1}^n V(x_i), \quad W_n(\mathbf{x}) := \frac{1}{2n^2}\sum_{i,j=1}^n W(x_i - x_j).$$

As a consequence, under the condition (1.12), we have

$$Z_n := \int_{\mathbf{x}\in(\mathbb{R}^d)^n} \exp\left(-\frac{2n}{\sigma^2} U_n(\mathbf{x})\right) \mathrm{d}\mathbf{x} < +\infty,$$

and the process $(\mathbf{X}_t)_{t\geq 0}$ has a unique stationary distribution P_n, which has density

$$p_n(\mathbf{x}) := \frac{1}{Z_n} \exp\left(-\frac{2n}{\sigma^2} U_n(\mathbf{x})\right) \tag{1.14}$$

with respect to the Lebesgue measure $\mathrm{d}\mathbf{x}$ on $(\mathbb{R}^d)^n$.

At this point, two important observations are to be made: on the one hand, the probability measure P_n is absolutely continuous with respect to Q_n, with a density such that[3]

$$\frac{\mathrm{d}P_n}{\mathrm{d}Q_n}(\mathbf{x}) \propto \exp\left(-\frac{2n}{\sigma^2} W_n(\mathbf{x})\right);$$

on the other hand, the functions V_n and W_n appearing in the definition of U_n satisfy the identity

$$V_n = \mathcal{V} \circ \pi_n, \qquad W_n = \mathcal{W} \circ \pi_n,$$

where $\mathcal{V}$ and $\mathcal{W}$ are the potential and interaction energies introduced in (1.10), while π_n is the empirical measure operator defined in (1.13).

As a consequence of these two facts, we deduce that the pushforward measure $\mathbb{P}_n := P_n \circ \pi^{-1}$, which is the law of μ_∞^n defined in (1.11) in the presence of an interaction potential W, satisfies

$$\frac{\mathrm{d}\mathbb{P}_n}{\mathrm{d}\mathbb{Q}_n}[\mu] \propto \exp\left(-\frac{2n}{\sigma^2}\mathcal{W}[\mu]\right).$$

[3] Only proportionality relations will be relevant in the sequel, so we no longer write normalisation constants.

Rewriting the LDP for $\mathbb{Q}_n$, given by Sanov's theorem, under the formal expression

$$\mathrm{d}\mathbb{Q}_n[\mu] \propto \exp\left(-n\mathcal{R}(\mu|\nu)\right),$$

we may expect to deduce from the identity

$$\mathrm{d}\mathbb{P}_n[\mu] = \mathrm{d}\mathbb{Q}_n[\mu]\frac{\mathrm{d}\mathbb{P}_n}{\mathrm{d}\mathbb{Q}_n}[\mu] \propto \exp\left(-n\mathcal{R}(\mu|\nu) - \frac{2n}{\sigma^2}\mathcal{W}[\mu]\right)$$

that the sequence $(\mathbb{P}_n)_{n\geq 1}$ satisfies a LDP with rate function $\mathcal{R}(\mu|\nu) + \frac{2}{\sigma^2}\mathcal{W}[\mu]$, up to a normalising additive constant. It then follows from the form of ν and the definition of the relative entropy that this rate function rewrites

$$\mathcal{R}(\mu|\nu) + \frac{2}{\sigma^2}\mathcal{W}[\mu] = \frac{2}{\sigma^2}\mathcal{S}[\mu] + \frac{2}{\sigma^2}\mathcal{V}[\mu] + \log(z) + \frac{2}{\sigma^2}\mathcal{W}[\mu],$$

where $\mathcal{S}$ is defined in (1.9), so that the rate function for $\mathbb{P}_n$ finally writes

$$\mathcal{I}[\mu] := \frac{2}{\sigma^2}\left(\mathcal{F}[\mu] - \mathcal{F}_\star\right),$$

with $\mathcal{F}$ the free energy introduced in (1.8) and $\mathcal{F}_\star := \inf_{\mu\in\mathcal{P}(\mathbb{R}^d)}\mathcal{F}[\mu]$.

Rigorous results

The rigorous formulation of such a transfer of LDPs to absolutely continuous measures is usually called the *Laplace–Varadhan lemma*, or *tilted LDP*. In its most basic formulation (see for instance [dH00, Theorem III.17, p. 34]), it requires the function $\mathcal{W}$ to be continuous and bounded from below on the topological space on which the LDP for $\mathbb{Q}_n$ holds. Therefore, if W is continuous and bounded on $\mathbb{R}^d$, then $\mathcal{W}$ is continuous on $\mathcal{P}(\mathbb{R}^d)$, endowed with the topology of weak convergence, so that combining Sanov's theorem with the Laplace–Varadhan lemma already allows to make the LDP for $\mathbb{P}_n$ rigorous on $\mathcal{P}(\mathbb{R}^d)$.

When W is not bounded, the function $\mathcal{W}$ is no longer continuous on $\mathcal{P}(\mathbb{R}^d)$, although under our assumptions, it remains bounded from below and lower semicontinuous. Still, continuity can be recovered on stronger topologies. For instance, for any $p \in [1, +\infty)$, let $\mathcal{P}_p(\mathbb{R}^d)$ denote the set of probability measures on $\mathbb{R}^d$ with a finite p-th order moment, equipped with the p-Wasserstein topology. The latter is defined as the weakest topology making all maps $\mu \mapsto \int f\mathrm{d}\mu$ continuous for $f : \mathbb{R}^d \to \mathbb{R}$ such that $|f(x)| \leq C(1 + |x|^p)$. As a consequence, if $W(x) \leq C(1 + |x|^p)$ then the mapping $\mathcal{W}$ can be shown to be continuous on $\mathcal{P}_p(\mathbb{R}^d)$. In order to recover the LDP for $\mathbb{P}_n$ on $\mathcal{P}_p(\mathbb{R}^d)$ through the Laplace–Varadhan lemma, it then becomes necessary to know whether Sanov's theorem holds on Wasserstein topologies. A complete answer was given by Wang, Wang and Wu [WWW10]: the sequence $(\mathbb{Q}_n)_{n\geq 0}$ satisfies a LDP on $\mathcal{P}_p(\mathbb{R}^d)$ if and only if

$$\forall\lambda > 0, \qquad \int_{x\in\mathbb{R}^d}\exp(\lambda|x|^p)\mathrm{d}\nu(x) = \frac{1}{z}\int_{x\in\mathbb{R}^d}\exp\left(\lambda|x|^p - \frac{2}{\sigma^2}V(x)\right)\mathrm{d}x < +\infty.$$

As a consequence, to obtain the LDP for $\mathbb{P}_n$ on some $\mathcal{P}_p(\mathbb{R}^d)$ by combining Sanov's theorem with the Laplace–Varadhan lemma, one has to assume that V grows to infinity faster that $|x|^p$ while W does not grow to infinity faster than $|x|^p$. In short, the external potential has to have a stronger confining effect than the interaction potential.

This dissymmetry between the roles of V and W is a clear consequence of the two-step structure of our argument, which is common in the literature on large deviations and, in the context of (1.6), was originally employed in the work by Dawson and Gärtner [DG89, Section 4] — see also the introduction of the article by Léonard [Léo87] for a discussion of the topological aspects. However, in the expression (1.14) for the invariant measure of $(\mathbf{X}_t)_{t\geq 0}$, V and W seem to have comparable contributions to

the tails of P_n: said otherwise, if $V(x) \propto |x|^p$ and $W(x) \propto |x|^q$ then U_n has a maximal growth rate of order $\max(p, q)$ at infinity. Using the so-called *weak convergence approach* to large deviations [DE97], Dupuis, Laschos and Ramanan [DLR20] provided a different proof of the LDP for $\mathbb{P}_n$, which implies in particular that if

$$\forall \lambda > 0, \qquad \int_{x,y \in \mathbb{R}^d} \exp\left(\lambda(|x|^p + |y|^p) - \frac{2}{\sigma^2}\left(V(x) + V(y) + W(x-y)\right)\right) \mathrm{d}x\mathrm{d}y < +\infty,$$

then the LDP for $\mathbb{P}_n$ holds on $\mathcal{P}_p(\mathbb{R}^d)$. In this formulation, which clearly generalises the result by Wang, Wang and Wu to the case $W \neq 0$, the dissymmetry between the external and confining potential has vanished: if both V and W grow faster than $|x|^p$ then the LDP holds on $\mathcal{P}_p(\mathbb{R}^d)$. This remark will be important in the proof of the results of the next section.

Remark 1.2.1 (Singular interactions)**.** *The assumption that W be smooth excludes from our study all models with singular interactions, such as Coulomb gases. The reason for this choice, beyond the fact that it makes several parts of the analysis simpler, is that we chose to focus on particle systems which exhibit features similar to systems of rank-based interacting diffusions, as will be detailed in the next section. However, the techniques evoked above, namely the combination of Sanov's theorem with the Laplace–Varadhan lemma, or the weak convergence approach to large deviations, may also applied to models with singular interactions, and rates in n which are different from the mean-field scaling: see [CGZ14, DLR20] and the references therein.*

1.2.2 Equilibrium large deviations for translation invariant systems

There is an immediate and obvious problem for the transposition of the results of Subsection 1.2.1 to the system of rank-based interacting diffusions (1.1): this system does not admit an invariant (probability) measure. Indeed, for this system, the centre of mass

$$\Xi_t := \frac{1}{n}\sum_{i=1}^n X_t^i$$

is a one-dimensional Brownian motion with drift $\frac{1}{n}\sum_{k=1}^n b_n(k)$ and variance $\frac{1}{n^2}\sum_{k=1}^n \sigma_n(k)^2$, and therefore it cannot converge to some invariant measure. Under assumptions on the coefficients $b_n(k)$ which will be detailed below (see also [PP08, JM08]), a stationary behaviour can however be recovered for the system *seen from its centre of mass* $\widetilde{X}_t^i := X_t^i - \Xi_t$. The same remark also applies to the McKean–Vlasov particle system (1.6) when the external potential V vanishes [Mal03]. We shall address these two classes of models simultaneously, by placing ourselves in a general framework in which an abstract interaction potential function $\mathcal{W}$ is required to satisfy a certain number of conditions, deriving our results in this framework, and then checking that both the rank-based model and the McKean–Vlasov model without external potential satisfy these conditions.

General framework

For $d \geq 1$, we let $\mathcal{W} : \mathcal{P}(\mathbb{R}^d) \to [0, +\infty]$ be a function satisfying the following conditions:

(TI) translation invariance: for any $y \in \mathbb{R}^d$, for any $\mu \in \mathcal{P}(\mathbb{R}^d)$, we have $\mathcal{W}[\tau_y\mu] = \mathcal{W}[\mu]$, with τ_y the translation operator defined by

$$\int_{x\in\mathbb{R}^d} f(x)\mathrm{d}\tau_y\mu(x) = \int_{x\in\mathbb{R}^d} f(x+y)\mathrm{d}\mu(x);$$

(σF) σ-finiteness: if μ has compact support then $\mathcal{W}[\mu] < +\infty$;

(LSC) lower semicontinuity: the function $\mathcal{W}$ is lower semicontinuous on $\mathcal{P}(\mathbb{R}^d)$ (endowed with the topology of weak convergence);

(GC) growth control: there exists $\ell \geq 1$ and $\kappa_\ell > 0$ such that $\mathcal{W}[\mu] = +\infty$ if $\mu \notin \mathcal{P}_\ell(\mathbb{R}^d)$, and

$$\forall \widetilde{\mu} \in \widetilde{\mathcal{P}}_\ell(\mathbb{R}^d), \qquad \mathcal{W}[\widetilde{\mu}] \geq \kappa_\ell \int_{x\in\mathbb{R}^d} |x|^\ell \mathrm{d}\widetilde{\mu}(x),$$

where $\widetilde{\mathcal{P}}_\ell(\mathbb{R}^d)$ denotes the set of centered probability measures on $\mathbb{R}^d$ with a finite ℓ-th order moment.

Given such a function $\mathcal{W}$, for all $n \geq 2$, we define the *energy* of a configuration $\mathbf{x} = (x_1, \dots, x_n) \in (\mathbb{R}^d)^n$ by

$$W_n(\mathbf{x}) := \mathcal{W}[\pi_n(\mathbf{x})],$$

where we recall the definition (1.13) of π_n.

For some temperature parameter $\sigma > 0$ which we shall keep fixed in the sequel, the (σ-finite) measure with density $\exp(-\frac{2}{\sigma^2} W_n(\mathbf{x}))$ is formally invariant for the system of SDEs

$$\mathrm{d}X_t^i = -n\nabla_{x_i} W_n(\mathbf{X}_t)\mathrm{d}t + \sigma \mathrm{d}B_t^i, \qquad i = 1, \dots, n, \tag{1.15}$$

but by Assumption (TI), it cannot be normalised to a probability measure on $(\mathbb{R}^d)^n$. However, under Assumptions (TI), (σF), (LSC) and (GC), this density is integrable with respect to the Lebesgue measure $\mathrm{d}\widetilde{\mathbf{x}}$ on the linear subspace

$$M_{d,n} := \{\widetilde{\mathbf{x}} = (\widetilde{x}_1, \dots, \widetilde{x}_n) \in (\mathbb{R}^d)^n : \widetilde{x}_1 + \cdots + \widetilde{x}_n = 0\},$$

and we denote by $\widetilde{P}_n$ the associated probability measure on $M_{d,n}$. The diffusion process defined on $M_{d,n}$ by

$$\widetilde{X}_t^i := X_t^i - \Xi_t, \qquad \Xi_t := \frac{1}{n}\sum_{i=1}^n X_t^i, \tag{1.16}$$

then turns out to be reversible with respect to $\widetilde{P}_n$.

Example 1.2.2 (MKV-model)**.** *Let $W : \mathbb{R}^d \to [0, +\infty)$ be an even and lower semicontinuous function and define the function $\mathcal{W}^{\mathrm{MKV}}$ by*

$$\mathcal{W}^{\mathrm{MKV}}[\mu] := \frac{1}{2}\int_{x,y\in\mathbb{R}^d} W(x-y)\mathrm{d}\mu(x)\mathrm{d}\mu(y).$$

This function satisfies Assumptions (TI), (σF) and (LSC). Besides, if there is $\ell \geq 1$ and $\kappa_\ell > 0$ such that $W(x) \geq 2\kappa_\ell |x|^\ell$, then Assumption (GC) is satisfied with these parameters. If, in addition, W is C^1, then the corresponding particle system (1.15) is the McKean–Vlasov particle system (1.6) with interaction potential W and no external potential.

Example 1.2.3 (RB-model)**.** *Let $B : [0,1] \to [0, +\infty)$ be a C^1 function such that*

$$B(0) = B(1) = 0; \qquad \forall u \in (0,1), \quad B(u) > 0; \qquad B'(0) > 0 > B'(1); \tag{1.17}$$

and let $\mathcal{W}^{\mathrm{RB}}$ be defined on $\mathcal{P}(\mathbb{R})$ by

$$\mathcal{W}^{\mathrm{RB}}[\mu] := \int_{x\in\mathbb{R}} B(F_\mu(x))\mathrm{d}x,$$

where $F_\mu := H * \mu$ denotes the cumulative distribution function of μ. This function satisfies Assumptions (TI), (σF), (LSC) and Assumption (GC) with $\ell = 1$. Let us insist on the fact that, whatever the choice of B, Assumption (GC) is never *satisfied with some $\ell > 1$. Besides, the corresponding particle system (1.15) is the system of rank-based interacting diffusions (1.1), with drift coefficients*

$$b_n(k) = n\int_{u=(k-1)/n}^{k/n} b(u)\mathrm{d}u, \qquad b := B', \tag{1.18}$$

and constant diffusion coefficients $\sigma_n(k) = \sigma$.

Remark 1.2.4 (On the coefficients in the RB-model)**.** *As far as the drift coefficients are concerned, the modification from* (1.2) *to the 'finite-difference approximation'* (1.18) *allows for simpler computation but does not affect the results: all LDP statements below would be equally valid with* $b_n(k) = b(k/n)$*. On the other hand, the assumption that the diffusion coefficients be constant is important as it provides an explicit formula for the invariant measure* $\widetilde{P}_n$*. This assumption could however be relaxed: indeed, it is known that if the coefficients* $\sigma_n^2(1), \dots, \sigma_n^2(n)$ *are in arithmetic progression, then the invariant measure* $\widetilde{P}_n$ *of the centered particle system remains explicit [IPB+11, Theorem 2]. More precisely, taking* $b_n(k)$ *given by either* (1.2) *or* (1.18)*, and* $\sigma_n^2(k) := \sigma_0^2 + \rho k/n$ *with* $\rho > -\sigma_0^2$*, we then have*

$$\widetilde{P}_n(\mathrm{d}\widetilde{\mathbf{x}}) \propto \exp\left(-\frac{2}{\sigma_0^2} W_n(\widetilde{\mathbf{x}})\right) \mathrm{d}\widetilde{\mathbf{x}},$$

for some function W_n *such that* $W_n = \mathcal{W}^{\mathrm{RB}}_{\sigma_0^2,\rho}[\pi_n] + o(1/n)$ *and*

$$\mathcal{W}^{\mathrm{RB}}_{\sigma_0^2,\rho}[\mu] = \int_{x\in\mathbb{R}} \frac{B(F_\mu(x))}{1 + \frac{\rho}{\sigma_0^2} F_\mu(x)} \mathrm{d}x,$$

see also the introduction of [Rey15]. In this case we also expect our LDP statements to remain true.

Remark 1.2.5 (Intersection between both models)**.** *Taking* $d = 1$ *and* $W(x) = |x|$ *in the* MKV*-model yields*

$$\mathcal{W}^{\mathrm{MKV}}[\mu] := \frac{1}{2} \int_{x,y\in\mathbb{R}} |x-y| \mathrm{d}\mu(x) \mathrm{d}\mu(y) = \int_{x\in\mathbb{R}} F_\mu(x)(1 - F_\mu(x)) \mathrm{d}x,$$

so that this model coincides with the RB*-model with* $B(u) = u(1-u)$*. In this case, the conservation law* (1.5) *on* u *writes*

$$\partial_t u = \frac{\sigma^2}{2} \partial_{xx} u - \partial_x(u(1-u)),$$

which is a variant of Burgers' equation and the solution to which may be computed analytically thanks to the Cole–Hopf transform [JM08, Example 2.5].

Remark 1.2.6 (On the conditions in (1.17))**.** *The first condition in* (1.17) *ensures that* $\mathcal{W}^{\mathrm{RB}}$ *is not identically equal to* $+\infty$*. Under this first condition, the second condition equivalently rewrites*

$$\forall u \in (0,1), \qquad \frac{1}{u} \int_{v=0}^{u} b(v) \mathrm{d}v > \frac{1}{1-u} \int_{v=u}^{1} b(v) \mathrm{d}v.$$

The latter identity has the following interpretation for the particle system (1.1) *with drift coefficients given by* (1.18)*: in the large* n *limit,* $\frac{1}{u}\int_{v=0}^{u} b(v)\mathrm{d}v$ *is the average drift of the group of the* nu *left-most particles, while* $\frac{1}{1-u}\int_{v=u}^{1} b(v)\mathrm{d}v$ *is the average drift of the group of the* $n(1-u)$ *right-most particles. If the former average is larger than the latter, then both groups tend to drift toward each other, which ensures the global stability of the system around its centre of mass. The discrete version of this condition is actually known to be necessary and sufficient for the existence of the invariant measure* $\widetilde{P}_n$*, see the discussion in [Rey17, Section 2.2]. In the terminology of scalar conservation laws, this stability condition is called* Oleinik's entropy condition*. Likewise, the third condition in* (1.17) *is called* Lax' entropy condition*.*

Main results

Under Assumptions (TI), (σF), (LSC) and (GC), let us define the pushforward measure

$$\widetilde{\mathbb{P}}_n := \widetilde{P}_n \circ \pi_n^{-1}.$$

Our purpose is now to study the large deviations of the sequence $(\widetilde{\mathbb{P}}_n)_{n\geq 2}$. Compared with the McKean–Vlasov particle system of Subsection 1.2.1, there are two main differences: there is no external potential

V, and $\widetilde{\mathbb{P}}_n$ gives full weight to the space $\widetilde{\mathcal{P}}(\mathbb{R}^d)$ of centered probability measures on $\mathbb{R}^d$. Therefore, a natural conjecture is that the sequence $(\widetilde{\mathbb{P}}_n)_{n\geq 2}$ satisfies a LDP on $\mathcal{P}(\mathbb{R}^d)$ with rate function

$$\widetilde{\mathcal{I}}[\mu] = \begin{cases} \dfrac{2}{\sigma^2}\left(\mathcal{F}[\mu] - \mathcal{F}_\star\right) & \text{if } \mu \in \widetilde{\mathcal{P}}(\mathbb{R}^d), \\ +\infty & \text{otherwise,} \end{cases} \tag{1.19}$$

where the free energy $\mathcal{F}$ is defined by

$$\mathcal{F}[\mu] := \mathcal{S}[\mu] + \mathcal{W}[\mu],$$

and $\mathcal{F}_\star := \inf_{\widetilde{\mu}\in\widetilde{\mathcal{P}}(\mathbb{R}^d)} \mathcal{F}[\widetilde{\mu}]$.

In order to formalise this statement, we proceed as follows. Let us first introduce the following supplementary assumption.

(CC) Chaos compatibility: for any $\mu \in \mathcal{P}(\mathbb{R}^d)$, if $(Y_n)_{n\geq 1}$ is a sequence of independent random variables with law μ on some probability space $(\Omega, \mathcal{A}, \mathbf{P})$, then

$$\lim_{n\to+\infty} \mathbf{E}\left[W_n(Y_1, \dots, Y_n)\right] = \mathcal{W}[\mu].$$

For any $\eta > 0$, let us consider the probability measure P_n^η defined on $(\mathbb{R}^d)^n$ by

$$P_n^\eta(\mathrm{d}\mathbf{x}) \propto \exp\left(-\frac{2n}{\sigma^2}\left(\eta V_n(\mathbf{x}) + W_n(\mathbf{x})\right)\right)\mathrm{d}\mathbf{x}, \qquad V_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^n |x_i|^\ell,$$

with the index $\ell \geq 1$ given by Assumption (GC). This is the invariant measure of the particle system (1.15) to which a small external potential $\eta|x|^\ell$ has been added, in order to break the translation invariance and recover the existence of a stationary distribution. The next result, obtained in [A1], follows from the adaptation of the proof of [DLR20, Theorem 2.9].

Proposition 1.2.7 (Large deviations for $\mathbb{P}_n^\eta$)**.** *Let Assumptions* (TI)*,* (σF)*,* (LSC)*,* (GC) *and* (CC) *hold. Let $\ell \geq 1$ be the index given by Assumption* (GC)*. Let $\eta > 0$, and for all $n \geq 1$, let $\mathbb{P}_n^\eta := P_n^\eta \circ \pi_n^{-1}$.*

(i) The sequence $(\mathbb{P}_n)_{n\geq 1}$ satisfies a LDP on $\mathcal{P}(\mathbb{R}^d)$ with rate function

$$\mathcal{I}^\eta[\mu] := \frac{2}{\sigma^2}\left(\mathcal{F}^\eta[\mu] - \mathcal{F}_\star^\eta\right),$$

where

$$\mathcal{F}^\eta[\mu] := \mathcal{S}[\mu] + \eta\mathcal{V}[\mu] + \mathcal{W}[\mu], \quad \mathcal{V}[\mu] := \int_{x\in\mathbb{R}^d} |x|^\ell \mathrm{d}\mu(x), \quad \mathcal{F}_\star^\eta := \inf_{\mu\in\mathcal{P}(\mathbb{R}^d)} \mathcal{F}^\eta[\mu].$$

(ii) If $\ell > 1$, then for any $p \in [1, \ell)$, the LDP holds on $\mathcal{P}_p(\mathbb{R}^d)$, equipped with the p-Wasserstein topology, with the same rate function.

For any $p \geq 1$, let $\mathrm{T} : \mathcal{P}_p(\mathbb{R}^d) \to \widetilde{\mathcal{P}}_p(\mathbb{R}^d)$ be the centering operator defined by

$$\mathrm{T}\mu = \tau_{-\xi}\mu, \qquad \xi := \int_{x\in\mathbb{R}^d} x\mathrm{d}\mu(x).$$

This operator is continuous on $\mathcal{P}_p(\mathbb{R}^d)$, therefore by the contraction principle, we deduce that under the assumptions of Proposition 1.2.7 (ii), for any $p \in [1, \ell)$, the pushforward measure $\widetilde{\mathbb{P}}_n^\eta := \mathbb{P}_n^\eta \circ \mathrm{T}^{-1}$ satisfies a LDP on $\mathcal{P}_p(\mathbb{R}^d)$ with rate function

$$\widetilde{\mathcal{I}}^\eta[\mu] := \begin{cases} \inf\limits_{\mu':\mathrm{T}\mu'=\mu} \mathcal{I}^\eta[\mu'] & \text{if } \mu \in \widetilde{\mathcal{P}}_p(\mathbb{R}^d), \\ +\infty & \text{otherwise.} \end{cases}$$

It is then easy to see that when $\eta \to 0$, $\widetilde{\mathcal{I}}^\eta$ converges, in an appropriate sense, to the function $\widetilde{\mathcal{I}}$ defined in (1.19). But on the other hand, when $\eta \to 0$, $\widetilde{\mathbb{P}}_n^\eta$ converges to $\widetilde{\mathbb{P}}_n$, and under the following last (and more technical) assumption:

(SH) sub-homogeneity: for all $\epsilon \in (0,1)$, for any $\mathbf{x} \in (\mathbb{R}^d)^n$, $(1-\epsilon)W_n(\mathbf{x}) \geq W_n((1-\epsilon)\mathbf{x})$;

this convergence can be controlled sufficiently accurately, at the exponential scale, so as to ensure the continuity of the LDP and to yield the following statement, which is the first main result of [A1].

Theorem 1.2.8 (LDP in the Wasserstein topology)**.** *Let Assumptions* (TI)*,* (σF)*,* (LSC)*,* (GC)*,* (CC) *and* (SH) *hold. If the index $\ell \geq 1$ given by Assumption* (GC) *is such that $\ell > 1$, then for any $p \in [1, \ell)$, the sequence $(\widetilde{\mathbb{P}}_n)_{n\geq 2}$ satisfies a LDP on $\mathcal{P}_p(\mathbb{R}^d)$ with rate function $\widetilde{\mathcal{I}}$ defined by* (1.19)*.*

Remark that since the injection from $\mathcal{P}_p(\mathbb{R}^d)$ to $\mathcal{P}(\mathbb{R}^d)$ is continuous, the LDP of Theorem 1.2.8 also holds on $\mathcal{P}(\mathbb{R}^d)$, with the same rate function.

The requirement that $\ell > 1$ in Theorem 1.2.8 is rather annoying since it excludes the RB-model, for which $\ell = 1$, and which was the initial objective of our study. In the case $\ell = 1$, Proposition 1.2.7 only provides a LDP on the space $\mathcal{P}(\mathbb{R}^d)$, on which the centering operator T is not continuous, and not even well defined. This prevents the application of the contraction principle. In fact, it can be directly observed that if $\ell = 1$, the function $\widetilde{\mathcal{I}}$ defined in (1.19) does not have compact level sets, so the conjectured LDP cannot hold.

In order to reconnect the function $\widetilde{\mathcal{I}}$ with the large deviations of $\widetilde{\mathbb{P}}_n$, let us adopt the following slightly different point of view. We first denote by $\overline{\mathcal{P}}(\mathbb{R}^d)$ the quotient space of $\mathcal{P}(\mathbb{R}^d)$ defined by identifying measures which are translations of each other. For any $\mu \in \mathcal{P}(\mathbb{R}^d)$, we then denote by $\mathrm{t}\mu \in \overline{\mathcal{P}}(\mathbb{R}^d)$ the equivalence class of μ. For any $n \geq 2$ and $t \geq 0$, there is a one-to-one correspondance between the empirical measure $\widetilde{\mu}_t^n = \frac{1}{n}\sum_{i=1}^n \delta_{\widetilde{X}_t^i}$ of the centered particle system (1.16), and the equivalence class $\mathrm{t}\mu_t^n$ of the empirical measure $\mu_t^n = \frac{1}{n}\sum_{i=1}^n \delta_{X_t^i}$ of the original particle system (1.15), since the former is the unique centered element of the latter. Therefore, the stationary behaviour of the centered particle system (1.16) is equivalently described by the probability measure

$$\overline{\mathbb{P}}_n := \widetilde{\mathbb{P}}_n \circ \mathrm{t}^{-1}$$

on $\overline{\mathcal{P}}(\mathbb{R}^d)$, which no longer involves neither the centering operator T nor even the notion of centre of mass. Providing $\overline{\mathcal{P}}(\mathbb{R}^d)$ with the *quotient topology*, defined as the strongest topology making the quotient map $\mathrm{t} : \mathcal{P}(\mathbb{R}^d) \to \overline{\mathcal{P}}(\mathbb{R}^d)$ continuous, we may now combine the LDP of Proposition 1.2.7 (i) with the contraction principle to obtain a LDP, on $\overline{\mathcal{P}}(\mathbb{R}^d)$, for $\overline{\mathbb{P}}_n^\eta := \mathbb{P}_n^\eta \circ \mathrm{t}^{-1}$. Replacing the pair $(\mathrm{T}, \widetilde{\mathcal{P}}_p(\mathbb{R}^d))$ with $(\mathrm{t}, \overline{\mathcal{P}}(\mathbb{R}^d))$, the same arguments as for the proof of Theorem 1.2.8 now yield the following statement, which is the second main result of [A1].

Theorem 1.2.9 (LDP in the quotient topology)**.** *Let Assumptions* (TI)*,* (σF)*,* (LSC)*,* (GC)*,* (CC) *and* (SH) *hold. The sequence $(\overline{\mathbb{P}}_n)_{n\geq 2}$ satisfies a LDP on $\overline{\mathcal{P}}(\mathbb{R}^d)$ with rate function $\overline{\mathcal{I}}$ defined by*

$$\overline{\mathcal{I}}[\overline{\mu}] = \frac{2}{\sigma^2}\left(\overline{\mathcal{F}}[\overline{\mu}] - \mathcal{F}_\star\right),$$

where the free energy $\overline{\mathcal{F}}[\overline{\mu}]$ is defined by $\overline{\mathcal{F}}[\overline{\mu}] = \mathcal{S}[\mu] + \mathcal{W}[\mu]$ for any $\mu \in \overline{\mu}$, both functions $\mathcal{S}$ and $\mathcal{W}$ being translation invariant.

The use of this quotient procedure was partially inspired by a recent work by Mukherjee and Varadhan [MV16] on the study of translation invariant functionals of the Brownian occupation measure.

Application to rank-based interacting diffusions

Let us complete this section by discussing the application of Theorems 1.2.8 and 1.2.9 to the MKV- and RB-models of Examples 1.2.2 and 1.2.3. We already noted that Assumptions (TI), (σF), (LSC) and (GC) are satisfied in these two models. It turns out that Assumption (CC) is satisfied without further condition for both models, and that Assumption (SH) always holds for the RB-model (in fact, the demanded inequality is an equality), while it holds for the MKV-model as soon as $(1-\epsilon)W(x) \geq W((1-\epsilon)x)$ for any $\epsilon \in (0,1)$ and $x \in \mathbb{R}^d$. We single out the application of Theorem 1.2.9 to the RB-model in the next statement, thereby completing our task to define a free energy function for this model through equilibrium large deviations.

Corollary 1.2.10 (Equilibrium large deviations for rank-based particle systems)**.** *Let $B : [0,1] \to [0,+\infty]$ be a C^1 function satisfying the conditions (1.17).*

(i) For any $\sigma > 0$, the system of rank-based interacting diffusions with drift coefficients $b_n(k)$ given by (1.18) and constant diffusion coefficients $\sigma_n(k) = \sigma$, seen from its centre of mass, possesses a unique stationary distribution

$$\widetilde{P}_n(\mathrm{d}\widetilde{\mathbf{x}}) \propto \exp\left(-\frac{2n}{\sigma^2} W_n(\widetilde{\mathbf{x}})\right) \mathrm{d}\widetilde{\mathbf{x}}$$

on the hyperplane $M_{1,n}$, where

$$W_n(\widetilde{\mathbf{x}}) = -\frac{1}{n}\sum_{k=1}^{n} b_n(k)\widetilde{x}_{(k)}, \qquad \widetilde{x}_{(1)} \leq \cdots \leq \widetilde{x}_{(n)}.$$

(ii) Let $\overline{\mathbb{P}}_n$ refer to the law of the equivalence class of the empirical measure of a random vector with distribution $\widetilde{P}_n$. The sequence $(\overline{\mathbb{P}}_n)_{n\geq 2}$ satisfies a LDP on $\overline{\mathcal{P}}(\mathbb{R})$ with rate function equal, up to an additive constant, to $\frac{2}{\sigma^2}\overline{\mathcal{F}}^{\mathrm{RB}}$, with

$$\overline{\mathcal{F}}^{\mathrm{RB}}[\overline{\mu}] := \mathcal{S}[\mu] + \int_{x\in\mathbb{R}} B(F_\mu(x))\mathrm{d}x,$$

for any $\mu \in \overline{\mu}$, where we recall that F_μ refers to the CDF of μ.

This LDP complements the Law of Large Numbers of [Rey15], where under the same assumptions the sequence $\widetilde{\mathbb{P}}_n = \widetilde{P}_n \circ \pi_n^{-1}$ was proved to converge to $\delta_{\widetilde{\mu}_\infty}$, with $\widetilde{\mu}_\infty$ the unique centered stationary distribution of the nonlinear diffusion process

$$\mathrm{d}X_t = b(F_{\mu_t}(X_t))\mathrm{d}t + \sigma \mathrm{d}B_t, \qquad \mu_t = \mathrm{Law}(X_t).$$

It may also be seen as an infinite time horizon complement to the LDP obtained by Dembo, Shkolnikov, Varadhan and Zeitouni [DSVZ16] on the trajectories $(\mu_t^n)_{t\in[0,T]}$ for the system (1.1–1.2) (with a general, non-constant diffusion coefficient $\sigma : [0,1] \to (0,+\infty)$). Last, it also has practical applications in Stochastic Portfolio Theory [Fer02, BFK05, JR15], where each process X^i in (1.1) represents the log-capitalisation of a stock, and such quantities as the *market weight* of a stock are invariant under translations, so that Corollary 1.2.10 can be employed to describe their stationary fluctuations, see Section 5.3 in [A1]. To conclude in this direction, let us mention that mean-field models such as the McKean–Vlasov equation, with or without external potential, also arise in mathematical finance as a model for systemic risk, see [FL13] and also [GPY13] for large deviation estimates.

1.3 Gradient flow approach to the long time behaviour of (1.5)

1.3.1 Case of the McKean–Vlasov equation

The McKean–Vlasov equation (1.7) formally rewrites

$$\partial_t \mu_t = \mathrm{div}\left(\mu_t \nabla \frac{\delta \mathcal{F}}{\delta \mu}[\mu_t]\right), \tag{1.20}$$

where $\mathcal{F}$ is the free energy function defined by (1.8), and $\frac{\delta \mathcal{F}}{\delta \mu}$ is (still formally) the Gâteaux derivative of $\mathcal{F}$ with respect to μ. It easily follows from this interpretation that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[\mu_t] = -\int_{\mathbb{R}^d} \left|\nabla \frac{\delta \mathcal{F}}{\delta \mu}[\mu_t]\right|^2 \mathrm{d}\mu_t \leq 0,$$

so that $\mathcal{F}$ acts as a Lyapunov function and the study of its minimisers, wells, curvature, saddle-points... becomes of interest in order to describe quantitatively the long time behaviour of μ_t.

This rather formal description finds its rigorous formulation in the theory of *gradient flows* in spaces of probability measures presented in the monograph by Ambrosio, Gigli and Savaré [AGS08] and prefigurated in the articles by Jordan, Kinderlehrer and Otto [JKO98] and Otto [Ott01]; more precisely, the identity (1.20) can be interpreted as the fact that $(\mu_t)_{t\geq 0}$ is the gradient flow of $\mathcal{F}$ in the space $\mathcal{P}_2(\mathbb{R}^d)$, metrised by the quadratic Wasserstein distance [Vil09, Chapter 15]. As a consequence, many results on the long time behaviour of μ_t may be expected to follow from the analogy between (1.20) and the finite-dimensional dynamical system

$$\dot{m}_t := -\nabla F(m_t),$$

for some function $F : \mathbb{R}^k \to \mathbb{R}$. In particular, if F is uniformly convex and has a unique minimiser m_∞, then both $F(m_t) - F(m_\infty)$ and the Euclidean norm $\|m_t - m_\infty\|$ converge at an exponential rate to 0. In the infinite-dimensional space $\mathcal{P}_2(\mathbb{R}^d)$, the suitable generalisation of the notion of convexity is called *displacement convexity* and was introduced by McCann in [McC97]. Under conditions over the potentials V and W ensuring that the function $\mathcal{F}$ is uniformly displacement convex, there exists a unique minimiser μ_∞ of $\mathcal{F}$, which obviously is the unique stationary solution of (1.7), and the exponential decay of both $\mathcal{F}[\mu_t] - \mathcal{F}[\mu_\infty]$ and $W_2(\mu_t, \mu_\infty)$ was proved by Carrillo, McCann and Villani [CMV03, CMV06].

1.3.2 Long time behaviour of conservation laws

Let $(X_t)_{t\geq 0}$ be a solution to the nonlinear SDE (1.3). As soon as, $\mathrm{d}s$-almost everywhere, the CDF $u(s,\cdot)$ of X_s is continuous on $\mathbb{R}$, the expectation of X_t satisfies

$$\mathbb{E}[X_t] = \mathbb{E}[X_0] + \int_{s=0}^{t} \mathbb{E}[b(u(s, X_s))]\mathrm{d}s = \mathbb{E}[X_0] + tB(1),$$

so that the first condition in (1.17) ensures that the expectation of X_t remains constant. Under this condition, the Oleinik entropy condition, namely the second condition in (1.17), ensures that the nonlinear Fokker–Planck (1.4), or equivalently the scalar conservation law (1.5), possesses a stationary solution μ_∞, which is unique up to spatial translation. The convergence of μ_t to μ_∞ has been extensively studied in relation with the notion of stability of traveling waves for the conservation law (1.5). In particular, it follows from results by Osher and Ralston [OR82], Freistühler and Serre [FS98], and Serre [Ser02], that if the diffusion coefficient σ is constant, then the CDF $u(t,\cdot)$ of μ_t converges, in $L^1(\mathbb{R})$, to the CDF u_∞ of the stationary solution μ_∞ with the same expectation as the initial condition. This result was then extended to a nonconstant diffusion coefficient by Gasnikov [Gas09].

The convergence of $u(t,\cdot)$ in $L^1(\mathbb{R})$ is actually directly related with the Wasserstein topology on $\mathcal{P}(\mathbb{R})$. Indeed, we recall that in general, for any $p \in [1, +\infty)$, the Wasserstein distance of order p between two probability measures $\mu, \nu \in \mathcal{P}_p(\mathbb{R}^d)$ is defined by

$$W_p(\mu,\nu) := \inf \mathbb{E}[|X - Y|^p]^{1/p},$$

where the infimum is taken over all pairs of random variables (X, Y) with marginal distributions μ and ν. In dimension $d = 1$, an optimal coupling (for all values of p) is given by

$$X = F_\mu^{-1}(U), \qquad Y = F_\nu^{-1}(U),$$

where U is a uniform random variable on $[0,1]$ and, for any CDF F, the *pseudo-inverse* F^{-1} is defined by

$$\forall u \in (0,1), \qquad F^{-1}(u) := \inf\{x \in \mathbb{R} : F(x) \geq u\}.$$

As a consequence, for any $\mu, \nu \in \mathcal{P}_p(\mathbb{R})$,

$$W_p(\mu,\nu) = \left(\int_{u=0}^{1} |F_\mu^{-1}(u) - F_\nu^{-1}(u)|^p \mathrm{d}u\right)^{1/p}, \tag{1.21}$$

and when $p = 1$, the right-hand side coincides with $\|F_\mu - F_\nu\|_{L^1(\mathbb{R})}$. Therefore, convergence results in $L^1(\mathbb{R})$ for (1.5) are equivalently expressed as convergence results in $\mathcal{P}_1(\mathbb{R})$ for (1.4). These results were extended to Wasserstein distances of order $p \geq 1$ in [JR13], in the spirit of previous works [CT04, CGT04, CDFL07].

1.3.3 Gradient flow approach for conservation laws

In order to connect the study of the long time behaviour of (1.4-1.5) with the gradient flow approach described above for the McKean–Vlasov equation, let us now observe that for a constant diffusion coefficient σ^2, the nonlinear Fokker–Planck equation (1.4) rewrites, at the same formal level as (1.20),

$$\partial_t \mu_t = \partial_x \left(\mu_t \partial_x \frac{\delta \mathcal{F}}{\delta \mu}[\mu_t] \right),$$

with the free energy function $\mathcal{F} := \mathcal{S} + \mathcal{W}$ given by

$$\mathcal{S}[\mu] := \frac{\sigma^2}{2} \int_{x \in \mathbb{R}} (\log \mu(x))\, \mu(x) \mathrm{d}x, \qquad \mathcal{W}[\mu] := \int_{x \in \mathbb{R}} B(F_\mu(x)) \mathrm{d}x.$$

Following the gradient flow approach [CMV03, CMV06, AGS08], rates of convergence of μ_t to μ_∞ can then be expected to be derived from the study of the displacement convexity of the function $\mathcal{F}$. The one-dimensional setting allows for a technical simplification here: indeed, the identity (1.21) shows that the mapping $\mu \mapsto F_\mu^{-1}$ induces an isometric embedding of the metric space $\mathcal{P}_p(\mathbb{R})$ into the linear space $L^p(0,1)$, such that displacement convexity in $\mathcal{P}_p(\mathbb{R})$ reduces to standard convexity in $L^p(0,1)$. Rewriting the entropy and the interaction energy under the form

$$\mathcal{S}[\mu] = -\frac{\sigma^2}{2} \int_{u=0}^{1} \left(\log(F_\mu^{-1})'(u) \right) \mathrm{d}u, \qquad \mathcal{W}[\mu] = -\int_{u=0}^{1} F_\mu^{-1}(u) b(u) \mathrm{d}u,$$

we then observe that $\mathcal{S}$ is convex but not uniformly convex, and that $\mathcal{W}$ appears as a linear perturbation of $\mathcal{S}$. Therefore, while the assumptions on B make this perturbation 'strong enough' for the function $\mathcal{F}$ to admit global minimisers (which $\mathcal{S}$ does not have), it does not have any effect on its curvature and this function is never uniformly convex. Hence, at least from this formal analysis, no exponential convergence of μ_t to μ_∞ can be expected to be observed without more restrictions on the initial condition μ_0.

In fact, it is known that the rate of convergence of solutions to (1.4) strongly depends on the tail of the initial condition μ_0 (see for instance [JGK93, MN94, How99, NZ02] and the references therein), therefore a general study of the rate of convergence of μ_t to μ_∞ within the gradient flow interpretation would probably require finer estimates on the dissipation of $\mathcal{S}[\mu_t]$ and $\mathcal{W}[\mu_t]$. This question is currently being investigated by means of Poincaré inequalities, which are known to be related with the curvature of $\mathcal{S}$ [CG03].

Chapter 2

Rate of convergence for sticky particle dynamics

This chapter presents the results of [A2], written in collaboration with Benjamin Jourdain.

2.1 Introduction

This chapter is dedicated to the study of systems of finitely many particles evolving on the real line at constant velocity between collisions, and sticking together into clusters at collisions, with preservation of total mass and momentum. Such collisions are called *perfectly inelastic*, and the resulting (deterministic) dynamics is called the *sticky particle dynamics* in one dimension. The latter is known to be relevant in the modelling of pressureless systems, which makes it of interest in astrophysics or gas dynamics [Zel70, VDFN94].

Let us denote by $m_1, \dots, m_n > 0$ the respective masses of the particles, and by $x_1^0 \leq \cdots \leq x_n^0$ and $v_1^0, \dots, v_n^0 \in \mathbb{R}$ their respective initial positions and velocities. If at some time $t \geq 0$, a cluster is composed by the particles of indices $k, k+1, \dots, l-1, l$, then its velocity $v_{k:l}$ is given by

$$v_{k:l} := \frac{m_k v_k^0 + \cdots + m_l v_l^0}{m_k + \cdots + m_l}, \tag{2.1}$$

and a necessary condition for the existence of the cluster is the fact that, for any $k' \in \{k+1, \dots, l\}$,

$$v_{k:k'-1} \geq v_{k':l}, \tag{2.2}$$

otherwise the cluster would split into diverging parts.

Let us then denote by $x_1(t) \leq \cdots \leq x_n(t)$ the respective positions of the particles at time t and introduce the *mass distribution*

$$\rho(t) := \sum_{k=1}^{n} m_k \delta_{x_k(t)}.$$

We finally call *velocity distribution* any measurable function $v : [0, +\infty) \times \mathbb{R}$ such that, $\mathrm{d}t$-almost everywhere, for all $k \in \{1, \dots, n\}$, $v(t, x_k(t)) = \dot{x}_k(t)$. The pair (ρ, v) turns out to solve, in the distributional sense, the system of partial differential equations

$$\begin{cases} \partial_t \rho + \partial_x(\rho v) = 0, \\ \partial_t(\rho v) + \partial_x(\rho v^2) = 0, \end{cases}$$

which respectively encode the preservation of mass and momentum. We refer to the recent survey by Hynd [Hyn19] for developments on the mathematical study of this system and bibliographical references. We also mention that there is an important litterature, in the probability theory community, dedicated to

the study of *sticky diffusions*, see for instance [BRHC20] and the references therein, but the questions of interest in this context are quite different.

Another description of the sticky particle dynamics in terms of partial differential equations was provided by Brenier and Grenier [BG98]. Let us assume, for simplicity, that the total mass of the system $m_1 + \cdots + m_n$ is normalised to 1. Let $B_n : [0,1] \to \mathbb{R}$ be defined by

$$\forall u \in [0,1], \qquad B_n(u) := \int_{v=0}^{u} \sum_{k=1}^{n} v_k^0 \mathbb{1}_{\{m_1+\cdots+m_{k-1}<v<m_1+\cdots+m_k\}} \mathrm{d}v,$$

and for all $t \geq 0$, let

$$u_n(t,x) := \sum_{k=1}^{n} m_k \mathbb{1}_{\{x_k(t)\leq x\}} \in [0,1]$$

be the cumulative distribution function (CDF) of the particle system. Then u_n is the unique entropy solution to the scalar conservation law

$$\begin{cases} \partial_t u_n + \partial_x B_n(u_n) = 0, \\ \qquad u_n(0,x) = u_n^0(x), \end{cases} \tag{2.3}$$

where $u_n^0(x) := \sum_{k=1}^n m_k \mathbb{1}_{\{x_k^0 \leq x\}}$. This follows from the fact that particles, or more generally clusters of particles, can be seen as *shocks* for the solution u_n, and collisions between these clusters satisfy the entropy condition. As a consequence of this observation, it turns out that if one takes a sequence of particle systems with parameters $(m_{k,n}, x_{k,n}^0, v_{k,n}^0)_{1\leq k\leq n}$ such that the initial condition u_n^0 and the flux function B_n converge to some functions $u^0 : \mathbb{R} \to [0,1]$ and $B : [0,1] \to \mathbb{R}$, then the associated CDF u_n converges to the entropy solution u to the scalar conservation law

$$\begin{cases} \partial_t u + \partial_x B(u) = 0, \\ \qquad u(0,x) = u^0(x). \end{cases} \tag{2.4}$$

This result can be seen either from a 'kinetic theory' point of view as the hydrodynamic description of large sticky particle systems, or from a 'numerical analysis' point of view as the convergence of a discretisation of the conservation law (2.4)[1]. From both points of view, the quantification of this convergence is of interest, and this is the purpose of this chapter.

We first establish a Wasserstein stability result for conservation laws with different flux functions, from which convergence rates are then deduced. The results presented in this chapter are slight extensions of [A2], in which *multitype* sticky particle dynamics, which are related to diagonal systems of conservation laws, are also addressed.

Remark 2.1.1 (Link with systems of rank-based interacting diffusions)**.** *When all masses are equal to $1/n$, the sticky particle dynamics is known [JR14] to describe the $\epsilon \to 0$ limit of the solution to the system of rank-based interacting diffusions (1.1) studied in Chapter 1, with coefficients $b_n(k) = v_k^0$ and $\sigma_n(k) = \epsilon$. From this perspective, the condition (2.2) for the existence of clusters is reminiscent of the stability condition discussed in Remark 1.2.6, and the convergence of u_n to u is a zero-noise version of propagation of chaos results.*

2.2 Stability and rate of convergence

Similarly to Chapter 1, we endow the space of CDFs on the line with Wasserstein distances, which we directly define, for $p \in [1, +\infty)$ and two CDFs $u, \overline{u} : \mathbb{R} \to [0,1]$, by

$$W_p(u,\overline{u}) := \left(\int_{v=0}^{1} |u^{-1}(v) - \overline{u}^{-1}(v)|^p \mathrm{d}v \right)^{1/p},$$

[1] The sticky particle dynamics is extremely simple to simulate exactly. In particular, an elementary convexity 'trick' enables one to compute the positions of particles at time $t \geq 0$ in $O(n)$ operations without having to simulate explicitly all trajectories and collisions on $[0,t]$, see Section 4 in [BG98] or Section 5.1 in [A2].

where u^{-1}, $\overline{u}^{-1}$ denote the pseudo-inverses of u, $\overline{u}$. We recall that for $p = 1$, the Wasserstein distance coincides with the $L^1(\mathbb{R})$ distance. The following result was proved in [A2], Proposition 1.4, only in the case $p = 1$, but the arguments can actually be adapted to the case $p \geq 1$ as is sketched below.

Theorem 2.2.1 (Wasserstein stability)**.** *Let u^0, $\overline{u}^0$ be CDFs on the real line, and $B, \overline{B} : [0,1] \to \mathbb{R}$ be Lipschitz continuous functions. Let u and $\overline{u}$ be the respective entropy solutions to the scalar conservation laws*

$$\begin{cases} \partial_t u + \partial_x B(u) = 0, \\ u(0,x) = u^0(x), \end{cases} \qquad \begin{cases} \partial_t \overline{u} + \partial_x \overline{B}(\overline{u}) = 0, \\ \overline{u}(0,x) = \overline{u}^0(x). \end{cases}$$

For all $0 \leq s \leq t$, for all $p \in [1, +\infty)$,

$$W_p(u(t,\cdot), \overline{u}(t,\cdot)) \leq W_p(u(s,\cdot), \overline{u}(s,\cdot)) + (t-s) \left(\int_{v=0}^1 |B'(v) - \overline{B}'(v)|^p \mathrm{d}v \right)^{1/p}.$$

In the case where $B = \overline{B}$, this result was first obtained by Bolley, Brenier and Loeper [BBL05], for all values of p.

The basic ingredient of the proof of Theorem 2.2.1 is the following discrete version of this stability estimate, for the sticky particle dynamics.

Proposition 2.2.2 (Wasserstein stability of the sticky particle dynamics)**.** *Let u_n and $\overline{u}_n$ denote the empirical CDFs of sticky particle dynamics with respective initial positions and velocities $x_1^0 \leq \cdots \leq x_n^0$, $v_1^0, \ldots, v_n^0$ and $\overline{x}_1^0 \leq \cdots \leq \overline{x}_n^0$, $\overline{v}_1^0, \ldots, \overline{v}_n^0$, and pairwise equal masses $m_1 = \overline{m}_1, \ldots, m_n = \overline{m}_n$. For all $0 \leq s \leq t$, for all $p \in [1, +\infty)$,*

$$W_p(u_n(t,\cdot), \overline{u}_n(t,\cdot)) \leq W_p(u_n(s,\cdot), \overline{u}_n(s,\cdot)) + (t-s) \left(\sum_{k=1}^n m_k |v_k^0 - \overline{v}_k^0|^p \right)^{1/p}.$$

Theorem 2.2.1 is then deduced from Proposition 2.2.2 by an approximation argument using the Brenier–Grenier convergence result, see Appendix A in [A2] for details.

Proof of Proposition 2.2.2. Let us denote by $x_1(t) \leq \cdots \leq x_n(t)$ and $\overline{x}_1(t) \leq \cdots \leq \overline{x}_n(t)$ the respective positions of particles in both systems. It follows from the definition of Wasserstein distances that, for any $t \geq 0$ and $p \in [1, +\infty)$,

$$W_p^p(u_n(t,\cdot), \overline{u}_n(t,\cdot)) = \sum_{k=1}^n m_k |x_k(t) - \overline{x}_k(t)|^p. \tag{2.5}$$

Let $c_k(t) := \{k' \in \{1, \ldots, n\} : x_{k'}(t) = x_k(t)\}$ denote the cluster in which the k-th particle lies at time $t \geq 0$ in the first system. For almost every $t \geq 0$, set

$$\gamma_k(t) := \sum_{k' \in c_k(t), k' \leq k} m_{k'} \left(v_{k'}^0 - \dot{x}_{k'}(t) \right), \qquad k = 1, \ldots, n,$$

and $\gamma_{n+1}(t) := 0$. Then it follows from (2.1) and (2.2) that $\gamma_k(t) \geq 0$, and if $x_k(t) < x_{k+1}(t)$ then $\gamma_k(t) = 0$; besides, by construction,

$$m_k \dot{x}_k(t) = m_k v_k^0 + \gamma_k(t) - \gamma_{k+1}(t), \qquad \mathrm{d}t\text{-almost everywhere.}$$

Obviously, a similar identity also holds for the second system. As a consequence,

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{k=1}^n m_k |x_k(t) - \overline{x}_k(t)|^p \leq p \sum_{k=1}^n m_k \mathrm{sgn}(x_k(t) - \overline{x}_k(t)) |x_k(t) - \overline{x}_k(t)|^{p-1} (v_k^0 - \overline{v}_k^0),$$

which by Hölder's inequality yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{k=1}^{n} m_k|x_k(t)-\overline{x}_k(t)|^p \leq p\left(\sum_{k=1}^{n} m_k|x_k(t)-\overline{x}_k(t)|^p\right)^{1-1/p}\left(\sum_{k=1}^{n} m_k|v_k^0-\overline{v}_k^0|^p\right)^{1/p},$$

and the claimed estimate finally follows from Gronwall's lemma combined with (2.5). □

The application of Theorem 2.2.1 to the study of the rate of convergence of the sticky particle dynamics is obvious: letting u_n and u be the respective entropy solutions to the scalar conservation laws (2.3) and (2.4), we get, for any $t \geq 0$ and $p \geq 1$,

$$W_p(u_n(t,\cdot),u(t,\cdot)) \leq W_p(u_n^0,u^0) + t\left(\int_{v=0}^{1}|B_n'(v)-B'(v)|^p\mathrm{d}v\right)^{1/p}.$$

From the numerical analysis point of view, this shows that if one wants to discretise (2.4) thanks to a sticky particle scheme, then the global discretisation error naturally decomposes as the sum of discretisation errors for the initial condition and the flux. In [A2] (see also [Jou02a, JR16]), all particles are taken to have the same mass $1/n$. In this case, the optimal discretisation of the initial condition was thoroughly studied by Bencheikh and Jourdain in the recent work [BJa]; apart from the case where u^0 is the CDF of a Dirac mass, the best rate of convergence that can be expected is $1/n$ (see also [XB19]). On the other hand, as soon as B' is Lipschitz continuous, then defining the initial velocities for the sticky particle dynamics by

$$v_k^0 = n\left(B\left(\frac{k}{n}\right) - B\left(\frac{k-1}{n}\right)\right) \quad \text{or} \quad B'\left(\frac{k}{n}\right)$$

also yields a rate $1/n$ for the flux term. Overall, we deduce that the sticky particle dynamics converges to the conservation law at rate $1/n$, with a constant which grows linearly in time, for Wasserstein distances of all orders. This rate is optimal in the sense that there are examples for which the discretisation error is indeed of order $1/n$. The sticky particle dynamics was also proved to display the same computational cost, for a given required level of precision, as such standard methods as upwind schemes, see Section 5 in [A2] for details.

The arguments detailed in this chapter can be generalised to study the rate of convergence, together with a simple numerical algorithm, for the *multitype* sticky particle dynamics introduced in [JR16] to approximate diagonal systems of conservation laws. In any case, the assumption that the initial condition u^0 be a CDF, and thus nonincreasing, is rather restrictive for practical applications. In [Jou02a], Jourdain introduced a system of sticky particle dynamics with signed masses and proved the convergence of the latter to the entropy solution of scalar conservation laws with bounded and BV initial conditions. The estimation of the rate of convergence for such a system (in $L^1(\mathbb{R})$, since in this case Wasserstein distances no longer make sense) is therefore a natural perspective for the continuation of the works presented in this chapter.

Chapter 3

Finite-Volume approximation of stationary distributions of stochastic conservation laws

This chapter presents the results of the articles [A3] and [A4], written in collaboration with Sébastien Boyaval and Sofiane Martel during Sofiane Martel's PhD thesis.

3.1 Introduction

3.1.1 Stochastic scalar conservation laws in statistical hydrodynamics

Stochastic conservation laws play a particular role in the study of the turbulence phenomenon. In particular, the field of *statistical hydrodynamics* [AFS08] aims at understanding the behaviour of the solution $u(t,x) \in \mathbb{R}^d$ to equations of fluid mechanics, such as the Euler or Navier–Stokes equation

$$\partial_t u + (u \cdot \nabla)u = \nu \Delta u - \nabla p + \xi, \qquad \operatorname{div} u = 0, \qquad \begin{cases} \nu = 0 & \text{(Euler)} \\ \nu > 0 & \text{(Navier–Stokes)} \end{cases} \tag{3.1}$$

perturbed by a source term $\xi(t,x)$ which is *stochastic*. In contrast with other domains of physics, such as statistical mechanics or quantum field theory, where white-in-space noise is a natural model and leads to *singular* SPDEs [Hai14, GIP15], here the noise term is usually sufficiently spatially correlated to make the realisations of the random field $\xi(t,x)$ smooth in the d-dimensional space variable [Zam21]. This does not however necessarily imply that the solution $u(t,x)$ is smooth itself, since when the *viscosity* parameter ν vanishes, the effect of the nonlinear *transport* term $(u \cdot \nabla)u$ may create shocks and result in the loss of spatial regularity.

When the solution $u(t,x)$ evolves as a Markov process, which typically requires the noise to be white-in-time, its *stationary distribution* is of particular interest since it describes the statistics of the fluid independently from the arbitrary choice of an initial condition. We refer for instance to [HM06, KS12] for a thorough exposition of the ergodic theory of the stochastic Navier–Stokes equation in dimension $d = 2$. In the sequel of this chapter, we focus on the case $d = 1$, so that (3.1) reduces to the one-dimensional stochastic Burgers equation

$$\partial_t u + u \partial_x u = \nu \partial_{xx} u + \xi, \tag{3.2}$$

the turbulent behaviour of which is sometimes referred to as *Burgulence* [FB01, BK07, Bor13b]. When $\nu > 0$, the Laplacian operator provides a dissipation mechanism which yields the existence of a stationary distribution [Sin91, Sin96]. Related quantitative estimates independent from ν were obtained in [Bor12, Bor13a]. In the *inviscid* case $\nu = 0$, E, Khanin, Mazel and Sinai showed in [EKMS00] that shocks in the entropy solution to (3.2) dissipate enough energy to maintain an ergodic behaviour.

The stochastic Burgers equation (3.2) is a particular case of a stochastic *conservation law*

$$\partial_t u + \partial_x A(u) = \nu \partial_{xx} u + \xi, \tag{3.3}$$

with the specific choice of a quadratic *flux* function $A(u) = u^2/2$. Still in the inviscid case $\nu = 0$, Debussche and Vovelle proved in [DV15] that under some *nondegeneracy* condition on A, which is in particular satisfied for uniformly convex flux functions, the solution u still admits a unique stationary distribution, thereby extending the results of [EKMS00] from the Burgers equation to the whole family of scalar conservation laws (3.3).

This result was the starting point of our collaboration with Sébastien Boyaval and of the PhD thesis of Sofiane Martel. Seeing scalar conservation laws of the form (3.3) as simplified models for more physically relevant *systems* of conservation laws, such as the shallow water equations[1], we wanted to construct a numerical scheme for (3.3) which would allow, under the assumptions of [DV15], to approximate the stationary distribution of the solution to this equation. We decided to study the Finite-Volume method [EGH00] which is particularly suitable for conservation laws.

3.1.2 Finite-Volume semidiscretisation and long time behaviour

Let us consider the stochastic scalar conservation law (3.3) on the one-dimensional torus $\mathbb{T} := \mathbb{R}/\mathbb{Z}$, which we identify with the interval $(0, 1]$. For the moment we do not give a precise meaning to the noise term $\xi(t, x)$. In order to explain the idea of the Finite-Volume method, we also leave the Laplacian term apart temporarily and thus assume that $\nu = 0$.

Fix $N \geq 1$, divide $\mathbb{T}$ into N intervals $I_i = ((i-1)/N, i/N]$ for $i \in \mathbb{T}_N := \mathbb{Z}/N\mathbb{Z}$ (which is identified with $\{1, \dots, N\}$), and call $x_i = i/N \in \mathbb{T}$ the *interface* between I_i and I_{i+1}. Averaging both sides of (3.3) on the interval I_i leads to the identity

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(N \int_{x=x_{i-1}}^{x_i} u(t,x)\mathrm{d}x\right) + N\left(A(u(t,x_i)) - A(u(t,x_{i-1}))\right) = N \int_{x=x_{i-1}}^{x_i} \xi(t,x)\mathrm{d}x.$$

Let us denote by $U_i^N(t)$ a quantity whose purpose is to approximate the average value of $u(t, x)$ on the interval I_i. The basic idea of the Finite-Volume method (in dimension 1) then consists in approximating the *flux* $A(u(t, x_i))$ at the interface x_i by a function $\overline{A}(U_i^N(t), U_{i+1}^N(t))$ of the approximate value of the solution on both sides of the interface. The function $\overline{A} : \mathbb{R}^2 \to \mathbb{R}$ is called a *numerical flux*, and it is typically required to satisfy the following assumptions:

(NF1) consistency: for all $v \in \mathbb{R}$, $\overline{A}(v, v) = A(v)$;

(NF2) monotonicity: $\overline{A}(v, w)$ is nondecreasing in v and nonincreasing in w.

Example 3.1.1 (The Engquist–Osher scheme)**.** *Let $A : \mathbb{R} \to \mathbb{R}$ be a C^1 flux function. Assume, without loss of generality, that $A(0) = 0$. The* Engquist–Osher *numerical flux, defined by*

$$\overline{A}(v, w) := A_+(v) - A_-(w), \qquad A_\pm(v) := \int_{v'=0}^{v} [A'(v')]_\pm \mathrm{d}v',$$

satisfies the assumptions (NF1) *and* (NF2)*.*

As a result, if $\nu = 0$ then the spatial discretisation of (3.3) by the Finite-Volume method leads to the system of differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t} U_i^N(t) + N\left(\overline{A}(U_i^N(t), U_{i+1}^N(t)) - \overline{A}(U_{i-1}^N(t), U_i^N(t))\right) = \xi_i^N(t), \qquad i \in \mathbb{T}_N, \tag{3.4}$$

[1] These equations constitute the basis of the industrial computer code TELEMAC developed by Laboratoire d'Hydraulique Saint-Venant, a joint laboratory between École des Ponts ParisTech, EDF R&D and CEREMA.

where $\xi_i^N(t)$ is the average of $\xi(t,x)$ on I_i. When $\nu > 0$, the Laplacian operator may be discretised by a simple finite difference approximation which adds the term $\nu N^2(U_{i+1}^N(t) - 2U_i^N(t) + U_{i-1}^N(t))$ to the right-hand side. From now on, we shall call *semidiscrete schemes* such systems of time-continuous differential equations as (3.4). A *fully discrete* scheme is then obtained by applying any classical time discretisation method to it.

If $\xi(t,x)$ is a Gaussian white-in-time noise, then (3.4) writes more naturally under the form of the Itô SDE

$$\mathrm{d}U_i^N(t) = -N\left(\overline{A}(U_i^N(t), U_{i+1}^N(t)) - \overline{A}(U_{i-1}^N(t), U_i^N(t))\right)\mathrm{d}t + \mathrm{d}W_i^N(t), \qquad i \in \mathbb{T}_N, \tag{3.5}$$

where $(W_1^N(t), \dots, W_N^N(t))_{t\geq 0}$ is a Wiener process with a certain covariance structure inherited from the spatial correlations of $\xi(t,x)$. In the purpose to approximate the stationary distribution of (3.3), the following two questions related with this semidiscrete scheme are then natural.

(i) Does the diffusion process $(U_1^N(t), \dots, U_N^N(t))_{t\geq 0}$ defined by (3.5) has a stationary distribution?

(ii) If so, does this stationary distribution converge, when $N \to +\infty$, to the stationary distribution of the original conservation law (3.3)?

The same questions obviously also arise for the fully discrete scheme, additionally taking the time discretisation into account.

3.1.3 Outline of the chapter

Unsurprisingly, these questions are easier to address when the viscosity ν is positive. We shall therefore give a complete treatment of this case first. In Section 3.2, we set up the framework of our study by introducing precisely the SPDE in which we are interested. In Section 3.3, we state our results on the Finite-Volume approximation of the stationary distribution. We finally discuss the inviscid case $\nu = 0$ in Section 3.4.

3.2 Strong solutions and stationary distribution in the viscous case

In this section, we discuss the well-posedness of (3.3) on the one-dimensional torus $\mathbb{T}$ when the viscosity parameter ν is positive, as well as the existence and uniqueness of a stationary distribution for its solution. Our purpose is to prepare the numerical analysis of this stationary distribution by the Finite-Volume method, which will be presented in Section 3.3. In this perspective, it shall be particularly convenient to look for solutions which are smooth enough for the higher order derivative $\partial_{xx}u$ appearing in the right-hand of (3.3) to be classically defined. This requires the noise term $\xi(t,x)$ to be sufficiently correlated in space, in contrast with seminal well-posedness results for the stochastic Burgers equation [DPDT94, BCJL94]. However, the latter works were (at least partially) motivated by the link between this equation and the celebrated KPZ equation [KPZ86, Cor12], in which white-in-space noise accounts for local fluctuations, a phenomenon which is not predominant in the statistical hydrodynamics context.

The regularity of the noise is imposed by defining $\xi(t,x)$ as the (formal) time derivative of a Wiener process taking its values in a given Sobolev space H on $\mathbb{T}$, as is explained in Subsection 3.2.1. This leads us to interpret (3.3) as a SDE with values in H, in accordance with the so-called *semigroup approach* to SPDEs [DPZ14]. In this context, we choose the Sobolev space H with an index large enough to enable us to work with *strong* solutions to (3.3). This notion is introduced in Subsection 3.2.2, where we also state our well-posedness result. Finally, the existence and uniqueness of a stationary distribution is addressed in Subsection 3.2.3.

This section summarises the results from [A3].

3.2.1 Sobolev spaces and Wiener process

Sobolev spaces

As a preliminary remark, let us observe that taking the integral of both sides of (3.3) on $\mathbb{T}$ yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x\in\mathbb{T}} u(t,x)\mathrm{d}x = \int_{x\in\mathbb{T}} \xi(t,x)\mathrm{d}x,$$

because of the periodicity of the boundary conditions. As a consequence, if both the initial condition u_0 and the noise $\xi(t,\cdot)$ have mean zero, then so is expected to have the solution $u(t,\cdot)$. This incites us, for all $p \geq 1$, to denote by $L^p_0(\mathbb{T})$ the set of L^p functions v on $\mathbb{T}$ such that

$$\int_{x\in\mathbb{T}} v(x)\mathrm{d}x = 0.$$

The restriction of the L^p norm to $L^p_0(\mathbb{T})$ is denoted by $\|\cdot\|_{L^p_0(\mathbb{T})}$.

For any integer $m \geq 0$, we denote by $W^{m,p}_0(\mathbb{T})$ the intersection of the Sobolev space $W^{m,p}(\mathbb{T})$ with $L^p_0(\mathbb{T})$. Thanks to the Poincaré inequality

$$\forall p \geq 1, \quad \forall v \in W^{1,p}_0(\mathbb{T}), \qquad \|v\|_{L^p_0(\mathbb{T})} \leq \|\partial_x v\|_{L^p_0(\mathbb{T})},$$

we define a norm on $W^{m,p}_0(\mathbb{T})$ by letting $\|v\|_{W^{m,p}_0(\mathbb{T})} := \|\partial^m_x v\|_{L^p_0(\mathbb{T})}$. In the particular case $p = 2$, the space $W^{m,2}_0(\mathbb{T})$ is denoted by $H^m_0(\mathbb{T})$ and the norm $\|\cdot\|_{H^m_0(\mathbb{T})}$ is defined accordingly. This norm is associated with the scalar product

$$\forall v, w \in H^m_0(\mathbb{T}), \qquad \langle v, w\rangle_{H^m_0(\mathbb{T})} := \int_{x\in\mathbb{T}} \partial^m_x v(x)\partial^m_x w(x)\mathrm{d}x,$$

which makes $H^m_0(\mathbb{T})$ a separable Hilbert space. More generally, for any real number $s \geq 0$, the fractional Sobolev space $H^s_0(\mathbb{T})$ is defined by Fourier series; it remains a separable Hilbert space.

Wiener processes

Let $\{(W^k(t))_{t\geq 0}, k \geq 1\}$ be a family of independent standard Brownian motions. Fix $s \geq 0$ and let $\{g^k, k \geq 1\}$ be a sequence of elements of $H^s_0(\mathbb{T})$ such that

$$D_s := \sum_{k\geq 1} \|g^k\|^2_{H^s_0(\mathbb{T})} < +\infty. \tag{3.6}$$

Then there exists a continuous, $H^s_0(\mathbb{T})$-valued process $(W^Q(t))_{t\geq 0}$ such that for all $T > 0$, the series $(\sum_{k\geq 1} g^k W^k(t))_{t\in[0,T]}$ converges in $L^2(\Omega; C([0,T]; H^s_0(\mathbb{T})))$ to $(W^Q(t))_{t\in[0,T]}$. Besides, this process is a Wiener process in $H^s_0(\mathbb{T})$ with covariance given by the trace class operator $Q : H^s_0(\mathbb{T}) \to H^s_0(\mathbb{T})$ defined by

$$\forall v, w \in H^s_0(\mathbb{T}), \qquad \langle Qv, w\rangle_{H^s_0(\mathbb{T})} = \sum_{k\geq 1} \langle g^k, v\rangle_{H^s_0(\mathbb{T})}\langle g^k, w\rangle_{H^s_0(\mathbb{T})}.$$

In short, we shall write that W^Q is an $H^s_0(\mathbb{T})$-*valued Wiener process* [DPZ14, Section 4.1], and call $\{g^k, k \geq 1\}$ the set of its *covariance functions*.

Remark 3.2.1. *The notation $W^Q = \sum_{k\geq 1} g^k W^k$ is inspired from [DV15] and allows to rewrite (3.3) under the form*

$$\partial_t u(t,x) + \partial_x A(u(t,x)) = \nu\partial_{xx} u(t,x) + \sum_{k\geq 1} g^k(x)\dot{W}^k(t),$$

which although more informal is perhaps the most intuitive formulation of the equation. A similar presentation is employed in [A3].

3.2.2 Mild and strong solutions

Let $s \geq 0$ and W^Q be an $H_0^s(\mathbb{T})$-valued Wiener process. From now on, we rewrite (3.3) as the Hilbert-valued SDE

$$\mathrm{d}u = (\nu \partial_{xx} u - \partial_x A(u))\,\mathrm{d}t + \mathrm{d}W^Q, \tag{3.7}$$

following the formalism of [DPZ14].

Mild solution

Let $S^\nu(t) = \exp(t\nu\partial_{xx})$ be the semigroup generated by the operator $\nu\partial_{xx}$; it is well-defined on (at least) all spaces $H_0^s(\mathbb{T})$, $s \geq 0$. Given $u_0 \in H_0^s(\mathbb{T})$, a *mild* solution to (3.7) with initial condition u_0 is a process $(u(t))_{t\geq 0}$ in $H_0^s(\mathbb{T})$ which satisfies the identity

$$u(t) = S^\nu(t)u_0 - \int_{s=0}^t S^\nu(t-s)\partial_x A(u(s))\mathrm{d}s + \int_{s=0}^t S^\nu(t-s)\mathrm{d}W^Q(s).$$

Since this expression does not involve the second-order derivative of u, mild solutions may be sought in Sobolev spaces $H_0^s(\mathbb{T})$ with index s smaller than 2, so that $\partial_{xx}u$ need not be defined in the classical sense. Recent results on the Sobolev regularity for mild solutions to equations of the form (3.3) can for instance be found in [JLP]; see also [GH18] in a related context.

Strong solution

Following [DPZ14, Section 5.1], we call *strong* solution to (3.7) a process $(u(t))_{t\geq 0}$ with values in $H_0^2(\mathbb{T})$ such that

$$u(t) = u_0 + \int_{s=0}^t (\nu\partial_{xx}u(s) - \partial_x A(u(s)))\,\mathrm{d}s + W^Q(t).$$

Strong solutions are mild solutions, and mild solutions which belong to $H_0^2(\mathbb{T})$ are strong solutions.

Boritchev [Bor12] studied strong solutions to (3.7) for flux functions A which are uniformly convex, and Hofmanová [Hof13] for globally Lipschitz continuous flux functions. Our first result (Theorem 1 in [A3]) is obtained under the following assumptions.

(F1) The function $A : \mathbb{R} \to \mathbb{R}$ is C^2 on $\mathbb{R}$.

(F2) There exist $C_A, p_A \geq 0$ such that $|A'(v)| \leq C_A(1 + |v|^{p_A})$ for all $v \in \mathbb{R}$.

(F3) The function A'' is locally Lipschitz continuous on $\mathbb{R}$.

Theorem 3.2.2 (Well-posedness of (3.7))**.** *Consider the equation (3.7) with $\nu > 0$. Assume that the flux function A satisfies the conditions (F1), (F2) and (F3), and that W^Q is an $H_0^2(\mathbb{T})$-valued Wiener process.*

(i) For any $u_0 \in H_0^2(\mathbb{T})$, there is a unique strong solution $(u(t))_{t\geq 0}$ to (3.7) with initial condition u_0.

(ii) For all $T > 0$, almost surely, the mapping $u_0 \mapsto (u(t))_{t\in[0,T]}$ is continuous from $H_0^2(\mathbb{T})$ to $C([0,T]; H_0^2(\mathbb{T}))$.

Following the semigroup approach [DPDT94, DPZ14], the first step of the proof of Theorem 3.2.2 consists in proving the existence of a mild solution by writing a fixed point problem in $H_0^1(\mathbb{T})$. Because the flux function is not necessarily globally Lipschitz continuous, this procedure only yields a local-in-time solution, which however is unique and depends continuously on u_0. This solution is then proved to be global thanks to uniform in time $L_0^p(\mathbb{T})$ and $H_0^1(\mathbb{T})$ estimates on u, which follow from the application of the (infinite-dimensional) Itô formula and rely crucially on the positivity of the viscosity. The regularity of u is finally improved from $H_0^1(\mathbb{T})$ to $H_0^2(\mathbb{T})$ by a bootstrapping argument [Bor12].

3.2.3 Stationary distribution

Our second theoretical result concerning (3.7) (Theorem 2 in [A3]) is related to stationary distributions.

Theorem 3.2.3 (Existence and uniqueness of a stationary distribution)**.** *Under the assumptions of Theorem 3.2.2, the process $(u(t))_{t\geq 0}$ has a unique stationary distribution μ.*

We briefly sketch the proof of Theorem 3.2.3. The energy estimate

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}\left[\|u\|^2_{L^2_0(\mathbb{T})}\right] = -2\nu\mathbb{E}\left[\|u\|^2_{H^1_0(\mathbb{T})}\right] + D_0,$$

combined with the compactness of the embedding of $H^1_0(\mathbb{T})$ into $L^2_0(\mathbb{T})$ allows to deduce the existence of μ from the Krylov–Bogoliubov Theorem [DPZ96, Theorem 3.1.1]. The uniqueness is obtained by a coupling argument on two solutions u and v driven by the same Wiener process W^Q. On the one hand, the presence of viscosity implies that on time intervals where W^Q remains small, both u and v are exponentially attracted to 0. On the other hand, it is a standard property of conservation laws that $\|u-v\|_{L^1_0(\mathbb{T})}$ does not increase, so that once u and v are close enough to 0, they remain close to each other forever. The use of such a so-called *small noise argument* to get the uniqueness of stationary distributions appears under various formulations in the study of conservation laws [DV15], related Hamilton–Jacobi equations [DS05] or the Navier–Stokes equation [Deb13]. Other possible approached are reviewed in [CP19].

3.3 Finite-Volume approximation of the stationary distribution

Under the assumptions of Theorem 3.2.3, let μ be the stationary distribution of the solution $(u(t))_{t\geq 0}$ to (3.7). Several quantities of interest in statistical hydrodynamics, transposed to the context of (3.7), write under the form

$$\mathcal{I}_F := \int_{v\in H^2_0(\mathbb{T})} F(v)\mu(\mathrm{d}v),$$

for some *observable* function $F : H^2_0(\mathbb{T}) \to \mathbb{R}$, see [Bor12, Mar19] for instance. By the ergodic theorem, we have

$$\mathcal{I}_F = \lim_{T\to+\infty} \frac{1}{T}\int_{t=0}^{T} F(u(t))\mathrm{d}t, \qquad \text{almost surely,}$$

so that $\mathcal{I}_F$ can be numerically computed by simulating one trajectory of $(u(t))_{t\in[0,T]}$ over a long enough time interval and taking the empirical average of F along this trajectory. This naturally raises the question of the efficiency of the discretisation of (3.7) with respect to the time horizon T.

For finite-dimensional SDEs, where only time is discretised [KP99], this issue was first addressed by Talay [Tal90], who obtained rates of convergence with respect to the time step by analysing the associated Kolmogorov equation. Other methods rely on Poisson equations [MST10], Meyn–Tweedie-like approaches [MSH02, LS16], or stochastic algorithms with decreasing time steps [LP02]. These results were extended to SPDEs in several rather recent works [Bré14, BK17, CHW17, CGW20, CHS21], in which the space variable is discretised either by a general Galerkin approximation or a specific Finite-Element method.

On the other hand, Finite-Volume schemes for stochastic conservation laws have been developed in [KR12, BCG16b, BCG16a, FGH18, DV19], but only on finite time intervals. In the present section, we describe the results obtained in [A4] on the approximation of μ by the Finite-Volume method, under the assumptions of Section 3.2. In Subsection 3.3.1, we present the study of the semidiscrete scheme, while Subsection 3.3.2 is dedicated to the fully discrete scheme.

Throughout this section, we use bold symbols to refer to vectors and matrices, and introduce the notation

$$\mathbb{R}^N_0 := \{\mathbf{v} = (v_1,\dots,v_N) \in \mathbb{R}^N : v_1 + \cdots + v_N = 0\}$$

to denote the space in which both the semidiscrete and the fully discrete schemes naturally take their values. We also define the *projection operator* $\Pi_N : L^1_0(\mathbb{T}) \to \mathbb{R}^N_0$ by

$$\forall i \in \mathbb{T}_N, \qquad (\Pi_N v)_i = N \int_{x=x_{i-1}}^{x_i} v(x)\mathrm{d}x.$$

3.3.1 Semidiscrete scheme

Following the discussion of Subsection 3.1.2, the semidiscrete scheme associated with (3.7) with $\nu > 0$ takes the form of the solution $(\mathbf{U}^N(t))_{t\geq 0} = (U_1^N(t), \dots, U_N^N(t))_{t\geq 0}$ to the SDE

$$\begin{aligned}\mathrm{d}U_i^N(t) = {} & \nu N^2 \left(U_{i+1}^N(t) - 2U_i^N(t) + U_{i-1}^N(t)\right)\mathrm{d}t \\ & - N\left(\overline{A}(U_i^N(t), U_{i+1}^N(t)) - \overline{A}(U_{i-1}^N(t), U_i^N(t))\right)\mathrm{d}t \\ & + \mathrm{d}W_i^{Q,N}(t),\end{aligned}$$

where the numerical flux function $\overline{A} : \mathbb{R}^2 \to \mathbb{R}$ satisfies Assumptions (NF1) and (NF2), and

$$\mathbf{W}^{Q,N} = \Pi_N W^Q. \tag{3.8}$$

If W^Q is an $L^2_0(\mathbb{T})$-valued Wiener process with covariance functions $\{g^k, k \geq 1\}$, then it is easy to check that $\mathbf{W}^{Q,N}$ is a Wiener process in $\mathbb{R}^N_0$ with covariance

$$\mathbb{E}\left[W_i^{Q,N}(t) W_j^{Q,N}(t)\right] = t \sum_{k\geq 1} g_i^k g_j^k, \qquad \mathbf{g}^k := \Pi_N g^k. \tag{3.9}$$

Some notation

We endow the space $\mathbb{R}^N$ with the scaled scalar product

$$\langle \mathbf{v}, \mathbf{w}\rangle := \frac{1}{N}\sum_{i=1}^N v_i w_i,$$

and for all $p \geq 1$ and $\mathbf{v} \in \mathbb{R}^N_0$, we denote

$$\|\mathbf{v}\|^p_{\ell^p_0(\mathbb{T}_N)} := \frac{1}{N}\sum_{i=1}^N |v_i|^p.$$

We define the discrete derivative operators $\mathbf{D}_N^{(1,-)}, \mathbf{D}_N^{(1,+)}, \mathbf{D}_N^{(2)} : \mathbb{R}^N \to \mathbb{R}^N_0$ by, for $\mathbf{v} \in \mathbb{R}^N$,

$$(\mathbf{D}_N^{(1,-)}\mathbf{v})_i = N(v_i - v_{i-1}), \quad (\mathbf{D}_N^{(1,+)}\mathbf{v})_i = N(v_{i+1} - v_i), \quad (\mathbf{D}_N^{(2)}\mathbf{v})_i = N^2(v_{i+1} - 2v_i + v_{i-1}).$$

Well-posedness and stationary distribution

Introducing the operator $\overline{\mathbf{A}}^N : \mathbb{R}^N \to \mathbb{R}^N$ defined by

$$(\overline{\mathbf{A}}^N(\mathbf{v}))_i = \overline{A}(v_i, v_{i+1}),$$

we may now rewrite the semidiscrete scheme under the compact form

$$\mathrm{d}\mathbf{U}^N(t) = \nu \mathbf{D}_N^{(2)}\mathbf{U}^N(t)\mathrm{d}t - \mathbf{D}_N^{(1,-)}\overline{\mathbf{A}}^N\left(\mathbf{U}(t)\right)\mathrm{d}t + \mathrm{d}\mathbf{W}^{Q,N}(t). \tag{3.10}$$

The conditions on the numerical flux yield the following important properties.

Lemma 3.3.1 (Dissipation and contraction of the drift)**.** *Let* $\mathbf{b}(\mathbf{v}) := \nu \mathbf{D}_N^{(2)}\mathbf{v} - \mathbf{D}_N^{(1,-)}\overline{\mathbf{A}}^N(\mathbf{v}) \in \mathbb{R}_0^N$ *be the drift of the SDE* (3.10)*. Under Assumptions* (NF1) *and* (NF2)*, we have:*

(i) for any $\mathbf{v} \in \mathbb{R}_0^N$, $\langle \mathbf{v}, \mathbf{b}(\mathbf{v})\rangle \leq -\nu \|\mathbf{D}_N^{(1)}\mathbf{v}\|^2_{\ell^2_0(\mathbb{T}_N)}$;

(ii) for any $\mathbf{v}, \mathbf{w} \in \mathbb{R}_0^N$, $\langle \mathbf{sgn}(\mathbf{v}-\mathbf{w}), \mathbf{b}(\mathbf{v}) - \mathbf{b}(\mathbf{w})\rangle \leq 0$, *where* $(\mathbf{sgn}(\mathbf{v}-\mathbf{w}))_i = \mathrm{sgn}(v_i - w_i)$.

Lemma 3.3.1 ensures that the SDE (3.10) possesses L^2_0 dissipation and L^1_0 contraction properties similar to the SPDE (3.7), which under the following regularity assumption:

(NF3) the function $\overline{A}$ is locally Lipschitz continuous on $\mathbb{R}^2$,

allows to prove the following result.

Proposition 3.3.2 (Well-posedness for (3.10))**.** *Let* $\nu > 0$, $\overline{A} : \mathbb{R}^2 \to \mathbb{R}$ *satisfy Assumptions* (NF1)*,* (NF2) *and* (NF3)*, and let* $\mathbf{W}^{Q,N}$ *be the* $\mathbb{R}_0^N$*-valued Wiener process obtained from some* $L^2_0(\mathbb{T})$*-valued Wiener process* W^Q *by* (3.8)*. For any* $\mathbf{U}_0^N \in \mathbb{R}_0^N$*, the SDE* (3.10) *possesses a unique strong solution* $(\mathbf{U}^N(t))_{t\geq 0}$ *with initial condition* $\mathbf{U}_0^N$*. This process takes its values in* $\mathbb{R}_0^N$ *and has a unique stationary distribution* ϑ_N*, which satisfies the uniform discrete* H^1_0 *estimate*

$$\mathbb{E}\left[\|\mathbf{D}_N^{(1,+)}\mathbf{U}_\infty^N\|^2_{\ell^2_0(\mathbb{T}_N)}\right] \leq \frac{D_0}{2\nu}, \qquad \mathbf{U}_\infty^N \sim \vartheta_N,$$

where we recall from (3.6) *that* $D_0 = \sum_{k\geq 1}\|g^k\|^2_{L^2_0(\mathbb{T})}$.

Convergence in the $N \to +\infty$ limit

Let $\Psi_N : \mathbb{R}_0^N \to L^\infty_0(\mathbb{T})$ denote the *reconstruction operator*, which to any $\mathbf{v} \in \mathbb{R}_0^N$ associates the piecewise constant function $\Psi_n\mathbf{v}$ defined by

$$\forall x \in (x_{i-1}, x_i], \qquad \Psi_N\mathbf{v}(x) = v_i.$$

Under the assumptions of Proposition 3.3.2, we denote by μ_N the pushforward measure of ϑ_N by Ψ_N. Under the assumptions of Theorem 3.2.3, our purpose is now to show that μ_N converges, when $N \to +\infty$, to the stationary distribution μ of the solution $(u(t))_{t\geq 0}$ to the SPDE (3.7).

A first step is provided by the uniform discrete H^1_0 estimate of Proposition 3.3.2, which by compactness of the embedding of $H^1_0(\mathbb{T})$ into $L^2_0(\mathbb{T})$ yields the tightness of the sequence $(\mu_N)_{N\geq 1}$ on $L^2_0(\mathbb{T})$. Under the following strengthening of Assumption (NF3):

(NF3') the function $\overline{A}$ is C^1 on $\mathbb{R}^2$, and there exist $C_{\overline{A}}, p_{\overline{A}} \geq 0$ such that

$$\forall v, w \in \mathbb{R}, \qquad |\partial_v \overline{A}(v,w)| \leq C_{\overline{A}}(1+|v|^{p_{\overline{A}}}), \quad |\partial_w \overline{A}(v,w)| \leq C_{\overline{A}}(1+|w|^{p_{\overline{A}}}),$$

and assuming that the SPDE (3.7) is driven by an $H^2_0(\mathbb{T})$-valued Wiener process W^Q, we derived in [A4] various *a priori* higher-order uniform discrete Sobolev estimates on ϑ_N, which first enabled us to prove that any limit μ^* of the sequence $(\mu_N)_{N\geq 1}$ gives full weight to $H^2_0(\mathbb{T})$. We then used the Skorokhod representation theorem to define on a common probability space:

- a random variable u_0^* with distribution μ^*;
- a sequence of random variables $(\mathbf{U}_0^N)_{N\geq 1}$ such that, for all $N \geq 1$, $\mathbf{U}_0^N \in \mathbb{R}_0^N$ is distributed according to ϑ_N, and up to the extraction of a subsequence (which we still denote by N for convenience), $\Psi_N\mathbf{U}_0^N$ converges almost surely to u_0^*;
- a Wiener process W^Q from which we defined $\mathbf{W}^{Q,N} = \Pi_N W^Q$;

and called:

- $(u^*(t))_{t\geq 0}$ the solution to (3.7) driven by W^Q with initial condition u_0^*;
- $(\mathbf{U}^N(t))_{t\geq 0}$ the solution to (3.10) driven by $\mathbf{W}^{Q,N}$ with initial condition $\mathbf{U}_0^N$;
- $(u^N(t))_{t\geq 0}$ the process defined by $u^N(t) = \Psi_N \mathbf{U}^N(t)$.

In this construction, the process $(u^N(t))_{t\geq 0}$ is stationary, and we aim to prove that so is the process $(u^*(t))_{t\geq 0}$. This fact is deduced from the following finite-time trajectorial convergence result: for any $t \geq 0$,

$$\lim_{N\to+\infty} \mathbb{E}\left[\|u^N(t) - u^*(t)\|^2_{L^2_0(\mathbb{T})}\right] = 0, \tag{3.11}$$

which is the main technical point of [A4]. This allows to identify all limits of $(\mu_N)_{N\geq 1}$ and yields the following final statement.

Theorem 3.3.3 (Convergence of the semidiscrete scheme)**.** *Under the assumptions of Theorem 3.2.3, let μ be the unique stationary distribution of the solution to the stochastic conservation law (3.7). Consider the associated semidiscrete scheme with a numerical flux function satisfying Assumptions (NF1), (NF2) and (NF3'). Let μ_N be the probability measure given by Proposition 3.3.2. We have*

$$\lim_{N\to+\infty} \mu_N = \mu,$$

weakly on $L^2_0(\mathbb{T})$.

Remark 3.3.4 (Convergence in Wasserstein distance)**.** *The fact that the finite-time trajectorial convergence (3.11) is established in the L^2 sense actually allows to express the convergence of μ_N to μ in the quadratic Wasserstein distance on the space of probability measures on $L^2_0(\mathbb{T})$.*

Remark 3.3.5 (On Assumptions (NF1), (NF2) and (NF3'))**.** *From a practical point of view, if the flux function A satisfies Assumptions (F1), (F2) and (F3) (and, without loss of generality, is assumed to be such that $A(0) = 0$), then the* Engquist–Osher *numerical flux introduced in Example 3.1.1 satisfies Assumptions (NF1), (NF2) and (NF3').*

Complementing the convergence result of Theorem 3.3.3 with a rate of convergence in N is the natural next step to be addressed. In the 'perturbative' case where the flux function A is assumed to be globally Lipschitz continuous with a small Lipschitz norm, the proof of the finite-time convergence result (3.11) can be adapted in order to become uniform in time and yield a rate of convergence, namely we obtain the existence of a constant C such that for all $N \geq 1$,

$$W_2(\mu_N, \mu) \leq \frac{C}{N},$$

where W_2 denotes the quadratic Wasserstein distance on the space of probability measures on $L^2_0(\mathbb{T})$. This rate is the same as for deterministic Finite-Volume schemes (see for instance [EGH00, Theorem 17.1]), which indicates that in contrast with standard results on the discretisation of SPDEs with white-in-space noise [Gyö99], here the noise is smooth enough not to deteriorate the order of convergence (in space).

However, this result remains a 'strong' error estimate, in the sense that a bound on the distance between the probability measures μ_N and μ is derived from a bound on the distance between the realisations $u^N(t)$ and $u^*(t)$. In order to go beyond this perturbative case, and compute directly a 'weak' type of error, one may consider coming back to the analysis of (infinite-dimensional) Kolmogorov or Poisson equations associated with (3.7) and (3.10), in the spirit of [Bré14] and [BK17], respectively. This is left as a perspective for future works.

3.3.2 Fully discrete scheme

We now fix $N \geq 1$ and address the time discretisation of the SDE (3.10) with the purpose to approximate the stationary distribution ϑ_N obtained in Proposition 3.3.2. The main difficulty here is that under the assumptions of the latter proposition, the drift $\mathbf{b}$ of this SDE need not be globally Lipschitz continuous. It is known that in such a case, the explicit Euler–Maruyama scheme may fail to preserve the ergodicity of the SDE. An example of such a situation is presented in [MSH02], where the authors introduce a *split-step* scheme which recovers suitable ergodic properties. We follow their approach, and for a given time step $\Delta t > 0$, define the sequence $(\mathbf{U}_n^{N,\Delta t})_{n\geq 0}$ by

$$\begin{cases} \mathbf{U}_{n+\frac{1}{2}}^{N,\Delta t} = \mathbf{U}_n^{N,\Delta t} + \Delta t \mathbf{b}\left(\mathbf{U}_{n+\frac{1}{2}}^{N,\Delta t}\right), \\ \mathbf{U}_{n+1}^{N,\Delta t} = \mathbf{U}_{n+\frac{1}{2}}^{N,\Delta t} + \Delta \mathbf{W}_{n+1}^{Q,N}, \end{cases} \tag{3.12}$$

where $\Delta \mathbf{W}_n^{Q,N} := \mathbf{W}^{Q,N}(n\Delta t) - \mathbf{W}^{Q,N}((n-1)\Delta t)$. Under our assumptions on $\mathbf{b}$, the existence and uniqueness of $\mathbf{U}_{n+\frac{1}{2}}^{N,\Delta t}$, which is defined implicitly, follows from a topological degree argument and holds without any smallness condition on Δt. Besides, it turns out that this scheme still preserves some kind of L^2 dissipation and L^1 contraction, which allows to prove the existence and uniqueness of a stationary distribution $\vartheta_{N,\Delta t}$, and the weak convergence of $\vartheta_{N,\Delta t}$ to ϑ_N when $\Delta t \to 0$ with similar arguments to Subsection 3.3.1. Overall, the main result of [A4] thus writes as follows.

Theorem 3.3.6 (Convergence of the fully discrete scheme)**.** *Under the assumptions of Theorem 3.2.3, let μ be the unique stationary distribution of the solution to the stochastic conservation law (3.7). Consider the associated fully discrete scheme (3.12) with a numerical flux function satisfying Assumptions (NF1), (NF2) and (NF3'). Let $\vartheta_{N,\Delta t}$ be the unique stationary distribution of this scheme, and let $\mu_{N,\Delta t}$ be the pushforward of $\vartheta_{N,\Delta t}$ by the reconstruction operator Ψ_N. We have*

$$\lim_{N\to+\infty} \lim_{\Delta t\to 0} \mu_{N,\Delta t} = \mu,$$

weakly on $L_0^2(\mathbb{T})$.

Once again, the lack of quantitative error estimate with respect to Δt is a major shortcoming of this result. A possible approach to progress in this direction might be to adapt the so-called *backward error analysis* of the split-step scheme (3.12) carried out by Kopec [Kop14] for gradient SDEs, which would yield a weak error of order Δt.

3.4 The inviscid case

Most arguments used in Sections 3.2 and 3.3 heavily rely on the positiveness of the viscosity parameter $\nu > 0$ and somehow eclipse the role of the transport mechanism by the flux function A in (3.7). Still, [EKMS00] and [DV15] show that the presence of viscosity is not necessary for the SPDE

$$\mathrm{d}u = -\partial_x A(u)\mathrm{d}t + \mathrm{d}W^Q \tag{3.13}$$

to be ergodic, so that identifying the role of the numerical flux in the long-time behaviour of the Finite-Volume scheme (3.10) when $\nu = 0$ remains a natural question. For the sake of simplicity we shall only discuss the space discretisation, that is to say the SDE

$$\mathrm{d}\mathbf{U}^N(t) = -\mathbf{D}_N^{(1,-)}\overline{\mathbf{A}}^N\left(\mathbf{U}^N(t)\right)\mathrm{d}t + \mathrm{d}\mathbf{W}^{Q,N}(t) \tag{3.14}$$

with the notation of Section 3.3.

Some parts of this section are discussed in the perspectives of [Mar19] but mostly remain works in progress.

3.4.1 Existence and uniqueness of the stationary distribution

Following [KR12], we say that a C^1 numerical flux function $\overline{A} : \mathbb{R}^2 \to \mathbb{R}$ is *strongly monotone* if there exists $\lambda > 0$ such that the function $\overline{A}^0 : \mathbb{R}^2 \to \mathbb{R}$ defined by

$$\overline{A}(v, w) = \overline{A}^0(v, w) + \lambda(v - w) \tag{3.15}$$

is monotone in the sense of Assumption (NF2). Notice that any numerical flux function $\overline{A}^0$ which satisfies Assumptions (NF1) and (NF2) can be turned into a strongly monotone numerical flux, which remains consistent (in the sense of Assumption (NF1)), simply by adding the term $\lambda(v - w)$ to it.

The assumption that $\overline{A}$ be strongly monotone induces some numerical viscosity in the scheme, since (3.14) may then be rewritten

$$\mathrm{d}\mathbf{U}^N(t) = \frac{\lambda}{N}\mathbf{D}_N^{(2)}\mathbf{U}^N(t)\mathrm{d}t - \mathbf{D}_N^{(1,-)}\overline{\mathbf{A}}^{0,N}\left(\mathbf{U}^N(t)\right)\mathrm{d}t + \mathrm{d}\mathbf{W}^{Q,N}(t),$$

with the notation of Section 3.3 and an obvious definition for $\overline{\mathbf{A}}^{0,N}$. As a consequence, the same arguments as in Section 3.3 may be employed to show that, for fixed N, this SDE has a unique strong solution, which possesses a unique stationary distribution. However, since the viscosity $\nu = \lambda/N$ vanishes when N goes to $+\infty$, the uniform discrete H_0^1 estimate of Proposition 3.3.2 no longer holds. This is not surprising since in the absence of viscosity, the solution to (3.13) is expected to develop shocks and therefore its stationary distribution should not be concentrated on $H_0^1(\mathbb{T})$.

3.4.2 $W_0^{1,1}$ estimate in the uniformly convex case

While $L_0^2(\mathbb{T})$ is a natural space for the energy estimates associated with the parabolic equation (3.7) with $\nu > 0$, the standard theory of hyperbolic conservation laws [Ser99, Ser00] indicates that $L_0^1(\mathbb{T})$ is likely to be better suited to (3.13) for which $\nu = 0$.

Under the assumptions that A be uniformly convex and subcubic, Boritchev [Bor13a, Corollary 4.3] obtained a $W_0^{1,1}$ estimate on the stationary distribution of (3.7) uniform in ν. Adapting his proof, which is based on a stochastic version of the so-called 'Kruzhkov maximum principle', one may show the following result.

Proposition 3.4.1 (Uniform discrete $W_0^{1,1}$ estimate)**.** *Assume that the flux function A is C^2 and such that $A''(v) \geq c_A > 0$, $|A'(v)| \leq C_A(1 + |v|^{p_A})$ for some $p_A < 2$. Let ϑ_N be the stationary distribution of the SDE (3.14) with the numerical flux function*

$$\overline{A}(v, w) = \overline{A}^0(v, w) + \lambda(v - w),$$

where $\lambda > 0$ and $\overline{A}^0$ is the Engquist–Osher numerical flux[2] associated with A. Assume finally that the covariance functions $\{g^k, k \geq 1\}$ appearing in the expression (3.9) on the covariance of the Wiener process $\mathbf{W}^{Q,N}$ satisfy the condition that

$$D_* := \sum_{k \geq 1} \|g^k\|^2_{W_0^{1,4}(\mathbb{T})} < +\infty.$$

If $\mathbf{U}_\infty^N$ is a random variable distributed according to ϑ_N, then for all $q \geq 1$, there exists a constant $C^{1,1,q}$ which depends on q, on C_A, c_A, p_A, on D_* and on λ but not on N such that

$$\mathbb{E}\left[\|\mathbf{D}_N^{(1,+)}\mathbf{U}_\infty^N\|^q_{\ell_0^1(\mathbb{T}_N)}\right] \leq C^{1,1,q}. \tag{3.16}$$

[2] See Example 3.1.1.

If one takes $q = 1$ in (3.16), one obtains a uniform discrete $W_0^{1,1}$ estimate[3] on ϑ_N which may play a similar role as the $W_0^{1,2}$ estimate from Proposition 3.3.2 and imply that the associated sequence $(\mu_N)_{N\geq 1}$ is tight on $L_0^1(\mathbb{T})$. As a consequence, one might then consider following the same program as in Section 3.3 and deriving the convergence of μ_N to the stationary distribution of (3.13) from a finite-time trajectorial convergence result in $L_0^1(\mathbb{T})$ for the Finite-Volume scheme (3.14). But, again, this method would probably not be appropriate to yield quantitative weak error estimates.

3.4.3 Kinetic formulation and averaging lemma

The ergodicity results by Debussche and Vovelle [DV15] for (3.13) hold under a *nondegeneracy condition* for the flux function A which can be seen as a relaxation of the uniform convexity assumption made in the previous subsection. They are obtained thanks to the *kinetic formulation* [LPT94, Per02] of (3.13), which we first briefly describe.

For all $v, \xi \in \mathbb{R}$, let us define

$$\chi(\xi, v) = \begin{cases} 1 & \text{if } 0 < \xi \leq v, \\ -1 & \text{if } v \leq \xi < 0, \\ 0 & \text{otherwise.} \end{cases}$$

A formal application of the Itô formula shows that if u is a solution to (3.13), then $f(t,x,\xi) := \chi(\xi, u(t,x))$ satisfies $\mathrm{d}f(t,x,\xi) = \partial_v \chi(\xi,u)\mathrm{d}u + \frac{1}{2}\partial_{vv}\chi(\xi_u)\mathrm{d}\langle u\rangle$, which then rewrites

$$\partial_t f + A'(\xi)\partial_x f = \partial_\xi \left(m - \frac{1}{2}\langle \dot{W}^Q \rangle \delta_{u=\xi} \right) + \delta_{u=\xi}\dot{W}^Q, \tag{3.17}$$

for some distribution $m(t,x,\xi)$ which depends on f. Kruzhkov's entropy condition is then essentially equivalent to $m(t,x,\xi)$ being a nonnegative measure, whose support can be described in terms of the discontinuities of u.

This formulation turns the nonlinear conservation law on u into a linear transport equation on f, which may be addressed by semigroup techniques; more precisely, calling $P(t,x,\xi)$ the right-hand side of (3.17), the Duhamel formula shows that

$$f(t,x,\xi) = \mathrm{e}^{-tA'(\xi)\partial_x} f_0(x,\xi) + \int_{s=0}^{t} \mathrm{e}^{-(t-s)A'(\xi)\partial_x} P(s,\xi,x)\mathrm{d}s, \tag{3.18}$$

with $f_0(x,\xi) = \chi(\xi, u_0(x))$. Of course, for a fixed value of ξ, the semigroup $\mathrm{e}^{-tA'(\xi)\partial_x}$ is generated by the linear transport equation with constant velocity $A'(\xi)$ and no regularisation nor mixing effect can be expected from its application. But the fact that u is recovered from f by the formula

$$u(t,x) = \int_{\xi\in\mathbb{R}} f(t,x,\xi)\mathrm{d}\xi$$

may bring forth such effects for the 'integrated semigroup' $\int_{\xi\in\mathbb{R}} \mathrm{e}^{-tA'(\xi)\partial_x}\mathrm{d}\xi$, as soon as A is 'sufficiently nonlinear', which is precisely ensured by nondegeneracy conditions. Quantifications of these effects are called *averaging lemmas* in kinetic theory [BD99, CP19]. The proof of the existence of a stationary distribution for (3.13) by Debussche and Vovelle [DV15] relies on such a lemma, which allows to control the $t \to +\infty$ behaviour of the convolution appearing in the right-hand side of (3.18).

A natural application of this formalism would therefore be to proceed similarly at the level of the Finite-Volume scheme in order to obtain uniform in N estimates on its stationary distribution. A kinetic formulation of Finite-Volume schemes for deterministic conservation laws was worked out by Makridakis and Perthame [MP03], and recently extended to the stochastic framework by Dotti and Vovelle [DV19]. The next step is the formulation of averaging lemmas adapted to these schemes. It is left for future works.

[3] Since we expect the solution u to (3.7) with $\nu = 0$ to display shocks under its stationary distribution, it would actually be more appropriate to call (3.16) a uniform discrete BV estimate rather than $W_0^{1,1}$.

Chapter 4

Eyring–Kramers formula for nonreversible diffusion processes

This chapter presents the results of the articles [A5] and [A6], written in collaboration with Freddy Bouchet. These articles were published in, or submitted to, statistical physics journals. Our arguments are not mathematically rigorous and our results are purely heuristic. Throughout the chapter, we shall emphasise the assumptions and approximations under which we work, and try to sketch the program towards a mathematical formalisation of these results.

4.1 Metastability and the Eyring–Kramers formula

4.1.1 Reversible diffusion processes

Many models of equilibrium statistical physics are described by the stochastic differential equation

$$\mathrm{d}X_t^\epsilon = -\nabla U(X_t^\epsilon)\mathrm{d}t + \sqrt{2\epsilon}\mathrm{d}W_t \tag{4.1}$$

in $\mathbb{R}^d$, where $U : \mathbb{R}^d \to \mathbb{R}$ is the *potential* of the system, $\epsilon > 0$ is a *temperature* parameter and $(W_t)_{t\geq 0}$ is a standard d-dimensional Brownian motion. If

$$Z^\epsilon := \int_{x\in\mathbb{R}^d} \exp\left(-\frac{U(x)}{\epsilon}\right)\mathrm{d}x < +\infty, \tag{4.2}$$

then the process $(X_t)_{t\geq 0}$ is reversible and ergodic with respect to the *Gibbs measure* with density

$$p_{\mathrm{st}}^\epsilon(x) = \frac{1}{Z^\epsilon}\exp\left(-\frac{U(x)}{\epsilon}\right) \tag{4.3}$$

with respect to the Lebesgue measure. In particular, it is recurrent, therefore it visits infinitely often any subset of $\mathbb{R}$ with positive Lebesgue measure. However, if ϵ is small and U possesses several local minima, it takes a long time for the process to exit neighbourhoods of such local minima: this is the *metastability* phenomenon. In this chapter, we focus on the asymptotics of the mean transition time between local minima in the small temperature regime $\epsilon \to 0$.

For the sake of simplicity, let us assume that U is smooth and possesses two local minima $\overline{x}_1$ and $\overline{x}_2$ which are separated by a unique saddle-point $x_\star$. We shall refer to this situation as the *double-well* case, see a two-dimensional example on Figure 4.1. Assume that $X_0^\epsilon = \overline{x}_1$, and for $0 < \delta \ll |\overline{x}_2 - x_\star|$, let

$$\tau^\epsilon := \inf\{t \geq 0, |X_t^\epsilon - \overline{x}_2| \leq \delta\}.$$

A first asymptotic description of the mean transition time $\mathbb{E}[\tau^\epsilon]$ is called *Arrhenius' law* [Arr89] and writes

$$\lim_{\epsilon\to 0} \epsilon \log \mathbb{E}[\tau^\epsilon] = U(x_\star) - U(\overline{x}_1) =: \Delta U. \tag{4.4}$$

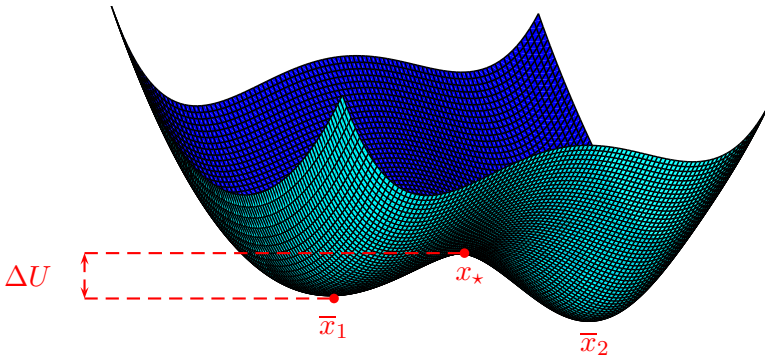

Figure 4.1: Example of a double-well potential in dimension $d = 2$. The potential barrier to escape from the well corresponding to the local minimum $\overline{x}_1$ is $\Delta U = U(x_\star) - U(\overline{x}_1)$.

In this expression, ΔU is called the *potential barrier* that the process has to 'climb' in order to escape from the potential 'well' containing $\overline{x}_1$. This statement provides an approximation of the mean transition time on a *logarithmic* scale and can be obtained thanks to the so-called *pathwise approach* to metastability [OV05], which exploits the following two features of the process $(X_t^\epsilon)_{t\geq 0}$:

(i) on a short time scale, the process reaches a seemingly stationary distribution, concentrated around $\overline{x}_1$: this is the *thermalisation* phase;

(ii) on a long time scale, the process performs seemingly independent and identically distributed attemps to jump from $\overline{x}_1$ to $\overline{x}_2$: this is the *tunnelling* phase.

Estimates on the mean transition time can then be deduced from estimates on the large deviations of the trajectory $(X_t^\epsilon)_{t\in[0,T]}$ on finite time intervals, which are provided by the Freidlin–Wentzell theory [FW12].

The *Eyring–Kramers formula*, named after the seminal articles [Eyr35, Kra40] in the physics litterature, gives the value of the *prefactor* for the mean transition time, that is to say terms in front of $\exp(\Delta U/\epsilon)$ which do not appear on the logarithmic scale. Denoting by $\nabla^2 U(x)$ the Hessian matrix of U at some point $x \in \mathbb{R}^d$, we assume that $\nabla^2 U(\overline{x}_1)$ is positive and that $\nabla^2 U(x_\star)$ has exactly one negative eigenvalue $-\mu_\star$ and $d-1$ positive eigenvalues. Then the Eyring–Kramers formula reads

$$\mathbb{E}[\tau^\epsilon] \sim \frac{2\pi}{\mu_\star}\sqrt{\frac{|\det \nabla^2 U(x_\star)|}{\det \nabla^2 U(\overline{x}_1)}}\exp\left(\frac{\Delta U}{\epsilon}\right), \tag{4.5}$$

when $\epsilon \to 0$. In dimension $d = 1$, the quantity $\mathbb{E}[\tau^\epsilon]$ can be explicitly determined by an ODE method, and the formula above follows from the application of the Laplace method. In higher dimensions, this formula was proved in 2004 by Bovier, Eckhoff, Gayrard and Klein [BEGK04] by a potential theoretic approach [BdH15], and simultaneously by Helffer, Klein and Nier [HKN04] through semiclassical analysis. We refer to the review article by Berglund [Ber13] for a short introduction to both approaches. In each case, the fact that the solution $(X_t^\epsilon)_{t\geq 0}$ to (4.1) is reversible with respect to the explicit stationary distribution p_{st}^ϵ given by (4.3) plays an important role, because then its infinitesimal generator L^ϵ is symmetric in $L^2(p_{\mathrm{st}}^\epsilon)$.

4.1.2 Extension to nonreversible processes

Let $n \geq 1$ and $\sigma \in \mathbb{R}^{d\times n}$. Define $a = \sigma\sigma^\top \in \mathbb{R}^{d\times d}$ and let $J \in \mathbb{R}^{d\times d}$ be an antisymmetric matrix. Under the assumption (4.2), the process $(X_t^\epsilon)_{t\geq 0}$ given by the SDE

$$\mathrm{d}X_t^\epsilon = -(a+J)\nabla U(X_t^\epsilon)\mathrm{d}t + \sqrt{2\epsilon}\sigma \mathrm{d}W_t, \tag{4.6}$$

where $(W_t)_{t\geq 0}$ is now a n-dimensional Brownian motion, remains ergodic with respect to the stationary distribution p^ϵ_{st} defined by (4.3), but when $J \neq 0$ it is no longer reversible. Yet, it still displays a metastable behaviour in the neighbourhood of each local minimum of U.

Such a process is of particular interest in various fields of application. For example, in numerical probability, it is widely accepted that in order to sample from the probability measure p^ϵ_{st}, adding the nonsymmetric term $-J\nabla U(X^\epsilon_t)$ in the drift of reversible processes increases the speed of their convergence, see for instance [HHMS93, HHMS05, LNP13, GM16, LS16]. A somehow related remark is that kinetic processes such as the *Langevin dynamics* $(q_t, p_t)_{t\geq 0}$ in $\mathbb{R}^n \times \mathbb{R}^n$, defined by

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = -\nabla u(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}W_t, \end{cases} \tag{4.7}$$

where $u : \mathbb{R}^n \to \mathbb{R}$ and $\gamma, \beta > 0$ are respectively called the *friction* and *inverse temperature* parameters [LS16], can formally be rewritten under the form (4.6) by letting $d = 2n$ and

$$x = \begin{pmatrix} q \\ p \end{pmatrix}, \quad U(x) = u(q) + \frac{|p|^2}{2}, \quad \sigma = \begin{pmatrix} 0 \\ \sqrt{\gamma} \end{pmatrix}, \quad \epsilon = \beta^{-1}, \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

A generalisation of the Eyring–Kramers formula to (4.6) was proposed by Ariel and Vanden-Eijnden in [AVE07]. It reads

$$\mathbb{E}[\tau^\epsilon] \sim \frac{2\pi}{\lambda_\star}\sqrt{\frac{|\det \nabla^2 U(x_\star)|}{\det \nabla^2 U(\overline{x}_1)}} \exp\left(\frac{\Delta U}{\epsilon}\right), \tag{4.8}$$

where $\lambda_\star$ refers to the positive eigenvalue of the matrix $-(a + J)\nabla^2 U(x_\star)$, which is assumed to be unique. A rigorous proof of this formula was recently obtained by Landim, Mariani and Seo [LMS19], based on a suitable extension of the potential theoretic approach to processes with nonsymmetric infinitesimal generators, developed in the series of papers [Slo, GL14, LS18]. The semiclassical analysis approach was also recently extended to (4.6) by Le Peutrec and Michel [LPM20].

The case of the Langevin dynamics (4.7) is not formally covered by these results, because the matrix a is degenerate. However, the asymptotic behaviour of the small eigenvalues of the infinitesimal generator of $(q_t, p_t)_{t\geq 0}$, which is closely related to the mean transition time between metastable states, was studied by Hérau, Hitrik and Sjöstrand in the works [HHS08a, HHS08b, HHS11].

4.2 Formal extension to general diffusion processes

In the work [A5] with Freddy Bouchet, we addressed the generalisation of the Eyring–Kramers formula to general diffusion processes of the form

$$\mathrm{d}X^\epsilon_t = b(X^\epsilon_t)\mathrm{d}t + \sqrt{2\epsilon}\sigma(X^\epsilon_t)\mathrm{d}W_t, \tag{4.9}$$

for arbitrary functions $b : \mathbb{R}^d \to \mathbb{R}^d$ and $\sigma : \mathbb{R}^d \to \mathbb{R}^{d\times n}$. We still assume that the process is ergodic with respect to some stationary distribution p^ϵ_{st}, but the latter no longer needs to have an explicit expression such as (4.3), and in general the process $(X^\epsilon_t)_{t\geq 0}$ need not be reversible with respect to p^ϵ_{st}.

4.2.1 'Double-well' case

For all $x \in \mathbb{R}^d$, we denote by $(\psi^x_t)_{t\geq 0}$ the *relaxation dynamics* defined by the ODE

$$\dot{\psi}^x_t = b(\psi^x_t), \qquad \psi^x_0 = x.$$

A simple set of assumptions under which the solution $(X^\epsilon_t)_{t\geq 0}$ to (4.9) displays a metastable behaviour is the following generalisation of the double-well case introduced in Section 4.1. The vector field b has exactly three zeroes $\overline{x}_1$, $\overline{x}_2$ and $x_\star$ in $\mathbb{R}^d$, and the space $\mathbb{R}^d$ is partitioned into two open sets D_1, D_2 and a $(d-1)$-dimensional closed surface S such that:

- for $i = 1, 2$, $\overline{x}_i \in D_i$ and for any $x \in D_i$, ψ_t^x remains contained in D_i and converges to $\overline{x}_i$ when $t \to +\infty$;
- $x_\star \in S$ and for any $x \in S$, ψ_t^x remains contained in S and converges to $x_\star$ when $t \to +\infty$;

see Figure 4.2.

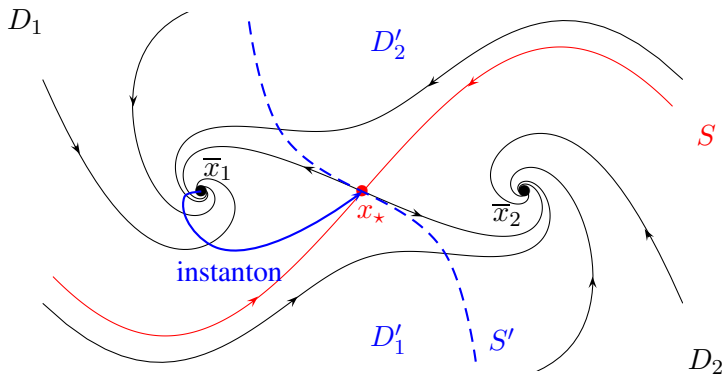

Figure 4.2: The partition of $\mathbb{R}^d$ into the sets D_1, D_2 and S, with the attractors $\overline{x}_1$, $\overline{x}_2$ and $x_\star$ of the ODE $\dot{x} = b(x)$, and the trajectories of the relaxation dynamics $(\psi_t^x)_{t\geq 0}$. The instanton joining $\overline{x}_1$ to $x_\star$ and the separatrix S' between D_1' and D_2', which will be introduced in Subsection 4.2.2, are plotted in blue.

In this setting, the Freidlin–Wentzell theory still provides a logarithmic description of the mean transition time between $\overline{x}_1$ and $\overline{x}_2$, which is comparable to the Arrhenius law (4.4) and in which the role of the potential U is played by a function V called the *quasipotential*. We first review some basic results of this theory in Subsection 4.2.2 and present the main steps of our heuristic derivation of the associated prefactor in Subsection 4.2.3.

4.2.2 Freidlin–Wentzell theory

From now on we assume that for all $x \in \mathbb{R}^d$, the matrix $a(x) := \sigma\sigma^\top(x)$ is nondegenerate. This assumption could however be relaxed, for precisions in this direction we refer to [Aze80]. The first building block of the theory of large deviations for (4.9) is the *action functional* defined, for $T_1 < T_2$, by

$$\forall \phi = (\phi_t)_{t\in[T_1,T_2]}, \qquad \mathcal{A}_{T_1,T_2}(\phi) = \begin{cases} \displaystyle\int_{t=T_1}^{T_2} \mathcal{L}(\phi_t, \dot{\phi}_t)\mathrm{d}t & \text{if } \phi \text{ is absolutely continuous,} \\ +\infty & \text{otherwise,} \end{cases}$$

where $\mathcal{L}(x, v)$ is the *Lagrangian* defined by

$$\mathcal{L}(x, v) := \frac{1}{4}\left\langle v - b(x), a(x)^{-1}\left(v - b(x)\right)\right\rangle.$$

For all $T > 0$, the action functional on $[0, T]$ is the rate function which describes the large deviations of the trajectory $(X_t^\epsilon)_{t\in[0,T]}$. As a consequence, when $X_0^\epsilon = \overline{x}_1$, the mean transition time $\mathbb{E}[\tau^\epsilon]$ satisfies

$$\lim_{\epsilon\to 0} \epsilon \log \mathbb{E}[\tau^\epsilon] = V(\overline{x}_1, x_\star),$$

where, for any $x \in \mathbb{R}^d$, the *quasipotential* $V(\overline{x}_1, \cdot)$ (with respect to $\overline{x}_1$) is defined by

$$V(\overline{x}_1, x) := \inf\left\{\mathcal{A}_{T_1,T_2}(\phi) : T_1 < T_2, \phi(T_1) = \overline{x}_1, \phi(T_2) = x\right\}.$$

Comparing this result with (4.4) shows that $V(\overline{x}_1, x_\star) = \Delta U = U(x_\star) - U(\overline{x}_1)$, but this identity can be recovered in a more direct, general and enlightening fashion as follows. Assume that the vector field b can be written under the form

$$b(x) = -a(x)\nabla U(x) + \ell(x), \qquad \langle \nabla U(x), \ell(x) \rangle = 0, \tag{4.10}$$

with the condition that $b(x) = 0$ if and only if $\nabla U(x) = 0$ (this is for instance the case in (4.6)). Equivalently, this amounts to finding a solution U to the Hamilton–Jacobi equation

$$\langle \nabla U(x), a(x)\nabla U(x) \rangle + \langle b(x), \nabla U(x) \rangle = 0 \tag{4.11}$$

which only admits as critical points the set of zeroes of b. For any $x \in \mathbb{R}^d$, define the *fluctuation dynamics* $(\varphi_t^x)_{t \le 0}$ by

$$\dot{\varphi}_t^x = a(\varphi_t^x)\nabla U(\varphi_t^x) + \ell(\varphi_t^x), \qquad \varphi_0^x = x.$$

Notice that, besides being defined on the set of nonpositive times and having x as a terminal condition, the fluctuation dynamics $(\varphi_t^x)_{t \le 0}$ differs from the relaxation dynamics $(\psi_t^x)_{t \ge 0}$ by the fact that the sign of the 'symmetric' part $a\nabla U$ of the vector field b has been reverted.

An elementary computation then shows that

$$\frac{\mathrm{d}}{\mathrm{d}t} U(\varphi_t^x) = \langle \nabla U(\varphi_t^x), a(\varphi_t^x)\nabla U(\varphi_t^x) \rangle \ge 0,$$

so that φ_t^x necessarily converges, when $t \to -\infty$, to a critical point of U, that is to say either $\overline{x}_1$, $\overline{x}_2$ or $x_\star$. We therefore assume that the space $\mathbb{R}^d$ can also be partitioned into two open sets D_1', D_2' and a $(d-1)$-dimensional closed surface S' such that:

- for $i = 1, 2$, $\overline{x}_i \in D_i'$ and for any $x \in D_i'$, φ_t^x remains contained in D_i' and converges to $\overline{x}_i$ when $t \to -\infty$;
- $x_\star \in S'$ and for any $x \in S'$, φ_t^x remains contained in S' and converges to $x_\star$ when $t \to -\infty$.

Notice that unless $\ell \equiv 0$, the sets D_1', D_2' and S' do not coincide with D_1, D_2 and S in general, see Figure 4.2.

For any $x \in D_1'$, an important result is then that

$$V(\overline{x}_1, x) = \int_{t=-\infty}^{0} \mathcal{L}(\varphi_t^x, \dot{\varphi}_t^x)\mathrm{d}t = U(x) - U(\overline{x}_1). \tag{4.12}$$

Indeed, for any absolutely continuous trajectory $\phi = (\phi_t)_{t \in [T_1, T_2]}$ such that $\phi_{T_1} = \overline{x}_1$, $\phi_{T_2} = x$, we have

$$\begin{aligned}
\mathcal{A}_{T_1,T_2}(\phi) &= \frac{1}{4}\int_{t=T_1}^{T_2} \Big\langle \dot{\phi}_t - b(\phi_t), a^{-1}(\phi_t)\Big(\dot{\phi}_t - b(\phi_t)\Big)\Big\rangle \,\mathrm{d}t \\
&= \frac{1}{4}\int_{t=T_1}^{T_2} \Big\langle \dot{\phi}_t + a(\phi_t)\nabla U(\phi_t) - \ell(\phi_t), a^{-1}(\phi_t)\Big(\dot{\phi}_t + a(\phi_t)\nabla U(\phi_t) - \ell(\phi_t)\Big)\Big\rangle \,\mathrm{d}t \\
&= \frac{1}{4}\int_{t=T_1}^{T_2} \Big\langle \dot{\phi}_t - a(\phi_t)\nabla U(\phi_t) - \ell(\phi_t), a^{-1}(\phi_t)\Big(\dot{\phi}_t - a(\phi_t)\nabla U(\phi_t) - \ell(\phi_t)\Big)\Big\rangle \,\mathrm{d}t \\
&\quad + \int_{t=T_1}^{T_2} \Big\langle \dot{\phi}_t - \ell(\phi_t), \nabla U(\phi_t)\Big\rangle \,\mathrm{d}t.
\end{aligned}$$

The first term in the right-hand side is nonnegative, while the orthogonality relation between ℓ and ∇U implies that the second term rewrites

$$\int_{t=T_1}^{T_2} \Big\langle \dot{\phi}_t, \nabla U(\phi_t)\Big\rangle \,\mathrm{d}t = U(\phi_{T_2}) - U(\phi_{T_1}) = U(x) - U(\overline{x}_1).$$

We deduce that $V(\overline{x}_1, x) \geq U(x) - U(\overline{x}_1)$. On the other hand, the second identity in (4.12) is an immediate consequence of the definition of $(\varphi_t^x)_{t\leq 0}$, and the final result (4.12) therefore follows from finite-time approximations of the optimal, but time-infinite, trajectory $(\varphi_t^x)_{t\leq 0}$.

As a consequence of (4.12), the fluctuation dynamics has the interpretation to be the *typical path* taken by the process $(X_t^\epsilon)_{t\geq 0}$ to reach the point $x \in \mathbb{R}^d$. Similarly, if there exists a *heteroclinic orbit* of the ODE $\dot{x} = a(x)\nabla U(x) + \ell(x)$ joining $\overline{x}_1$ to $x_\star$, that is to say a trajectory $(\rho_t)_{t\in\mathbb{R}}$ such that

$$\dot{\rho}_t = a(\rho_t)\nabla U(\rho_t) + \ell(\rho_t), \qquad \rho_{-\infty} = \overline{x}_1, \quad \rho_{+\infty} = x_\star,$$

then the transitions of $(X_t^\epsilon)_{t\geq 0}$ from $\overline{x}_1$ to $x_\star$ concentrate around this path in the $\epsilon \to 0$ limit. The path $(\rho_t)_{t\in\mathbb{R}}$ is then called an *instanton*, see Figure 4.2.

Overall, we have shown that assuming the existence of a solution U to the Hamilton–Jacobi equation (4.11) allows to define, through the fluctuation dynamics, two sets D_1' and D_2' in which we have the respective identities $V(\overline{x}_1, x) = U(x) - U(\overline{x}_1)$ and $V(\overline{x}_2, x) = U(x) - U(\overline{x}_2)$. As a consequence, it is natural to expect, conversely, that a solution U to (4.11) might be constructed by piecing together the quasipotentials $V(\overline{x}_1, \cdot)$ and $V(\overline{x}_2, \cdot)$, suitably balanced by additive constants representing the relative 'heights', in terms of quasipotential, of the attractors $\overline{x}_1$ and $\overline{x}_2$, in suitably chosen regions D_1' and D_2'. This idea was implemented by Freidlin and Wentzell to construct the rate function of the stationary distribution p_{st}^ϵ [FW12, Section 6.4]. It is also related with the presence of singularities in large deviation functions arising in nonequilibrium statistical mechanics [BK15] and the weak KAM theory for Lagrangian dynamics [Fat]. A clarification of these connections would be an important step in the formalisation of the results presented in this section.

4.2.3 Eyring–Kramers formula

Derivation of the formula

In order to compute the prefactor of the mean transition time, we follow the pathwise approach and assume that there is a time scale separation between the thermalisation and tunnelling phases. It is commonly accepted that at thermalisation, the statistical behaviour of the process in D_1 should be described by its *quasistationary distribution*, the definition of which is given below. This statement already appeared in Kramers' original paper [Kra40], although a precise definition of a quasi-stationary distribution was not introduced there, and we refer to [LBLLP12, BG16, DGLLPN19] for rigorous justifications. In our present context, the quasistationary distribution $p_{\mathrm{qst}}^\epsilon$ of $(X_t^\epsilon)_{t\geq 0}$ in D_1 can be defined by the so-called Yaglom limit

$$p_{\mathrm{qst}}^\epsilon(\cdot) = \lim_{t\to+\infty} \mathbb{P}(X_t^\epsilon \in \cdot | \tau_{D_1}^\epsilon > t),$$

where $\tau_{D_1}^\epsilon = \inf\{t \geq 0 : X_t^\epsilon \notin D_1\}$, see [CMSM13]. Our time scale separation assumption can then be reformulated as the assertion that this convergence occurs much faster than the order of magnitude of $\tau_{D_1}^\epsilon$ (which, by the Freidlin–Wentzell theory, is actually of the same order as the transition time τ^ϵ), so that on this short time scale, the event $\{\tau_{D_1}^\epsilon > t\}$ has a probability close to 1 and conditionning by this event does not really affect the law of X_t^ϵ.

The quasistationary distribution is the Perron–Frobenius eigenvector of the infinitesimal generator L^ϵ of $(X_t^\epsilon)_{t\geq 0}$ in D_1, with Dirichlet boundary conditions. Using nonrigorous WKB and boundary layer approximations, similar to some developments in [Gar09, Sch10], we first obtained an approximation of the quasistationary *flux* $\epsilon\nabla p_{\mathrm{qst}}^\epsilon$ in the neighbourhood of $x_\star$. Linearising b and σ in this neighbourhood, we then computed explicitly the probability that the process arriving from D_1 actually crosses the surface S and reaches the neighbourhood of $\overline{x}_2$ — this computation is reminiscent of the capacity estimates in [BEGK04]. Combining these two results, we finally obtained the Eyring–Kramers formula

$$\mathbb{E}[\tau^\epsilon] \sim \frac{2\pi}{\lambda_\star}\sqrt{\frac{|\det H_\star|}{\det \nabla_x^2 V(\overline{x}_1, \overline{x}_1)}}\exp\left(\frac{V(\overline{x}_1, x_\star)}{\epsilon} + \int_{t=-\infty}^{+\infty} F(\rho_t)\mathrm{d}t\right). \tag{4.13}$$

In this expression, $\lambda_\star$ is the positive eigenvalue of the matrix $\nabla b(x_\star)$. The matrix $H_\star$ plays the role of the Hessian of the quasipotential $V(\overline{x}_1, x)$ at the point $x = x_\star$, but in general the quasipotential is not smooth at $x_\star$, so that we have to define

$$H_\star = \lim_{t\to+\infty} \nabla_x^2 V(\overline{x}_1, \rho_t),$$

where we recall that $(\rho_t)_{t\in\mathbb{R}}$ is the instanton joining $\overline{x}_1$ to $x_\star$. Finally, the function F is defined by

$$F(x) = \operatorname{div} \ell(x) + \langle \operatorname{div} a(x), \nabla_x V(\overline{x}_1, x)\rangle, \tag{4.14}$$

where the vector field ℓ is defined by the assumption that b admits the transverse decomposition (4.10). Similar results, based on various formal techniques, were already obtained in the physics litterature, see for instance [CL67, Lud75, MS77, SM79, Gra87, MS93, MS97].

Integral term

The integral of F along the instanton is perhaps the most surprising term in this formula, when compared with (4.5) or (4.8). Since, under the assumption that there exist a solution U to the Hamilton–Jacobi equation (4.11), the stationary distribution p^ϵ_{st} is given by the explicit expression (4.3) if and only if $F = 0$, this term can be interpreted as a measure of how far the system is from being described, in its stationary state, by a Gibbs measure. In the sequel of this paragraph, we give the intuition of the origin of this term by computing the prefactor of the stationary distribution rather than the quasistationary distribution.

We therefore now leave the 'double-well' situation apart and rather assume that the vector field b possesses a unique zero $\overline{x}$, which is an attractor of all relaxation paths $(\psi^x_t)_{t\geq 0}$, $x \in \mathbb{R}^d$. In this case, the quasipotential $U(x) := V(\overline{x}, x)$ is a solution to the Hamilton–Jacobi (4.11) and therefore the transverse decomposition (4.10) holds in $\mathbb{R}^d$. The Freidlin–Wentzell theory also asserts that the stationary distribution p^ϵ_{st} satisfies a large deviation principle with rate function U. Defining the prefactor $C^\epsilon(x)$ by the identity

$$p^\epsilon_{\mathrm{st}}(x) = C^\epsilon(x)\sqrt{\frac{\det \nabla^2 U(\overline{x})}{(2\pi\epsilon)^d}}\exp\left(-\frac{U(x)}{\epsilon}\right),$$

so that by Laplace's method we may anticipate that $C^\epsilon(\overline{x}) = 1$, injecting this expression into the stationary Fokker–Planck equation associated with $(X^\epsilon_t)_{t\geq 0}$ and using the Hamilton–Jacobi equation (4.11), we get the equation

$$\epsilon\Delta C^\epsilon = \langle \nabla C^\epsilon, a\nabla U + \ell\rangle + C^\epsilon F,$$

with F defined by (4.14). Let us assume that in the $\epsilon \to 0$ limit, C^ϵ converges to some function C solution to the *transport equation*

$$0 = \langle \nabla C, a\nabla U + \ell\rangle + CF.$$

Since $a\nabla U + \ell$ is the vector field driving the fluctuation dynamics $(\varphi^x_t)_{t\leq 0}$, the latter is a characteristics for this equation in the sense that

$$\frac{\mathrm{d}}{\mathrm{d}t}\log C(\varphi^x_t) = -F(\varphi^x_t).$$

As a consequence, the prefactor writes

$$C(x) = C(\varphi^x_0) = C(\varphi^x_{-\infty})\exp\left(-\int_{t=-\infty}^{0} F(\varphi^x_t)\mathrm{d}t\right),$$

and since all fluctuation paths are also attracted to $\overline{x}$, we conclude that $C(\varphi^x_{-\infty}) = C(\overline{x}) = 1$.

In the double-well situation, in order to compute the prefactor at the point $x_\star$ then the characteristics is the instanton, which finally explains the occurrence of the integral along $(\rho_t)_{t\in\mathbb{R}}$ in (4.13).

Summary of cases and results

In a very recent work, Lee and Seo [LS] gave a proof, based on a new approach to potential theory for nonreversible processes, of the formula (4.13) in the case where both terms in the right-hand side of (4.14) vanish, so that there is no integral term in (4.13), and the stationary distribution of the process $(X_t^\epsilon)_{t\geq 0}$ remains explicitly given by the Gibbs measure (4.3). This situation is more general than the case of (4.6) described in Subsection 4.1.2, as is summarised on Table 4.1.

Assumptions on ℓ	(a) $\ell \equiv 0$	(b) $\ell = -J\nabla U$	(c) $\operatorname{div} \ell \equiv 0$	(d) General case
Reversibility	Yes	No	No	No
Invariant measure (4.3)	Yes	Yes	Yes	No
EK formula (heuristic)	[Eyr35, Kra40]	[AVE07]	[A5]	
EK formula (proof)	[BEGK04, HKN04]	[LMS19, LPM20]	[LS]	To be done!

Table 4.1: Various assumptions over ℓ under which Eyring–Kramers (EK) formulæ were investigated.
Case (a): $b = -\nabla U$ and σ is the identity.
Case (b): $b = -(a + J)\nabla U$, with J an antisymmetric matrix and $a = \sigma\sigma^\top$ does not depend on x.
Case (c): $b = a\nabla U + \ell$, with $\langle \ell, \nabla U\rangle = 0$, $\operatorname{div} \ell \equiv 0$ and $a = \sigma\sigma^\top$ does not depend on x.
Case (d): $b = a\nabla U + \ell$, with $\langle \ell, \nabla U\rangle = 0$ and $a = \sigma\sigma^\top$ may depend on x.
Notice that the cases are progressively ordered, in the sense that (a) $\subset$ (b) $\subset$ (c) $\subset$ (d).

4.2.4 Riccati equations for the computation of the prefactor

In this paragraph, we present the results from [A6] which address the numerical computation of the different terms involved in the formula (4.13). For the sake of simplicity, we take here $n = d$, and σ is the identity matrix. We still work under the assumption that there exist a solution U to the Hamilton–Jacobi equation (4.11), which is identified with the quasipotential $V(\overline{x}_1, x)$ in the domain D_1' and allows to decompose the vector field b under the form (4.10), but neither U nor ℓ are assumed to be known: only b is explicit. This already enables one to compute the eigenvalue $\lambda_\star$ in (4.13).

The numerical evaluation of the quasipotential $V(\overline{x}_1, x)$ is a common topic in computational statistical physics. In particular, the *geometric Minimum Action Method* (gMAM) [HVE08], based on [ERVE02, ERVE04], employs the Hamiltonian formalism of the Freidlin–Wentzell theory to compute fluctuation paths $(\varphi_t^x)_{t\geq 0}$, from which the quasipotential $V(\overline{x}_1, x)$ is deduced as the action of this path. With such a method, one may then compute the instanton $(\rho_t)_{t\in\mathbb{R}}$ and deduce the value of the quasipotential $V(\overline{x}_1, x_\star)$. It remains to compute the Hessian matrices $\nabla_x^2 V(\overline{x}_1, \overline{x}_1)$, $H_\star = \lim_{t\to+\infty} \nabla_x^2 V(\overline{x}_1, \rho_t)$, and the integral

$$\int_{t=-\infty}^{+\infty} F(\rho_t)\mathrm{d}t = \int_{t=-\infty}^{+\infty} \operatorname{div} \ell(\rho_t)\mathrm{d}t = \int_{t=-\infty}^{+\infty} (\operatorname{div} b(\rho_t) + \Delta_x V(\overline{x}_1, \rho_t))\,\mathrm{d}t.$$

All quantities which remain unknown depend on the matrix process $(H_t)_{t\in\mathbb{R}}$ defined by $H_t = \nabla_x^2 V(\overline{x}_1, \rho_t)$. It turns out that, as a consequence of the Hamilton–Jacobi equation, the process $(H_t)_{t\in\mathbb{R}}$ satisfies the matrix Riccati equation

$$\dot{H}_t = -2H_t^2 + Q_t^\top H_t + H_t Q_t + R_t, \tag{4.15}$$

where both matrices Q_t and R_t are explicit in terms of b and ρ_t. This fact was already noticed for example in [Lud75, MS97], and recent studies also established connections between matrix Riccati equations and large deviation prefactors for (4.9) [FG, GSVE]. Similar statements also appear in the litterature of deterministic optimal control [CFS15].

As a consequence, the matrix Riccati equation (4.15), after a geometric reparametrisation in order to replace the time interval $(-\infty, +\infty)$ with the instanton length $[0, L]$, can be solved by an Euler scheme as soon as its initial condition $H_{-\infty} = \nabla_x^2 V(\overline{x}_1, \overline{x}_1)$ is given. We compute the latter by remarking that it solves the stationary version of (4.15), which is called a *Continuous Algebraic Riccati Equation* in optimal control, and for which both numerical solvers and semi-analytic solutions are available.

Chapter 5

Quasistationary distributions in molecular dynamics

This chapter presents the results of the article [A7], written in collaboration with Tony Lelièvre and Loucas Pillaud-Vivien during Loucas Pillaud-Vivien's masters internship, and of the articles [A8] and [A9], written in collaboration with Tony Lelièvre and Mouad Ramil during Mouad Ramil's PhD thesis.

5.1 Introduction

Let $(\mathrm{x}_t)_{t\geq 0}$ be a homogeneous, time-continuous Markov process taking its values in some measurable space E. For a given probability measure μ on E (resp. a given point $x \in \mathsf{E}$), we use the notation $\mathbb{P}_\mu$ (resp. $\mathbb{P}_x$) to indicate that x_0 has distribution μ (resp. δ_x). For any measurable subset D of E, we denote by $\mathcal{P}(\mathsf{D})$ the set of probability measures on D and by $\mathcal{M}(\mathsf{D})$ the set of signed measures on D with finite total variation.

5.1.1 Quasistationary distributions

Let D be a nonempty, measurable subset of E and let us define

$$\tau_{\mathsf{D}} := \inf\{t > 0 : \mathrm{x}_t \notin \mathsf{D}\}.$$

A probability measure π on D is called a *quasistationary distribution* (QSD) for $(\mathrm{x}_t)_{t\geq 0}$ if

$$\forall t \geq 0, \qquad \mathbb{P}_\pi(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t) = \pi(\cdot). \tag{5.1}$$

Generically, QSDs are known to describe the $t \to +\infty$ limit of conditional probability measures of the form $\mathbb{P}_\mu(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t)$ for $\mu \in \mathcal{P}(\mathsf{D})$, which makes them particularly relevant to study the *metastability* phenomenon, described in the next subsection (see also Chapter 4). We refer to [CMSM13] for an extensive introduction to the study of QSDs.

The combination of the definition (5.1) with the Markov property provides QSDs with several useful properties. Indeed, if π is a QSD, then it is easily seen that there exists $\lambda \in [0, +\infty)$ such that under $\mathbb{P}_\pi$, the random variable τ_{D} is exponentially distributed with parameter λ. We shall call this quantity the *rate* associated with π, the case $\lambda = 0$ meaning that $\tau_{\mathsf{D}} = +\infty$ almost surely, so that π is actually a stationary distribution for $(\mathrm{x}_t)_{t\geq 0}$. If $\lambda > 0$, then under $\mathbb{P}_\pi$, τ_{D} is independent from $\mathrm{x}_{\tau_{\mathsf{D}}}$. Last, let us define the (nonconservative) semigroup $(P_t^{\mathsf{D}})_{t\geq 0}$ acting on measurable and bounded functions $f : \mathsf{D} \to \mathbb{R}$ by

$$P_t^{\mathsf{D}} f(x) := \mathbb{E}_x\left[f(\mathrm{x}_t)\mathbb{1}_{\{\tau_{\mathsf{D}} > t\}}\right],$$

and define the left product of P_t^{D} with measures $\rho \in \mathcal{M}(\mathsf{D})$ by

$$\rho P_t^{\mathsf{D}} f := \int_{x\in\mathsf{D}} P_t^{\mathsf{D}} f(x)\rho(\mathrm{d}x).$$

Then for any $t \geq 0$, π is a left eigenvector of P_t^{D}, with associated eigenvalue $\mathrm{e}^{-\lambda t}$, which generally implies that π is a left eigenvector of the infinitesimal generator of $(P_t^{\mathsf{D}})_{t\geq 0}$, with associated eigenvalue $-\lambda$. This spectral description often proves useful in order to study the existence and uniqueness of QSDs.

5.1.2 Metastability

Loosely speaking, a *metastable set* for the process $(\mathrm{x}_t)_{t\geq 0}$ is a subset D of E in which the process typically remains trapped over 'long periods of time'. For instance, many models of molecular dynamics, such as protein folding, are encoded by multimodal probability distributions on a phase space E, of which natural sampling processes $(\mathrm{x}_t)_{t\geq 0}$ admit the modes as metastable sets [LS16, Sections 6.3 and 6.4].

A more formal description of metastability is the fact that, starting from some point $x \in \mathsf{D}$, the convergence of the conditional distribution $\mathbb{P}_x(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t)$ to the QSD of $(\mathrm{x}_t)_{t\geq 0}$ in D occurs on a much shorter time scale than the order of magnitude of τ_{D}. Based on this remark, *accelerated dynamics algorithms* [Lel15] replace the simulation of the whole trajectory of $(\mathrm{x}_t)_{t\geq 0}$ in metastable sets with simulations under the QSD. This allows to use the properties of $(\tau_{\mathsf{D}}, \mathrm{x}_{\tau_{\mathsf{D}}})$ stated above, and is also more amenable to parallelisation (see Subsection 5.2.4).

On the theoretical side, the justification of these algorithms raises two important questions.

(i) Given a set D, does there exist a QSD π in D? Is it unique, and what is the speed of convergence of $\mathbb{P}_x(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t)$ to π?

(ii) How to numerically sample from π?

5.1.3 Outline of the chapter

In Section 5.2, we deal with the case where $(\mathrm{x}_t)_{t\geq 0}$ is a continuous-time Markov chain with values in a finite state space E. Under an irreducibility assumption on this chain in D, it is known that there is a unique QSD π and the convergence of $\mathbb{P}_x(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t)$ to π is exponential, which answers the first question above. We address the second and establish limit theorems for the *Fleming–Viot particle system* which provides a numerical method to sample from π. These results were established during Loucas Pillaud-Vivien's masters internship and are reported in the article [A7].

In Section 5.3, we then address the first question for *Langevin processes*, which are commonly employed in molecular dynamics. These are diffusion processes in the phase space $\mathsf{E} = \mathbb{R}^d \times \mathbb{R}^d$ of position-velocity pairs, which have the peculiarity of being degenerate. Besides, the relevant metastable sets are typically of the form $\mathsf{D} = \mathsf{O} \times \mathbb{R}^d$ and are therefore not bounded. Both the degeneracy of the process and the unboundedness of the set D require to develop appropriate tools to study quasistationarity. This work was carried out in Mouad Ramil's PhD thesis [Ram20], from which the articles [A8] and [A9] described below are extracted.

5.2 Limit theorems for Fleming–Viot particle systems

5.2.1 The finite state space framework

In this section, we let E be a finite set and $(\mathrm{x}_t)_{t\geq 0}$ be a continuous-time Markov chain with infinitesimal generator L given by

$$Lf(x) = \sum_{y\in\mathsf{E}} p(x,y)[f(y) - f(x)],$$

for any $x \in \mathsf{E}$ and $f : \mathsf{E} \to \mathbb{R}$. Up to a global time change, there is no loss of generality in assuming that the $\mathsf{E} \times \mathsf{E}$ matrix P with coefficients $\{p(x,y), x, y \in \mathsf{E}\}$ is stochastic, that is to say that

$$\forall x, y \in \mathsf{E}, \quad p(x,y) \geq 0, \qquad \forall x \in \mathsf{E}, \quad \sum_{y\in\mathsf{E}} p(x,y) = 1.$$

We fix a nonempty subset D of E and take the convention to identify measures on D with row vectors. Recall that we denote by $\mathcal{P}(\mathsf{D})$ the space of probability measures on D. The following proposition follows from the Perron–Frobenius theorem and [DS67].

Proposition 5.2.1 (QSD in D)**.** *Assume that the $\mathsf{D} \times \mathsf{D}$ matrix P_{D} with coefficients $\{p(x,y), x, y \in \mathsf{D}\}$ is irreducible.*

(i) There exists $\lambda \in [0,1)$ such that $1-\lambda$ is the spectral radius of P_{D}.

(ii) There is a unique $\pi \in \mathcal{P}(\mathsf{D})$ such that $\pi P_{\mathsf{D}} = (1-\lambda)\pi$.

(iii) π is the unique QSD of the process $(\mathrm{x}_t)_{t\geq 0}$ in D.

(iv) Under $\mathbb{P}_\pi$, τ_{D} is exponential with parameter λ.

Besides, for any $\mu \in \mathcal{P}(\mathsf{D})$, $\mathbb{P}_\mu(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t)$ converges exponentially fast to π.

One might consider using Proposition 5.2.1 to approximate π numerically by implementing the following rejection sampling procedure: simulate $n \gg 1$ independent copies of $(\mathrm{x}_t)_{t\geq 0}$ — in the sequel, we shall call these copies *particles* —, and at time $t \gg 1$, approximate π with the empirical measure of those particles for which $\tau_{\mathsf{D}} > t$. But of course, for a large value of t, the event $\{\tau_{\mathsf{D}} > t\}$ becomes more and more unlikely so that the required number of particles to simulate has to grow as well.

5.2.2 The Fleming–Viot particle system

Two classes of algorithms adapt the rejection sampling idea described above to improve its efficiency.

First, one may simulate a single particle $(\mathrm{x}_t)_{t\geq 0}$, and when it attempts to exit D at some time t, move it to some random location chosen in D according to the occupation measure $\frac{1}{t}\int_{s=0}^{t} \delta_{\mathrm{x}_s} \mathrm{d}s$. When $t \to +\infty$, the law of x_t is expected to converge to π [AFP88, GJ13, BC15, BCP18].

Second, one may simulate n particles $(\mathrm{x}_t^1)_{t\geq 0}, \ldots, (\mathrm{x}_t^n)_{t\geq 0}$, and when one of these particles attempts to exit D, move it to the position of one of the $n-1$ remaining particles, uniformly chosen. The process $(\mathrm{x}_t^1, \ldots, \mathrm{x}_t^n)_{t\geq 0}$ in D^n is called the *Fleming–Viot particle system* [BHIM96, BHM00]. In our finite state space setting, the following results are due to Asselah, Groisman and Ferrari [AFG11].

Proposition 5.2.2 (Laws of Large Numbers for Fleming–Viot particle systems)**.** *Under the assumptions of Proposition 5.2.1, we have:*

(i) for any probability measure μ on D, if the particles are initially iid according to μ then for any $t \geq 0$, the empirical measure $\frac{1}{n}\sum_{i=1}^n \delta_{\mathrm{x}_t^i}$ converges to $\mathbb{P}_\mu(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t)$ when $n \to +\infty$;

(ii) for any $n \geq 2$, the process $(\mathrm{x}_t^1, \ldots, \mathrm{x}_t^n)_{t\geq 0}$ possesses a unique stationary distribution, under which the empirical measure $\frac{1}{n}\sum_{i=1}^n \delta_{\mathrm{x}_\infty^i}$ converges to π when $n \to +\infty$.

We refer to [BHM00, GK04, Rou06, FM07, Löb09, Vil14, CT16, OV17, JM, CV19] for various extensions of these statements to Markov processes in countably infinite or continuous state spaces.

5.2.3 Central Limit Theorem for the stationary distribution in finite state spaces

The convergence of the empirical measure $\frac{1}{n}\sum_{i=1}^n \delta_{\mathrm{x}_t^i}$ to $\mathbb{P}_\mu(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t)$ is complemented by a Central Limit Theorem, first obtained by Del Moral and Miclo [DMM03] and then generalised by Cérou, Delyon, Guyader and Rousset [CDGR20]. More precisely, the random variable

$$\xi_t^n := \sqrt{n}\left(\frac{1}{n}\sum_{i=1}^n \delta_{\mathrm{x}_t^i} - \mathbb{P}_\mu(\mathrm{x}_t \in \cdot | \tau_{\mathsf{D}} > t)\right),$$

which takes its values in the space $\mathcal{M}_0(\mathsf{D})$ of signed measures on D with finite total variation and mass zero, converges in distribution to some centered Gaussian random variable, with an explicit covariance operator K_t^μ. This result holds in a very general setting. In [A7], we established a stationary version of this theorem for finite state space Markov chains.

Theorem 5.2.3 (Central Limit Theorem for the stationary distribution of the Fleming–Viot particle system)**.** *Under the assumptions of Proposition 5.2.1, let $n \geq 2$, $(\mathrm{x}_\infty^1, \ldots, \mathrm{x}_\infty^n)$ be distributed according to the stationary distribution of the Fleming–Viot particle system, and*

$$\xi_\infty^n := \sqrt{n}\left(\frac{1}{n}\sum_{i=1}^n \delta_{\mathrm{x}_\infty^i} - \pi\right).$$

When $n \to +\infty$, ξ_∞^n converges in distribution to some centered Gaussian random variable in $\mathcal{M}_0(\mathsf{D})$, with an explicit covariance operator K_∞.

The operator K_∞ turns out to be the limit, when $t \to +\infty$, of the operator K_t^μ, for any initial distribution μ. This makes Theorem 5.2.3 consistent with a formal $t \to +\infty$ limit of the results of [DMM03, CDGR20]. Our proof of Theorem 5.2.3 relies on the following remark. In the Fleming–Viot particle system, the particles are exchangeable, so that the empirical measure

$$\eta_t^n := \frac{1}{n}\sum_{i=1}^n \delta_{\mathrm{x}_t^i}$$

defines a Markov process in $\mathcal{P}(\mathsf{D})$, whose infinitesimal generator is easily seen to write

$$\mathbf{L}^n\phi(\eta) = \sum_{x,y\in\mathsf{D}} n\eta(x)\left(p(x,y) + \frac{nq(x)\eta(y)}{n-1}\right)\left[\phi\left(\eta^{x,y}\right) - \phi(\eta)\right], \qquad \phi : \mathcal{P}(\mathsf{D}) \to \mathbb{R},$$

where $\eta^{x,y} := \eta + \frac{1}{n}(\delta_y - \delta_x)$ and $q(x) := \sum_{y\in\mathsf{E}\setminus\mathsf{D}} p(x,y)$. Indeed, in a configuration η, there are $n\eta(x)$ particles located in x, and each of these particles may move to y 'directly' at rate $p(x,y)$, or try to exit D at rate $q(x)$ and then be moved to y with probability $n\eta(y)$ (the number of particles in y) divided by $n-1$ (the total number of particles among which the location of the exiting particle is chosen).

We then define $\xi_t^n := \sqrt{n}(\eta_t^n - \pi) \in \mathcal{M}_0(\mathsf{D})$. Since it is an affine, bijective transformation of η_t^n, the process $(\xi_t^n)_{t\geq 0}$ remains Markov and its infinitesimal generator $\mathbf{M}^n$ can be written explicitly. It turns out that for any smooth function $\psi : \mathcal{M}_0(\mathsf{D}) \to \mathbb{R}$, $\mathbf{M}^n\psi$ converges, when $n \to +\infty$, to $\overline{\mathbf{M}}\psi$, where $\overline{\mathbf{M}}$ is the infinitesimal generator of a linear diffusion process $(\overline{\xi}_t)_{t\geq 0}$ in $\mathcal{M}_0(\mathsf{D})$. The unique stationary distribution of $(\overline{\xi}_t)_{t\geq 0}$ is known to be Gaussian with a covariance operator K_∞ given as the solution to a Lyapunov equation involving the coefficients of $\overline{\mathbf{M}}$.

We now claim that the sequence of the stationary distributions of $(\xi_t^n)_{t\geq 0}$ is tight on $\mathcal{M}_0(\mathsf{D})$. The proof of this claim is a bit technical but merely relies on the combination of Proposition 5.2.2 (ii) with estimates on $\mathbf{M}^n$. It is then easy to deduce from the convergence of $\mathbf{M}^n\psi$ to $\overline{\mathbf{M}}\psi$ that necessarily, any limit of this sequence is a stationary distribution for $(\overline{\xi}_t)_{t\geq 0}$, which completes the proof.

Remark 5.2.4 (Nonasymptotic variance estimate)**.** *Let η_∞^n be the empirical measure of n particles distributed according to the stationary distribution of the Fleming–Viot particle process. Theorem 5.2.3 shows that the asymptotic rate of convergence of η_∞^n to π is $1/\sqrt{n}$. It is then natural to wonder whether a nonasymptotic rate may be derived, that is to say whether there exists $C \in [0, +\infty)$ such that for all $n \geq 1$,*

$$\mathbb{E}\left[\|\eta_\infty^n - \pi\|^2\right] \leq \frac{C}{n}, \tag{5.2}$$

for some norm $\|\cdot\|$ on $\mathcal{M}_0(\mathsf{D})$. Notice that such an estimate would make the tightness of $(\xi_\infty^n)_{t\geq 0}$ immediate in the proof of Theorem 5.2.3.

Versions of (5.2) were for example obtained in [FM07, CT16] for continuous-time Markov chains with countably infinite state spaces, but under specific mixing conditions on their jump rates. On the other hand, Angeli, Grosskinsky and Johansen [AGJ] recently studied interacting particle systems associated with nonlinear Feynman–Kac semigroups for pure jump Markov processes, based on a previous work by Rousset [Rou06]. In our finite state space setting, their results imply (5.2) (and actually a quantitative, uniform in time propagation of chaos estimate for η_t^n) for the following variant of the Fleming–Viot particle system: when a particle tries to exit D, its location is drawn according to the current empirical measure η_t^n of the system, so that it has an extra $1/n$ probability to remain in its current location.

5.2.4 Limit theorems for first exit times

Let us come back to the issue of simulating the trajectory of a metastable stochastic process $(\mathrm{x}_t)_{t\geq 0}$. Assume that given a metastable set D, one is interested in the sampling of the pair $(\tau_{\mathsf{D}}, \mathrm{x}_{\tau_{\mathsf{D}}})$ under $\mathbb{P}_x$, for some $x \in \mathsf{D}$. This assumption is for instance motivated by the so-called *Transition State Theory*, the purpose of which is to reduce the dynamics of a metastable process in a continuous and possibly high-dimensional state space to a pure jump Markov process between metastable sets. The rates of this pure jump process then naturally depend on the law of $(\tau_{\mathsf{D}}, \mathrm{x}_{\tau_{\mathsf{D}}})$, see the introduction of [DGLLPN19] and the references therein.

Based on the metastability assumption on D, one may first replace $\mathbb{P}_x$ with $\mathbb{P}_\pi$, where π is the QSD of $(\mathrm{x}_t)_{t\geq 0}$ in D. One may then simulate n independent realisations $(\mathrm{x}_t^1)_{t\geq 0}, \ldots, (\mathrm{x}_t^n)_{t\geq 0}$ of the process under $\mathbb{P}_\pi$, call $\tau_{\mathsf{D}}^1, \ldots, \tau_{\mathsf{D}}^n$ the corresponding exit times and define

$$I = \operatorname*{arg\,min}_{1\leq i\leq n} \tau_{\mathsf{D}}^i.$$

Then, since $\tau_{\mathsf{D}}^1, \ldots, \tau_{\mathsf{D}}^n$ are independent and exponentially distributed, and they are independent from $\mathrm{x}^1_{\tau_{\mathsf{D}}^1}, \ldots, \mathrm{x}^n_{\tau_{\mathsf{D}}^n}$, we have that

$$\left(n\tau_{\mathsf{D}}^I, \mathrm{x}^I_{\tau_{\mathsf{D}}^I}\right) = \left(\tau_{\mathsf{D}}, \mathrm{x}_{\tau_{\mathsf{D}}}\right), \qquad \text{in distribution.} \tag{5.3}$$

In other words, this *paralellisation* procedure divides by n the time needed to observe an exit event. This algorithm is called the *Parallel Replica Dynamics* [LBLLP12, PUV15].

Of course, it requires one to be initially able to sample n independent realisations $\mathrm{x}_0^1, \ldots, \mathrm{x}_0^n$ from the QSD π. Based on such convergence results as Proposition 5.2.2 (ii), a possible approach may be to take the vector $(\mathrm{x}_0^1, \ldots, \mathrm{x}_0^n)$ distributed under the stationary distribution of the Fleming–Viot particle system. Because of the fact that, in this case, the particles are not initially independent, the relation (5.3) no longer holds for finite values of n, but it may be shown to hold asymptotically, at least in the case of continuous-time Markov chains in finite state spaces.

Proposition 5.2.5 (Limit theorem for exit times)**.** *Let the assumptions of Proposition 5.2.2 be in force. Let $(\mathrm{x}_0^1, \ldots, \mathrm{x}_0^n)$ be distributed under the stationary distribution of the Fleming–Viot particle system, and conditionally on $(\mathrm{x}_0^1, \ldots, \mathrm{x}_0^n)$, let $(\mathrm{x}_t^1)_{t\geq 0}, \ldots, (\mathrm{x}_t^n)_{t\geq 0}$ evolve as independent copies of $(\mathrm{x}_t)_{t\geq 0}$. With the notation introduced above, we have*

$$\lim_{n\to+\infty} \left(n\tau_{\mathsf{D}}^I, \mathrm{x}^I_{\tau_{\mathsf{D}}^I}\right) = \left(\tau_{\mathsf{D}}, \mathrm{x}_{\tau_{\mathsf{D}}}\right), \qquad \textit{in distribution.}$$

We do not detail the whole proof but outline the justification of the convergence of $n\tau_{\mathsf{D}}^I$ to τ_{D}. For any $t \geq 0$, using the conditional independence of the processes given the initial condition, we have

$$\mathbb{P}\left(n\tau_{\mathsf{D}}^I > t\right) = \mathbb{E}\left[\prod_{i=1}^n \mathbb{P}(\tau_{\mathsf{D}}^i > t/n | \mathrm{x}_0^i)\right] = \mathbb{E}\left[\exp\left(n \sum_{x\in\mathsf{D}} \log u\left(t/n, x\right) \eta_0^n(x)\right)\right],$$

where $u(s,x) := \mathbb{P}_x(\tau_{\mathsf{D}} > s)$ and η_0^n is the empirical measure of $\mathrm{x}_0^1, \ldots, \mathrm{x}_0^n$. On the one hand, Proposition 5.2.2 (ii) asserts that η_0^n converges to π. On the other hand, from Proposition 5.2.1 it is easy to show that, denoting by I_{D} the $\mathsf{D}\times\mathsf{D}$ identity matrix and by $\mathbf{1}_{\mathsf{D}}$ the function $x \mapsto 1$ on D (which is identified with a column vector), we have

$$n \sum_{x\in\mathsf{D}} \log u\left(t/n, x\right) \pi(x) = n \sum_{x\in\mathsf{D}} \log\left(\left(\mathrm{e}^{t(P_{\mathsf{D}} - I_{\mathsf{D}})/n} \mathbf{1}_{\mathsf{D}}\right)(x)\right) \pi(x) \simeq -\lambda t$$

when $n \to +\infty$. In this finite state space setting, we therefore deduce that $n\tau_{\mathsf{D}}^I$ converges to an exponential random variable with parameter λ. The arguments virtually carry out in a general state space, but then one has to study the asymptotic behaviour of

$$n \int_{x\in\mathsf{D}} \log u\left(t/n, x\right) \eta_0^n(\mathrm{d}x).$$

In this expression, the integrand $n \log u\,(t/n, x)$ depends on n, and generically converges towards a (quite singular) distribution supported by $\partial\mathsf{D}$, to which the empirical measures η_0^n do not give any mass. It is therefore likely that quantitative estimates on the convergence of η_0^n to π will then be needed to control this quantity. We leave this problem as a work in progress.

5.3 Quasistationary distribution for Langevin processes

5.3.1 Metastability in molecular dynamics

Let $F : \mathbb{R}^d \to \mathbb{R}^d$ be a smooth function, which shall play the role of a *force field*, and $(B_t)_{t\geq 0}$ be a d-dimensional Brownian motion. The *overdamped Langevin process* $(\overline{q}_t)_{t\geq 0}$ in $\mathbb{R}^d$, defined by the stochastic differential equation

$$\mathrm{d}\overline{q}_t = F(\overline{q}_t)\mathrm{d}t + \overline{\sigma}\mathrm{d}B_t, \tag{5.4}$$

and the *Langevin process* $(q_t, p_t)_{t\geq 0}$ in $\mathbb{R}^d \times \mathbb{R}^d$, defined by the system of stochastic differential equations

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = F(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sigma \mathrm{d}B_t, \end{cases} \tag{5.5}$$

are ubiquitous in molecular dynamics [LS16]. An important reason for this fact is that, in the case where $F = -\nabla V$, $\overline{\sigma} = \sqrt{2\beta^{-1}}$ with $\beta > 0$, $\gamma > 0$ and $\sigma = \sqrt{2\gamma\beta^{-1}}$, the overdamped Langevin process is reversible and ergodic with respect to the so-called *Gibbs measure*

$$\overline{\nu}(\mathrm{d}q) := \frac{1}{\overline{Z}_\beta} \mathrm{e}^{-\beta V(q)} \mathrm{d}q, \qquad \overline{Z}_\beta := \int_{q\in\mathbb{R}^d} \mathrm{e}^{-\beta V(q)} \mathrm{d}q,$$

while the Langevin process is ergodic (but not reversible) with respect to the product measure

$$\nu(\mathrm{d}q\mathrm{d}p) := \overline{\nu}(\mathrm{d}q)\mathrm{M}_\beta(\mathrm{d}p), \tag{5.6}$$

where M_β is the centered Gaussian measure with covariance matrix $\beta^{-1} I_d$, also called the *Maxwell distribution* with inverse temperature β. Therefore, both processes may be employed to sample from the Gibbs measure $\overline{\nu}$, which is often the quantity of interest for the statistical description of a physical system.

When the potential V has several local minima, both processes $(\overline{q}_t)_{t\geq 0}$ and $(q_t, p_t)_{t\geq 0}$ exhibit metastability in sets with respective forms $\mathsf{D} = \mathsf{O}$ and $\mathsf{D} = \mathsf{O} \times \mathbb{R}^d$, where O is a well of V. Accelerated algorithms are thus needed to simulate trajectories over long time intervals, which motivates the theoretical study of QSDs in such sets. Known results for the overdamped Langevin process are recalled in Subsection 5.3.2, and the study of the Langevin process carried out in [A8] and [A9] is summarised in Subsection 5.3.3.

5.3.2 QSD for overdamped Langevin processes

Let us introduce precisely our assumptions on the force field F and the set $\mathsf{O} \subset \mathbb{R}^d$.

(F) The function $F : \mathbb{R}^d \to \mathbb{R}^d$ is C^∞.

(O) The subset $\mathsf{O} \subset \mathbb{R}^d$ is open, bounded, connected and has a C^2 boundary.

Under these assumptions, and for any temperature parameter $\overline{\sigma} > 0$, the stochastic differential equation (5.4) admits a unique strong solution, which is defined at least up to the stopping time

$$\overline{\tau}_{\mathsf{O}} := \inf\{t > 0 : \overline{q}_t \notin \mathsf{O}\},$$

as soon as the initial condition is taken in O. The associated infinitesimal generator writes

$$\overline{L}f = \frac{\overline{\sigma}^2}{2}\Delta f + F \cdot \nabla f, \qquad f \in C^2(\mathbb{R}^d),$$

and we introduce the operator

$$\overline{L}^* \rho = \frac{\overline{\sigma}^2}{2}\Delta \rho - \operatorname{div}(F\rho), \qquad \rho \in C^2(\mathbb{R}^d).$$

In the next statement, which should be compared with Proposition 5.2.1 in the finite state space setting, we gather results from [GQZ88, LBLLP12, CCPV18, CV].

Theorem 5.3.1 (QSD for the overdamped Langevin process)**.** *Let Assumptions* (F) *and* (O) *hold, and take* $\overline{\sigma} > 0$ *in* (5.4)*.*

(i) The solution to (5.4) *admits a unique QSD* $\overline{\pi}$ *in* O*, and the associated rate* $\overline{\lambda}$ *is positive.*

(ii) The measure $\overline{\pi}$ *admits a density* $\overline{\psi} \in C(\overline{\mathsf{O}}) \cap C^\infty(\mathsf{O})$ *with respect to the Lebesgue measure on* $\mathbb{R}^d$*. This density is positive on* O *and satisfies*

$$\begin{cases} \overline{L}^* \overline{\psi} = -\overline{\lambda}\overline{\psi} & \text{on } \mathsf{O}, \\ \overline{\psi} = 0 & \text{on } \partial\mathsf{O}. \end{cases}$$

(iii) Let $\theta \in \mathbb{R}$ *and* $\rho \in C(\overline{\mathsf{O}}) \cap C^2(\mathsf{O})$*, such that* $\rho \neq 0$ *and*

$$\begin{cases} \overline{L}^* \rho = -\theta\rho & \text{on } \mathsf{O}, \\ \rho = 0 & \text{on } \partial\mathsf{O}. \end{cases}$$

Then $\theta \geq \overline{\lambda}$*, and the conditions*

(a) $\theta = \overline{\lambda}$*,*

(b) ρ *has constant sign over* O*,*

(c) ρ *is a multiple of* $\overline{\psi}$*,*

are equivalent.

(iv) There exists $\overline{C} \geq 0$ *and* $\overline{\alpha} > 0$ *such that, for any* $\mu \in \mathcal{P}(\mathsf{O})$*,*

$$\forall t \geq 0, \qquad \|\mathbb{P}_\mu(\overline{q}_t \in \cdot | \overline{\tau}_\mathsf{O} > t) - \overline{\pi}(\cdot)\|_{\mathrm{TV}} \leq \overline{C}\mathrm{e}^{-\overline{\alpha}t},$$

with $\|\cdot\|_{\mathrm{TV}}$ *the total variation norm on* $\mathcal{M}(\mathsf{O})$*.*

Theorem 5.3.1 relies on two main classes of arguments, analytic and probabilistic (often used in combination with each other). For example, the existence of a nonnegative eigenvector for $\overline{L}^*$, which then yields the existence of a QSD, and the exponential convergence of conditional distributions toward the QSD, can be obtained from a spectral analysis of the operator $\overline{L}$ with homogeneous Dirichlet condition ([LBLLP12] in the reversible case), or the associated semigroup ([GQZ88] in the general case). In both cases, the fact that the domain O be bounded and the operator $\overline{L}$ be uniformly elliptic plays an important role. Similar results may be obtained with a more probabilistic approach based on Lyapunov functionals, where the boundedness of O is less crucial [CV]. Uniqueness, on the other hand, follows from minorisation conditions or Harnack inequalities.

5.3.3 QSD for Langevin processes

Statement of the main result

Under Assumptions (F) and (O), for any temperature parameter $\sigma > 0$ and friction parameter $\gamma \in \mathbb{R}$, the stochastic differential equation (5.5) admits a unique strong solution defined at least up to the stopping time

$$\tau_{\mathsf{D}} := \inf\{t > 0 : q_t \notin \mathsf{O}\}$$

as soon as the initial condition is taken in the cylindrical domain of the phase space

$$\mathsf{D} := \mathsf{O} \times \mathbb{R}^d.$$

The associated infinitesimal generator now writes

$$Lf = \frac{\sigma^2}{2}\Delta_p f + (F(q) - \gamma p) \cdot \nabla_p f + p \cdot \nabla_q f, \qquad f \in C^2(\mathbb{R}^d \times \mathbb{R}^d),$$

and we define

$$L^*\rho = \frac{\sigma^2}{2}\Delta_p \rho - \operatorname{div}_p\left((F(q) - \gamma p)\,\rho\right) - \operatorname{div}_q\left(p\rho\right), \qquad \rho \in C^2(\mathbb{R}^d \times \mathbb{R}^d).$$

Since the Laplacian in L and L^* only acts on the velocity variable, these operators are called *degenerate*. This makes the analysis of the exit event from D different from the overdamped Langevin process, as is illustrated on the following result which is proved in [A8]. In this statement, for any $q \in \partial\mathsf{O}$, we denote by $n(q)$ the outward normal vector to O.

Proposition 5.3.2 (Exit from D)**.** *Under Assumptions* (F) *and* (O)*, for any $x = (q, p) \in \mathsf{D}$ and $T \geq 0$, we have*

$$\mathbb{P}_x\left(n(q_{\tau_{\mathsf{D}}}) \cdot p_{\tau_{\mathsf{D}}} \leq 0, \tau_{\mathsf{D}} \leq T\right) = 0.$$

In other words, when the process leaves O, it is with a strictly outgoing velocity. As a consequence of this probabilistic fact, boundary conditions in related partial differential equations are generally not set on the whole boundary $\partial\mathsf{D}$. In order to make this statement more precise, let us first introduce the following partition of $\partial\mathsf{D}$:

$$\begin{aligned}
\Gamma^+ &:= \{(q, p) \in \partial\mathsf{O} \times \mathbb{R}^d : n(q) \cdot p > 0\},\\
\Gamma^- &:= \{(q, p) \in \partial\mathsf{O} \times \mathbb{R}^d : n(q) \cdot p < 0\},\\
\Gamma^0 &:= \{(q, p) \in \partial\mathsf{O} \times \mathbb{R}^d : n(q) \cdot p = 0\}.
\end{aligned}$$

The main result of [A9] reads as follows.

Theorem 5.3.3 (QSD for the Langevin process)**.** *Let Assumptions* (F) *and* (O) *hold, and take $\sigma > 0$, $\gamma \in \mathbb{R}$ in* (5.5)*.*

(i) The solution to (5.5) *admits a unique QSD π in D, and the associated rate λ is positive.*

(ii) The measure π admits a density $\psi \in C(\overline{\mathsf{D}}) \cap C^\infty(\mathsf{D})$ with respect to the Lebesgue measure on $\mathbb{R}^d \times \mathbb{R}^d$. This density is positive and bounded on $\mathsf{D} \cup \Gamma^+$ and satisfies

$$\begin{cases} L^*\psi = -\lambda\psi & \text{on } \mathsf{D},\\ \psi = 0 & \text{on } \Gamma^- \cup \Gamma^0. \end{cases}$$

(iii) Let $\theta \in \mathbb{R}$ and $\rho \in C(\overline{\mathsf{D}}) \cap C^2(\mathsf{D})$, such that $\rho \neq 0$ and

$$\begin{cases} L^*\rho = -\theta\rho & \text{on } \mathsf{D},\\ \rho = 0 & \text{on } \Gamma^- \cup \Gamma^0. \end{cases}$$

Then $\theta \geq \lambda$, and the conditions

(a) $\theta = \lambda$,

(b) ρ *has constant sign over* D,

(c) ρ *is a multiple of* ψ,

are equivalent.

(iv) There exists $C \geq 0$, $\alpha > 0$ *and a positive, continuous and bounded function* ϕ *on* D *such that, for any* $\mu \in \mathcal{P}(\mathsf{D})$,

$$\forall t \geq 0, \qquad \|\mathbb{P}_\mu\left((q_t, p_t) \in \cdot | \tau_{\mathsf{D}} > t\right) - \pi(\cdot)\|_{\mathrm{TV}} \leq \frac{C}{\int_{\mathsf{D}} \phi \mathrm{d}\mu} \mathrm{e}^{-\alpha t},$$

with $\|\cdot\|_{\mathrm{TV}}$ *the total variation norm on* $\mathcal{M}(\mathsf{D})$.

Outline of the proof

In the sequel, we denote by $C_{\mathrm{b}}(\overline{\mathsf{D}})$ the set of continuous and bounded functions on $\overline{\mathsf{D}}$ and endow this set with the sup norm. For any $t \geq 0$, let us define the operator P_t^{D} by

$$\forall f \in C_{\mathrm{b}}(\overline{\mathsf{D}}), \qquad P_t^{\mathsf{D}} f(x) := \mathbb{E}_x\left[f(q_t, p_t) \mathbb{1}_{\{t < \tau_{\mathsf{D}}\}}\right].$$

The following statement is one of the main results of [A8].

Proposition 5.3.4 (Transition density)**.** *Let the assumptions of Theorem 5.3.3 hold.*

(i) There exists a continuous function $\mathrm{p}^{\mathsf{D}} : (0, +\infty) \times \overline{\mathsf{D}} \times \overline{\mathsf{D}} \to [0, +\infty)$ *such that, for any* $t > 0$, $x \in \overline{\mathsf{D}}$ *and* $f \in C_{\mathrm{b}}(\overline{\mathsf{D}})$,

$$P_t^{\mathsf{D}} f(x) = \int_{y \in \mathsf{D}} \mathrm{p}^{\mathsf{D}}(t, x, y) f(y) \mathrm{d}y.$$

(ii) For any $t > 0$ *and* $x, y \in \overline{\mathsf{D}}$,

- $\mathrm{p}^{\mathsf{D}}(t, x, y) > 0$ *if* $x \notin \Gamma^+ \cup \Gamma^0$ *and* $y \notin \Gamma^- \cup \Gamma^0$,
- $\mathrm{p}^{\mathsf{D}}(t, x, y) = 0$ *if* $x \in \Gamma^+ \cup \Gamma^0$ *or* $y \in \Gamma^- \cup \Gamma^0$.

(iii) The function p^{D} *is* C^∞ *on* $(0, +\infty) \times \mathsf{D} \times \mathsf{D}$ *and satisfies the forward and backward Kolmogorov equations*

$$\partial_t \mathrm{p}^{\mathsf{D}} = L_y^* \mathrm{p}^{\mathsf{D}} = L_x \mathrm{p}^{\mathsf{D}}.$$

The proof of Proposition 5.3.4 is primarily based on the Feynman–Kac representation formula for strong solutions to the problem

$$\begin{cases} \partial_t u = Lu & \text{in } \mathsf{D}, \\ u = f & \text{for } t = 0, \\ u = g & \text{on } \Gamma^+, \end{cases} \tag{5.7}$$

as

$$u(t, x) = \mathbb{E}_x\left[\mathbb{1}_{\{t < \tau_{\mathsf{D}}\}} f(q_t, p_t) + \mathbb{1}_{\{t \geq \tau_{\mathsf{D}}\}} g(q_{\tau_{\mathsf{D}}}, p_{\tau_{\mathsf{D}}})\right].$$

This representation is established as follows. First, weak solutions of (5.7) are constructed by parabolic approximation and localisation in velocity, in order to bypass the degeneracy of the operator L and the unboundedness of the set D. Second, the hypoellipticity of the operator L is used to obtain the regularity of these solutions. Third, these solutions are identified with the probabilistic representation thanks to Itô's formula. This essentially yields the points (i) and (iii) of Proposition 5.3.4. For further results in the litterature regarding weak and strong solutions to the problem (5.7), we refer to [Car98, HJV14, HJJ18, AM].

The point (ii) relies on quite different arguments. The positivity of the transition density in $\mathsf{D} \times \mathsf{D}$ follows from a Harnack inequality for the operator $\partial_t - L$, which is originally due to Imbert, Golse, Mouhot and Vasseur [GIMV19] but was suitably generalised in [A8]. The behaviour of the transition density on $\partial\mathsf{D}$ combines a detailed analysis of the trajectories of the process $(q_t, p_t)_{t\geq 0}$ near the boundary, the use of an *adjoint* process related with time-reversal, and the following Gaussian upper bound on p^{D}.

Proposition 5.3.5 (Gaussian upper bound)**.** *Let the assumptions of Theorem 5.3.3 hold. For any $\alpha \in (0,1)$ and $T > 0$, there exists a finite constant $C(\alpha, T)$ (which also depends on F, σ^2, γ and O) such that, for all $t \in (0, T]$ and $x, y \in \overline{\mathsf{D}}$,*

$$\mathrm{p}^{\mathsf{D}}(t, x, y) \leq C(\alpha, T)\widehat{\mathrm{p}}^{(\alpha)}(t, x, y), \tag{5.8}$$

where $\widehat{\mathrm{p}}^{(\alpha)}(t, x, y)$ is the transition density of the Gaussian process $(\widehat{q}_t^{(\alpha)}, \widehat{p}_t^{(\alpha)})_{t\geq 0}$ defined by

$$\begin{cases} \mathrm{d}\widehat{q}_t^{(\alpha)} = \widehat{p}^{(\alpha)}\mathrm{d}t, \\ \mathrm{d}\widehat{p}_t^{(\alpha)} = -\gamma\widehat{p}_t^{(\alpha)}\mathrm{d}t + \dfrac{\sigma}{\sqrt{\alpha}}\mathrm{d}B_t. \end{cases} \tag{5.9}$$

Proposition 5.3.5 generalises a result by Konakov, Menozzi and Molchanov [KMM10], which would only cover the case $\gamma = 0$ in our setting, based on the use of the parametrix method [Bal81, Fri64]. We actually prove that the bound (5.8) holds for the transition density $\mathrm{p}(t, x, y)$ of the solution $(q_t, p_t)_{t\geq 0}$ to (5.5) in the whole phase space $\mathbb{R}^d \times \mathbb{R}^d$, under the condition that F be globally bounded. It is then clear that the upper bound transfers to $\mathrm{p}^{\mathsf{D}}(t, x, y)$ because by construction, $\mathrm{p}^{\mathsf{D}}(t, x, y) \leq \mathrm{p}(t, x, y)$, and the transition density $\mathrm{p}^{\mathsf{D}}(t, x, y)$ does not depend on the values of F outside O, so under Assumption (F), the latter function can be modified in order to be globally bounded.

The first step of the proof of Proposition 5.3.5 consists in establishing the *mild formulation* of the forward Kolmogorov equation satisfied by $\mathrm{p}(t, x, y)$:

$$\mathrm{p}(t, x, y) = \widehat{\mathrm{p}}(t, x, y) + \int_{s=0}^{t} \int_{x'=(q',p')\in\mathbb{R}^d\times\mathbb{R}^d} \mathrm{p}(s, x, x')F(q') \cdot \nabla_{p'}\widehat{\mathrm{p}}(t - s, x', y)\mathrm{d}x',$$

where $\widehat{\mathrm{p}}(t, x, y) := \widehat{\mathrm{p}}^{(1)}(t, x, y)$ is the transition density of the process (5.9) taken with $\alpha = 1$. The double integral in the right-hand side above is then controllable in terms of $\widehat{\mathrm{p}}^{(\alpha)}(t, x, y)$ for any $\alpha \in (0, 1)$, so that iterating this mild formulation yields the claimed estimate.

Beyond the completion of the proof of Proposition 5.3.4, the Gaussian upper bound (5.8) turns out to be the cornerstone of the proof of Theorem 5.3.3. Indeed, an explicit computation shows that, for any $\alpha \in (0, 1)$ and $t > 0$,

$$\widehat{\mathrm{p}}^{(\alpha)}(t, \cdot, \cdot) \in L^1 \cap L^\infty(\mathsf{D} \times \mathsf{D}),$$

which is far from being obvious since D is not bounded. The combination of this remark with the estimate (5.8) then yields the following result, proved in [A9].

Proposition 5.3.6 (Compactness of the semigroup $(P_t^{\mathsf{D}})_{t\geq 0}$)**.** *Let the assumptions of Theorem 5.3.3 hold.*

(i) For any $t \geq 0$ and $p, q \in [1, +\infty]$, P_t^{D} maps $L^p(\mathsf{D})$ continuously into $L^q(\mathsf{D})$ and into $C_{\mathrm{b}}(\overline{\mathsf{D}})$.

(ii) For any $t > 0$ and $p \in [1, +\infty]$, P_t^{D} is compact from $L^p(\mathsf{D})$ to $L^p(\mathsf{D})$, and from $C_{\mathrm{b}}(\overline{\mathsf{D}})$ to $C_{\mathrm{b}}(\overline{\mathsf{D}})$.

Similar results, in a much more general (and abstract) framework, are due to Nier [Nie18]. Proposition 5.3.6 allows to apply the Krein–Rutman theorem, which is an infinite-dimensional generalisation of the Perron–Frobenius theorem used to obtain Proposition 5.2.1, to the semigroup $(P_t^{\mathsf{D}})_{t\geq 0}$ acting on $C_{\mathrm{b}}(\overline{\mathsf{D}})$. This gives the existence of a QSD π as well as its spectral interpretation as an eigenvector, associated with the smallest eigenvalue λ, of $-L^*$. On the other hand, the regularity and positivity of the density ψ are a consequences of the regularity and positivity of the transition density p^{D}, which respectively follow from hypoellipticity and the Harnack inequality. The positivity of ψ implies in particular

that π is the unique QSD. Last, the compactness of P_t^{D} and the Krein–Rutman theorem imply that there exists $\alpha^* \in (0, +\infty]$ such that

$$\mathrm{e}^{-(\lambda+\alpha^*)} = \sup_{z \in \sigma(P_1^{\mathsf{D}}) \setminus \{\mathrm{e}^{-\lambda}\}} |z|,$$

where $\sigma(P_1^{\mathsf{D}})$ denotes the spectrum of the operator P_1^{D} of $C_{\mathrm{b}}(\overline{\mathsf{D}})$. The exponential convergence of $\mathbb{P}_\mu((q_t, p_t) \in \cdot | \tau_{\mathsf{D}} > t)$ to π can then be proved to hold for any rate of convergence $\alpha < \alpha^*$.

Remark 5.3.7 (Spectral gap)**.** *The definition of α^* in terms of P_1^{D} may seem unusual, as spectral quantities are often*[1] *defined in terms of the infinitesimal generator L, complemented with suitable boundary condition on $\partial\mathsf{D}$. The spectrum of the latter operator is not directly studied in [A9], however the definition of α^* can be formally seen to be equivalent to the* spectral gap *identity*

$$\lambda + \alpha^* = \inf_{\theta \in \sigma(-L) \setminus \{\lambda\}} \mathrm{Re}(\theta).$$

Remark 5.3.8 (Overdamped limit)**.** *Assume that F is globally Lipschitz continuous on $\mathbb{R}^d$, and that for some $\beta > 0$, $\overline{\sigma} = \sqrt{2\beta^{-1}}$ in (5.4) while $\gamma > 0$ and $\sigma = \sqrt{2\gamma\beta^{-1}}$ in (5.5). Then it is known that for any $T > 0$, the time-rescaled trajectory $(q_{\gamma t})_{t \in [0,T]}$ converges in distribution to $(\overline{q}_t)_{t \in [0,T]}$, in the* overdamped *limit $\gamma \to +\infty$. Using a refinement of this statement, Mouad Ramil [Ram] proved that the QSD π of the Langevin process, given by Theorem 5.3.3, converges to the product measure $\overline{\pi} \otimes \mathrm{M}_\beta$, where $\overline{\pi}$ is the QSD of the overdamped Langevin process given by Theorem 5.3.1 and M_β is the Maxwell distribution with inverse temperature β.*

The parallel between this result and the relation (5.6) between the stationary distributions of the Langevin and overdamped Langevin processes is striking. However, it is worth noting that while the identity $\nu = \overline{\nu} \otimes \mathrm{M}_\beta$ holds for any $\gamma > 0$ (in fact, ν does not depend on γ), the identity '$\pi = \overline{\pi} \otimes \mathrm{M}_\beta$' only holds in the $\gamma \to +\infty$ limit: indeed, since Theorem 5.3.3 shows that the density ψ of π satisfies $\psi > 0$ on Γ^+ and $\psi = 0$ on $\Gamma^- \cup \Gamma^0$, the measure π does not admit a product structure.

During the preparation of [A8] and [A9], the work [GNW] was released by Guillin, Nectoux and Wu. In this article, the existence of a QSD is established for a large class of hypoelliptic processes with a Hamiltonian structure comparable to (5.5), at least in the case $F = -\nabla V$. Their proof is based on the use of Lyapunov functionals, which allows to relax the assumption that the set O be bounded; in return, the uniqueness of a QSD is merely proved to hold in the class of distributions satisfying certain integrability conditions with respect to the Lyapunov functional, which even if O is bounded, does not cover in general the whole space of probability measures on the set $\mathsf{O} \times \mathbb{R}^d$.

Perspectives

An important difference between the statements of Theorem 5.3.1 and Theorem 5.3.3 is that in the former, the convergence rate of $\mathbb{P}_\mu(\overline{q}_t \in \cdot | \overline{\tau}_{\mathsf{O}} > t)$ to $\overline{\pi}$ is uniform in the initial distribution μ, while in the latter the prefactor depends on μ, and blows up when μ concentrates near the boundary of D. Whether this prefactor can be made uniform in μ is known to be related with so-called *two-sided estimates* on the transition density p^{D}, see [CCPV18, CV] and the appendix of [BGL]. Establishing such estimates for Langevin process is therefore a natural program for future research.

From the practical point of view, the law of the exit point $(q_{\tau_{\mathsf{D}}}, p_{\tau_{\mathsf{D}}})$ under $\mathbb{P}_\pi$ is of major interest in the implementation of accelerated algorithms. It can be derived through the following formal computation. Let $g : \Gamma^+ \cup \Gamma^0 \to \mathbb{R}$ be a continuous and bounded function, and set $u(q,p) := \mathbb{E}_{q,p}[g(q_{\tau_{\mathsf{D}}}, p_{\tau_{\mathsf{D}}})]$. It can be proved that $u \in C(\overline{\mathsf{D}}) \cap C^\infty(\mathsf{D})$, and

$$\begin{cases} Lu = 0 & \text{in } \mathsf{D}, \\ u = g & \text{on } \Gamma^+. \end{cases}$$

[1] from the PDE point of view, one would even say 'always'

As a consequence, the Green formula yields

$$\begin{aligned}\mathbb{E}_\pi\left[g(q_{\tau_\mathsf{D}}, p_{\tau_\mathsf{D}})\right] &= \int_{(q,p)\in\mathsf{D}} u(q,p)\psi(q,p)\mathrm{d}q\mathrm{d}p \\ &= -\frac{1}{\lambda}\int_{(q,p)\in\mathsf{D}} u(q,p)L^*\psi(q,p)\mathrm{d}q\mathrm{d}p \\ &= \frac{1}{\lambda}\int_{(q,p)\in\partial\mathsf{O}\times\mathbb{R}^d} p\cdot n(q)u(q,p)\psi(q,p)\sigma_{\partial\mathsf{O}}(\mathrm{d}q)\mathrm{d}p - \frac{1}{\lambda}\int_{(q,p)\in\mathsf{D}} Lu(q,p)\psi(q,p)\mathrm{d}q\mathrm{d}p \\ &= \frac{1}{\lambda}\int_{(q,p)\in\Gamma^+} p\cdot n(q)g(q,p)\psi(q,p)\sigma_{\partial\mathsf{O}}(\mathrm{d}q)\mathrm{d}p,\end{aligned}$$

where $\sigma_{\partial\mathsf{O}}$ denotes the surface measure on O, since $Lu = 0$ on D, $u = g$ on Γ^+ and $\psi = 0$ on $\Gamma^- \cup \Gamma^0$. Therefore, one may expect the pair $(q_{\tau_\mathsf{D}}, p_{\tau_\mathsf{D}})$ to admit the law

$$\frac{1}{\lambda}\mathbb{1}_{\{(q,p)\in\Gamma^+\}} p\cdot n(q)\psi(q,p)\sigma_{\partial\mathsf{O}}(\mathrm{d}q)\mathrm{d}p$$

under $\mathbb{P}_\pi$. However, the rigorous justification of this integration by parts seems to require gradient estimates on either ψ or u, which will be the subject of future works.

Chapter 6

Uncertainty propagation in a graph of numerical models

This chapter presents the results of the articles [A11] and [A12], written in collaboration with Adrien Touboul during his PhD thesis.

6.1 Introduction

6.1.1 Uncertainty propagation in Computer Experiments

The mathematical and numerical study of a process of interest (physical, biological, social, industrial...) generally involves one or several *models* for the process, which are turned into *computer codes* and fed *parameters*. Models almost always represent an incomplete description of the process, their transformation into computer codes generates numerical errors, and the parameters are often either inherently variable, or only known up to a certain degree of precision. Loosely speaking, the field of *Uncertainty Quantification* aims at taking into account all these discrepancies between the outcome of the numerical analysis and the 'real-world' process, in a quantitative manner. It is naturally based on standard mathematical tools, ranging from probability theory and statistics to numerical analysis, optimisation and computer science, but as a research area by itself it is quite young, see the references [Sul15, GHO17] for an introduction from an academic point of view, as well as [DRDT08] for examples of industrial applications.

In the specific context of *computer experiments*, where the numerical code is represented as a deterministic function

$$f : \left\{ \begin{array}{ccc} \mathsf{E} \times \mathsf{T} & \to & \mathsf{F} \\ (x, \theta) & \mapsto & y \end{array} \right.$$

for which we call x the *input*, θ the *parameter* and y the *output*, the purpose of *Uncertainty Propagation* is to quantify to which extent the uncertainty on the parameter propagates to uncertainty on the output. Let us emphasise that in this introduction, we take the convention that θ is uncertain but x is not[1]. For example, a basic task — but already nontrivial in practice if the evaluation of the function f is costly — consists in postulating that Θ is a random variable with a prescribed probability distribution μ_Θ and computing quantities of interest on the law of $Y = f(x, \Theta)$, such as moments, the probability to reach a certain subset of F, or quantiles. If the uncertain parameter $\Theta = (\Theta_1, \dots, \Theta_d)$ is multivariate, the related issue of *Sensitivity Analysis* aims at determining which components of Θ have the most influence on the variation of Y. This can be done through the estimation of such quantities as

$$\mathrm{Var}\left(\mathbb{E}\left[f(x, \Theta_1, \dots, \Theta_d) | \Theta_{i_1}, \dots, \Theta_{i_k}\right]\right), \qquad \{i_1, \dots, i_k\} \subset \{1, \dots, d\},$$

[1] This notational convention is more or less the opposite of the standard practice, according to which x often denotes uncertain inputs. The consistency of this convention will be recovered in the next subsection, where both x and θ will be random, but originating from different uncertainty sources.

which are used in the definition of so-called *Sobol indices*.

6.1.2 Multicomponent models

In certain industrial fields, such as aircraft conception, design stages involve a large number of interacting agents, which may represent subcontractors in charge of the design of different components of the product, or at a finer scale, computer codes modelling different physical phenomena. The propagation of uncertainty in such complex systems has motivated several recent research works, see for instance [AW10, AAW14, MPGP19, SLC19, MG] and references therein. The PhD thesis of Adrien Touboul, hosted by the project *Agility and Design Margins* at IRT SystemX, addresses this issue with user cases provided by the aeronautics and automotive sectors.

At the abstract level, the design stage is represented by a finite set $\mathcal{V}$ of computer codes (which we shall also call *numerical models*), such that the outputs of certain codes are taken as inputs of other codes. This naturally provides the model with a directed graph structure $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. More precisely, each vertex $v \in \mathcal{V}$ is associated with a deterministic function

$$f_v : \left\{ \begin{array}{ccc} \mathsf{E}_v \times \mathsf{T}_v & \to & \mathsf{F}_v \\ (x_v, \theta_v) & \mapsto & y_v \end{array} \right.$$

and a pair of vertices (u, v) belongs to the set of edges $\mathcal{E}$ if the output y_u of f_u is then taken as an input $x_{u,v}$ for the function f_v. Thus, each edge $(u, v) \in \mathcal{E}$ is associated with a function

$$g_{u,v} : \left\{ \begin{array}{ccc} \mathsf{F}_u & \to & \mathsf{E}_{u,v} \\ y_u & \mapsto & x_{u,v} \end{array} \right.$$

which represents the actual information contained in y_u which is taken as an input for v, and the vertices satisfy the compatibility condition

$$\forall v \in \mathcal{V}, \qquad \mathsf{E}_v = \prod_{u \in \mathcal{I}(v)} \mathsf{E}_{u,v},$$

where $\mathcal{I}(v) := \{u \in \mathcal{V} : (u, v) \in \mathcal{E}\}$ denotes the set of *parents* of v in $\mathcal{G}$. When $\mathcal{I}(v) = \varnothing$, we call v a *root* of $\mathcal{G}$ and we denote by $\mathcal{R} \subset \mathcal{V}$ the set of roots. Likewise, we denote by $\mathcal{L} \subset \mathcal{V}$ the set of *leaves*, that is to say vertices v such that there is no edge of the form (v, w).

In the sequel, we shall work under the standing assumption that $\mathcal{G}$ is a *Directed Acyclic Graph*, that is to say that is does not contain oriented cycles. This excludes the situation, called *strong coupling* in the industrial context, where two numerical models take as input the output of each other. This structural assumption induces a partial order on $\mathcal{V}$ which then allows to define inductively, given $(\theta_v)_{v \in \mathcal{V}}$:

- for any root v, the variable $y_v = f_v(\theta_v)$;
- for any edge (u, v) for which y_u is defined, $x_{u,v} = g_{u,v}(y_u)$;
- for any vertex v such that the variables $x_{u,v}$, $u \in \mathcal{I}(v)$ are defined, the variable $y_v = f_v(x_v, \theta_v)$, with $x_v = (x_{u,v})_{u \in \mathcal{I}(v)}$.

Thus, the vector $y_{\mathcal{V}} := (y_v)_{v \in \mathcal{V}}$ is well-defined as a (composite) function of $\theta_{\mathcal{V}} := (\theta_v)_{v \in \mathcal{V}}$, which we denote by

$$F_{\mathcal{V}} : \left\{ \begin{array}{ccc} \prod_{v \in \mathcal{V}} \mathsf{T}_v & \to & \prod_{v \in \mathcal{V}} \mathsf{F}_v, \\ \theta_{\mathcal{V}} & \mapsto & y_{\mathcal{V}}. \end{array} \right.$$

These definitions are illustrated on Figure 6.1.

We shall from now on assume that all sets E_v, T_v and F_v are endowed with a σ-field (and in particular that the σ-field over E_v is the product of the σ-fields over $\mathsf{E}_{u,v}$, $u \in \mathcal{I}(v)$), and that all functions f_v, $g_{u,v}$ are measurable. We define the *canonical probability space* $(\Omega, \mathcal{F}, \mathbb{P})$ by $\Omega = \prod_{v \in \mathcal{V}} \mathsf{T}_v$, $\mathcal{F}$ the associated product σ-field, and $\mathbb{P} = \otimes_{v \in \mathcal{V}} \mu_{\Theta_v}$. On this canonical space, elements of Ω are generically denoted by

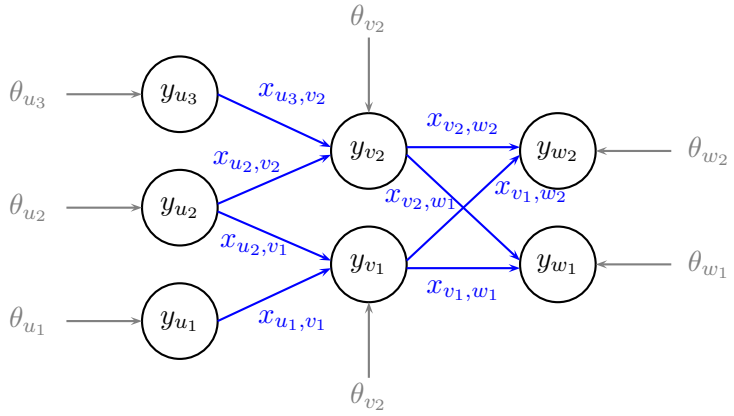

Figure 6.1: An example of a graph of numerical models with 7 vertices. The vertices u_1, u_2, u_3 are roots, and the vertices w_1, w_2 are leaves.

$\Theta_{\mathcal{V}} := (\Theta_v)_{v\in\mathcal{V}}$ and, for any $v \in \mathcal{V}$ and $(u, v) \in \mathcal{E}$, the random variables $X_{u,v}$, X_v, Y_v are defined according to the procedure above. Our purpose is then to estimate quantities of interest related with the joint law of $Y_{\mathcal{V}} := (Y_v)_{v\in\mathcal{V}}$. Notice that for sensitivity analysis, quantities of interest related with the joint law of $\{\Theta_{\mathcal{V}}, Y_{\mathcal{V}}\}$ are also relevant.

6.1.3 Reweighting methods

Let $\Phi : \prod_{v\in\mathcal{V}} \mathsf{F}_v \to \mathbb{R}$ be a measurable (and, say, bounded) function. In order to estimate the quantity of interest

$$\mathrm{QI} := \mathbb{E}\left[\Phi\left(Y_{\mathcal{V}}\right)\right],$$

an obvious direct Monte Carlo procedure consists in fixing $n \geq 1$ and proceeding sequentially, following the graph structure of $\mathcal{G}$, as follows:

- each root v generates n independent realisations $\Theta_{v,1}, \ldots, \Theta_{v,n}$ according to μ_{Θ_v} and computes a sample $Y_{v,1} = f_v(\Theta_{v,1}), \ldots, Y_{v,n} = f_v(\Theta_{v,n})$ which we denote by $\mathbf{Y}_{v,n}$;
- for each $v \in \mathcal{V}$ such that the samples $\mathbf{Y}_{u,n}$, $u \in \mathcal{I}(v)$ have been computed, the vertex v generates n independent realisations $\Theta_{v,1}, \ldots, \Theta_{v,n}$ according to μ_{Θ_v} and computes a sample $Y_{v,1} = f_v(X_{v,1}, \Theta_{v,1}), \ldots, Y_{v,n} = f_v(X_{v,n}, \Theta_{v,n})$ which we denote by $\mathbf{Y}_{v,n}$, with $X_{v,j} = (g_{u,v}(Y_{u,j}))_{u\in\mathcal{I}(v)}$ for any $j \in \{1, \ldots, n\}$;

and QI is estimated by

$$\widehat{\mathrm{QI}}_n^{\mathrm{MC}} := \frac{1}{n}\sum_{j=1}^{n} \Phi\left(Y_{\mathcal{V},j}\right), \qquad Y_{\mathcal{V},j} := (Y_{v,j})_{v\in\mathcal{V}}.$$

Since this estimator directly rewrites

$$\widehat{\mathrm{QI}}_n^{\mathrm{MC}} = \frac{1}{n}\sum_{j=1}^{n} \Phi\left(F_{\mathcal{V}}(\Theta_{\mathcal{V},j})\right), \qquad \Theta_{\mathcal{V},j} := (\Theta_{v,j})_{v\in\mathcal{V}},$$

and the vectors $\Theta_{\mathcal{V},j}$, $j \in \{1, \ldots, n\}$ are iid according to $\mathbb{P}$, it is clear that it is (strongly) consistent, in the sense that when $n \to +\infty$, it converges almost surely to QI. Notice that all random variables involved in this procedure need not be defined on the canonical probability space, but on the contrary it is more natural to define them on some *experimental* probability space on which each vertex $v \in \mathcal{V}$ is assumed to be able to generate a sequence $(\Theta_{v,j})_{j\geq 1}$ of independent realisations of μ_{Θ_v}.

This direct Monte Carlo procedure is generally difficult to implement in practice for large networks because it requires each vertex v to wait for the results of all upstream codes before running its own code, and if the evaluation of f_v is time consuming then the whole process becomes intractable. In this chapter, we study a decomposition method, partially inspired by [AW10, AAW14], in which all vertices work in parallel with a *synthetic sample* $X'_{v,1}, \dots, X'_{v,n_v}$ which is generated locally, independently from the results of other codes, during some *offline* phase. We however assume that during this offline phase, each vertex remains able to sample independent realisations $\Theta_{v,1}, \dots, \Theta_{v,n_v}$ from the 'true' distribution μ_{Θ_v}. The offline phase results in a family of samples $\mathbf{S}_{v,n_v} = (X'_{v,j}, Y'_{v,j})_{1 \leq j \leq n_v}$, with $Y'_{v,j} = f_v(X'_{j,v}, \Theta_{j,v})$, which are sent to a *simulation architect*. In an *online* phase, the simulation architect then has to construct an estimator of QI based only on the collection of samples $\mathbf{S}_{\mathcal{V}} := (\mathbf{S}_{v,n_v})_{v \in \mathcal{V}}$.

6.1.4 Outline and main results

We address the estimation of QI in this offline/online context by looking for estimators of the form

$$\widehat{\mathrm{QI}}_{n_{\mathcal{V}}} = \sum_{j_{\mathcal{V}} \in \mathcal{N}_{\mathcal{V}}} w_{j_{\mathcal{V}}}(\mathbf{S}_{\mathcal{V}}) \Phi\left(Y'_{\mathcal{V},j_{\mathcal{V}}}\right), \tag{6.1}$$

with

$$n_{\mathcal{V}} := (n_v)_{v \in \mathcal{V}}, \quad j_{\mathcal{V}} := (j_v)_{v \in \mathcal{V}}, \quad \mathcal{N}_{\mathcal{V}} := \prod_{v \in \mathcal{V}} \{1, \dots, n_v\}, \quad Y'_{\mathcal{V},j_{\mathcal{V}}} := (Y'_{v,j_v})_{v \in \mathcal{V}}. \tag{6.2}$$

In this formula, $(w_{j_{\mathcal{V}}}(\mathbf{S}_{\mathcal{V}}))_{j_{\mathcal{V}} \in \mathcal{N}_{\mathcal{V}}}$ is some family of *weights* which somehow represent how likely each observation $Y'_{\mathcal{V},j_{\mathcal{V}}}$ should be under $\mathbb{P}$. We shall proceed in two steps.

In Section 6.2, which summarises the contents from [A12], we assume that for each vertex v and any $x_v \in \mathsf{E}_v$, we are given a method to compute an estimator of the Markov kernel

$$\ell_v(x_v, \mathrm{d}y_v) := \mathbb{P}(Y_v \in \mathrm{d}y_v | X_v = x_v) = \mu_{\Theta_v} \circ f_v(x_v, \cdot)^{-1}(\mathrm{d}y_v)$$

of the form

$$\sum_{j=1}^{n_v} W_{v,j}(\mathbf{S}_{v,n_v}, x_v) \delta_{Y'_{v,j}}(\mathrm{d}y_v).$$

When v is a root, that is to say $\mathsf{E}_v = \varnothing$, we adapt the notation above and assume that we are given estimators of

$$\ell_v(\mathrm{d}y_v) := \mathbb{P}(Y_v \in \mathrm{d}y_v) = \mu_{\Theta_v} \circ f_v^{-1}(\mathrm{d}y_v)$$

of the form

$$\sum_{j=1}^{n_v} W_{v,j} \delta_{Y'_{v,j}}(\mathrm{d}y_v).$$

We call such a method a *Weighted Linear Approximation Method* (WLAM). The main results of Section 6.2 are the formula (6.5), which defines the global weight $w_{j_{\mathcal{V}}}(\mathbf{S}_{\mathcal{V}})$ as a function of the local weights $W_{v,j}(\mathbf{S}_{v,n_v}, x_v)$ and Theorem 6.2.7 which shows the consistency of this formula.

In Section 6.3, we then construct a particular instance of a WLAM, based on the Nearest Neighbour regression method studied in [A11]. Combining this construction with the results from Section 6.2 finally yields a consistent estimator of QI.

6.2 Reweighting procedure

In this section, we provide a practical algorithm to compute a family of weights $(w_{j_{\mathcal{V}}}(\mathbf{S}_{\mathcal{V}}))_{j_{\mathcal{V}} \in \mathcal{N}_{\mathcal{V}}}$ which makes the estimator $\widehat{\mathrm{QI}}_{n_{\mathcal{V}}}$ defined in (6.1) consistent, in a certain sense, when the sizes n_v, $v \in \mathcal{V}$ of all samples go to $+\infty$. The building brick of our method is the notion of WLAM introduced in Subsection 6.2.1 on a single vertex, and then applied to the graph in Subsection 6.2.2.

6.2.1 Weighted Linear Approximation Method

In this subsection we work at the level of a single vertex and therefore remove the subscript v from our notation. We thus let E, T and F be three measurable spaces, $f : \mathsf{E} \times \mathsf{T} \to \mathsf{F}$ be a measurable function, and μ_Θ be a probability measure on T.

We assume that, on some *canonical* probability space $(\Omega, \mathcal{F}, \mathbb{P})$, two independent random variables X and Θ are defined, with respective distribution μ_X and μ_Θ, and let $Y = f(X, \Theta)$. For any $x \in \mathsf{E}$, the conditional distribution of Y given $X = x$, which is the pushforward measure of μ_Θ by the function $f(x, \cdot)$, is then denoted by $\ell(x, \mathrm{d}y)$ (and simply $\ell(\mathrm{d}y)$ if $\mathsf{E} = \varnothing$).

We also assume that, on some *experimental* probability space $(\Omega^*, \mathcal{F}^*, \mathbb{P}^*)$, a sequence of independent random variables $(\Theta_j)_{j\geq 1}$ distributed according to μ_Θ is defined.

Last, we denote by $\mathfrak{B}_\mathsf{F}$ the space of real-valued, bounded and measurable functions on F.

Definition and consistency

Definition 6.2.1 (WLAM)**.** *In the setting described above, an* n-Weighted Linear Approximation Method *(n-WLAM) is a pair* $(\mathbf{W}_n, \mathbf{X}'_n)$ *such that:*

- $\mathbf{X}'_n = (X'_j)_{1\leq j\leq n}$ *is a collection of* E*-valued random variables, defined on the probability space* $(\Omega^*, \mathcal{F}^*, \mathbb{P}^*)$*, and independent from the sequence* $(\Theta_j)_{j\geq 1}$*;*
- $\mathbf{W}_n = (W_j)_{1\leq j\leq n} : (\mathsf{E} \times \mathsf{F})^n \times \mathsf{E} \to [0, +\infty)^n$ *is a function such that, for any* $\mathbf{s}_n \in (\mathsf{E} \times \mathsf{F})^n$ *and* $x \in \mathsf{E}$*,*

$$\sum_{j=1}^{n} W_j(\mathbf{s}_n, x) = 1.$$

In the particular case where $\mathsf{E} = \varnothing$, an n-WLAM is simply a vector $\mathbf{W}_n = (W_j)_{1\leq j\leq n}$ of nonnegative numbers whose sum equals to 1.

An n-WLAM naturally induces a random Markov kernel $\widehat{\ell}_n(x, \mathrm{d}y)$ from E to F, defined by

$$\forall x \in \mathsf{E}, \qquad \widehat{\ell}_n(x, \mathrm{d}y) = \sum_{j=1}^{n} W_j(\mathbf{S}_n, x)\delta_{Y'_j}(\mathrm{d}y),$$

where the sample $\mathbf{S}_n$ is defined on the experimental probability space by $\mathbf{S}_n = (X'_j, Y'_j)_{1\leq j\leq n}$, with $Y'_j = f(X'_j, \Theta_j)$.

Definition 6.2.2 (Consistency)**.** *Let* $\mathfrak{B}$ *be a linear subspace of* $\mathfrak{B}_\mathsf{F}$*. A sequence of* n*-WLAMs,* $n \geq 1$*, is called* $\mathfrak{B}$-consistent *if, for any* $x \in \mathsf{E}$ *and* $\phi \in \mathfrak{B}$*,*

$$\lim_{n\to+\infty} \int_{y\in\mathsf{F}} \phi(y)\widehat{\ell}_n(x, \mathrm{d}y) = \int_{y\in\mathsf{F}} \phi(y)\ell(x, \mathrm{d}y), \qquad \text{in probability on } (\Omega^*, \mathcal{F}^*, \mathbb{P}^*).$$

In the sequel we shall always implicitly consider sequences of n-WLAMs, to which we shall simply refer as 'WLAM'.

Definition 6.2.2 rewrites, for any $\phi \in \mathfrak{B}$, for any $x \in \mathsf{E}$,

$$\lim_{n\to+\infty} \sum_{j=1}^{n} W_j(\mathbf{S}_n, x)\phi(Y'_j) = \mathbb{E}[\phi(Y)|X = x],$$

in probability. In other words, a WLAM can be reinterpreted as a *linear nonparametric regression estimator* for $\mathbb{E}[\phi(Y)|X = x] = \mathbb{E}[\phi(f(x, \Theta))]$ [Tsy09, Definition 1.7 in Section 1.5], which is consistent for any function ϕ in the class $\mathfrak{B}$.

Examples and comments

Example 6.2.3 (Case $\mathsf{E} = \varnothing$)**.** *If $\mathsf{E} = \varnothing$, the WLAM $\mathbf{W}_n$ defined by $W_j = 1/n$ for any $j \in \{1, \dots, n\}$ is $\mathfrak{B}_\mathsf{F}$-consistent.*

Example 6.2.4 (Discrete case)**.** *Assume that E is a discrete space and let $\mu_{X'}$ be a probability measure on E such that $\mu_{X'}(x) > 0$ for any $x \in \mathsf{E}$. Consider the WLAM composed by a sample $\mathbf{X}'_n$ of independent random variables $X'_1, \dots, X'_n$ distributed according to $\mu_{X'}$, and the function $\mathbf{W}_n$ defined by*

$$W_j(\mathbf{S}_n, x) = \begin{cases} \dfrac{1}{n} & \text{if } \Sigma(x) = 0, \\ \dfrac{\mathbb{1}_{\{x = X'_j\}}}{\Sigma(x)} & \text{if } \Sigma(x) > 0, \end{cases}$$

where $\Sigma(x) := \sum_{j=1}^n \mathbb{1}_{\{x = X'_j\}}$. This WLAM is $\mathfrak{B}_\mathsf{F}$-consistent.

Example 6.2.5 (Nadaraya–Watson WLAM)**.** *If $\mathsf{E} = \mathbb{R}^d$, a natural generalisation of Example 6.2.4 would be to draw an iid synthetic sample $X'_1, \dots, X'_n$ according to some probability measure $\mu_{X'}$, and set*

$$W_j(\mathbf{S}_n, x) = \frac{\delta_{X'_j}(\mathrm{d}x)}{\Sigma(\mathrm{d}x)}, \qquad \Sigma(\mathrm{d}x) := \sum_{j=1}^n \delta_{X'_j}(\mathrm{d}x),$$

but of course this expression does not make sense. Smoothing the Dirac masses by convolution with a kernel $K > 0$ and a bandwidth $h > 0$, we get

$$W_j(\mathbf{S}_n, x) = \frac{K(h^{-1}(x - X'_j))}{\Sigma_h(x)}, \qquad \Sigma_h(x) := \sum_{j=1}^n K(h^{-1}(x - X'_j)).$$

For any $\phi \in \mathfrak{B}_\mathsf{F}$, the quantity

$$\int_{y \in \mathsf{F}} \phi(y) \widehat{\ell}_n(x, \mathrm{d}y) = \sum_{j=1}^n W_j(\mathbf{S}_n, x) \phi(Y'_j)$$

then turns out to be the Nadaraya–Watson *estimator of the regression function $\mathbb{E}[\phi(Y)|X = x]$ [Tsy09, Section 1.5]. From standard results in kernel density estimation, it can be checked that if $\mu_{X'}$ has a positive and continuous density with respect to the Lebesgue measure on $\mathbb{R}^d$, and the bandwidth $h = h_n$ is chosen so that $h_n \to 0$, $nh_n \to +\infty$, then this WLAM is $\mathfrak{B}$-consistent, for any class $\mathfrak{B}$ of measurable and bounded functions ϕ for which the mapping $x \mapsto \mathbb{E}[\phi(f(x, \Theta))]$ is continuous.*

A WLAM based on another popular nonparametric regression method, the Nearest Neighbour method, will be discussed in detail in Section 6.3. In contrast, parametric regression methods, such as linear or logistic, may only be expected to yield consistent WLAMs for drastically restricted classes of functions ϕ and f.

In the previous examples, the weights $W_j(\mathbf{S}_n, x)$ only depend on the sample $\mathbf{S}_n$ through $\mathbf{X}'_n$, but there are nonparametric regression methods, such as regression trees [HTF09, Section 9.2.2], for which weights also depend on $(Y'_1, \dots, Y'_n)$. Last, let us also emphasise the fact that while in the examples above, the design $\mathbf{X}'_n$ is iid, our framework also allows to work with deterministic, user-chosen designs, as long as they fulfill the consistency property of Definition 6.2.2.

Toward WLAM composition

As a consequence of Definition 6.2.2, if a WLAM $(\mathbf{W}_n, \mathbf{X}'_n)_{n \geq 1}$ is $\mathfrak{B}$-consistent, then for any measurable and bounded function $\Phi : \mathsf{E} \times \mathsf{F} \to \mathbb{R}$ such that $\Phi(x, \cdot) \in \mathfrak{B}$ for all $x \in \mathsf{E}$, we have

$$\lim_{n \to +\infty} \int_{x \in \mathsf{E}} \sum_{j=1}^n W_j(\mathbf{S}_n, x) \Phi(x, Y'_j) \mu_X(\mathrm{d}x) = \mathbb{E}[\Phi(X, Y)],$$

in probability. This suggests that if the probability measure μ_X is approximated by a finite sum of Dirac masses

$$\widehat{\mu}_{X,m} = \sum_{i=1}^{m} w_i \delta_{X_i},$$

then the joint law of (X, Y) should be approximated by the probability measure

$$\sum_{i=1}^{m}\sum_{j=1}^{n} w_i W_j(\mathbf{S}_n, X_i)\delta_{(X_i,Y'_j)}. \tag{6.3}$$

This remark will be generalised in the next subsection.

6.2.2 Computing weights on the graph

In this subsection, we come back to the study of the graph of numerical models $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and assume that each vertex $v \in \mathcal{V}$ is provided with a consistent WLAM $(\mathbf{W}_{v,n_v}, \mathbf{X}'_{v,n_v})$ defined on some experimental probability space $(\Omega_v^*, \mathcal{F}_v^*, \mathbb{P}_v^*)$. We denote by $\mathbf{S}_{v,n_v} = (X'_{v,j}, Y'_{v,j})_{1\leq j\leq n_v}$ the associated sample, defined on the product $(\Omega_{\mathcal{V}}^*, \mathcal{F}_{\mathcal{V}}^*, \mathbb{P}_{\mathcal{V}}^*)$ of all experimental spaces.

Our purpose is now to describe an 'online' algorithm taking as an input the WLAMs of all vertices and returning a family of weights $(w_{j_{\mathcal{V}}}(\mathbf{S}_{\mathcal{V}}))_{j_{\mathcal{V}}\in\mathcal{N}_{\mathcal{V}}}$ making the estimator $\widehat{\mathrm{QI}}_{n_{\mathcal{V}}}$ of QI defined in (6.1) consistent.

Markov property and factorisation formula

Let us recall that we denote by $\mathcal{L} \subset \mathcal{V}$ the set of leaves, and introduce the sub-σ-field of the canonical probability space

$$\mathcal{F}_- := \sigma\left((\Theta_v)_{v\in\mathcal{V}\setminus\mathcal{L}}\right),$$

which is generated by the family of random variables Θ_v which are not located on leaves. Clearly, for any $v \in \mathcal{L}$, the random variable X_v is $\mathcal{F}_-$-measurable, while Θ_v is independent from $\mathcal{F}_-$. Therefore, since the random variables $(\Theta_v)_{v\in\mathcal{L}}$ are independent, the conditional distribution of $(Y_v)_{v\in\mathcal{L}}$ given $\mathcal{F}_-$ is the product measure[2]

$$\prod_{v\in\mathcal{L}} \ell_v(X_v, \mathrm{d}y_v),$$

where we recall that, for each $v \in \mathcal{L}$, $X_v = (g_{u,v}(Y_u))_{u\in\mathcal{I}(v)}$. This fact can be seen as a Markov property for the graph structure of $\mathcal{G}$.

We deduce that the joint law $\mu_{Y_{\mathcal{V}}}(\mathrm{d}y_{\mathcal{V}})$ of the complete vector $Y_{\mathcal{V}} = (Y_v)_{v\in\mathcal{V}}$ satisfies the disintegration formula

$$\mu_{Y_{\mathcal{V}}}(\mathrm{d}y_{\mathcal{V}}) = \mu_{Y_{\mathcal{V}\setminus\mathcal{L}}}(\mathrm{d}y_{\mathcal{V}\setminus\mathcal{L}}) \prod_{v\in\mathcal{L}} \ell_v(x_v, \mathrm{d}y_v), \qquad x_v = (g_{u,v}(y_u))_{u\in\mathcal{I}(v)},$$

where $\mu_{Y_{\mathcal{V}\setminus\mathcal{L}}}(\mathrm{d}y_{\mathcal{V}\setminus\mathcal{L}})$ refers to the law of the vector $Y_{\mathcal{V}\setminus\mathcal{L}} = (Y_v)_{v\in\mathcal{V}\setminus\mathcal{L}}$. Since $\mathcal{G}$ is a Directed Acyclic Graph with a finite number of vertices, it is easily seen that $\mathcal{L} \neq \varnothing$. Therefore, the disintegration formula may be iterated to yield inductively

$$\mu_{Y_{\mathcal{V}}}(\mathrm{d}y_{\mathcal{V}}) = \prod_{v\in\mathcal{R}} \ell_v(\mathrm{d}y_v) \prod_{v\in\mathcal{V}\setminus\mathcal{R}} \ell_v(x_v, \mathrm{d}y_v), \qquad x_v = (g_{u,v}(y_u))_{u\in\mathcal{I}(v)}, \tag{6.4}$$

where we recall that $\mathcal{R}$ denotes the set of roots of $\mathcal{V}$.

[2] In this expression, the terms corresponding to vertices v which are roots should write $\ell_v(\mathrm{d}y_v)$ rather than $\ell_v(X_v, \mathrm{d}y_v)$. In order not to overload the presentation, we shall often keep this distinction implicit in the sequel.

Definition of weights and consistency theorem

We recall that, for each root $v \in \mathcal{R}$, the law $\ell_v(\mathrm{d}y_v)$ of Y_v is approximated by

$$\widehat{\ell}_{v,n_v}(\mathrm{d}y_v) = \sum_{j=1}^{n_v} W_{v,j}\delta_{Y'_{v,j}}(\mathrm{d}y_v),$$

and for any $v \in \mathcal{V} \setminus \mathcal{R}$ and $x \in \mathsf{E}_v$, the conditional distribution $\ell_v(x_v, \mathrm{d}y_v)$ of Y_v given $X_v = x$ is approximated by

$$\widehat{\ell}_{v,n_v}(x, \mathrm{d}y_v) = \sum_{j=1}^{n_v} W_{v,j}(\mathbf{S}_{v,n_v}, x)\delta_{Y'_{v,j}}(\mathrm{d}y_v).$$

It is therefore natural to approximate the joint law $\mu_{Y_\mathcal{V}}(\mathrm{d}y_\mathcal{V})$, which satisfies the factorisation formula (6.4), by the measure

$$\widehat{\mu}_{Y_\mathcal{V},n_\mathcal{V}}(\mathrm{d}y_\mathcal{V}) := \prod_{v\in\mathcal{R}} \widehat{\ell}_{v,n_v}(\mathrm{d}y_v) \prod_{v\in\mathcal{V}\setminus\mathcal{R}} \widehat{\ell}_{v,n_v}(x_v, \mathrm{d}y_v), \qquad x_v = (g_{u,v}(y_u))_{u\in\mathcal{I}(v)}.$$

The latter rewrites

$$\widehat{\mu}_{Y_\mathcal{V},n_\mathcal{V}}(\mathrm{d}y_\mathcal{V}) = \sum_{j_\mathcal{V}\in\mathcal{N}_\mathcal{V}} w_{j_\mathcal{V}}(\mathbf{S}_\mathcal{V})\delta_{Y'_{\mathcal{V},j_\mathcal{V}}},$$

where we recall the notation from (6.2) and, for any $j_\mathcal{V} \in \mathcal{N}_\mathcal{V}$, we set

$$w_{j_\mathcal{V}}(\mathbf{S}_\mathcal{V}) := \prod_{v\in\mathcal{R}} W_{v,j_v} \prod_{v\in\mathcal{V}\setminus\mathcal{R}} W_{v,j_v}(\mathbf{S}_{v,n_v}, (g_{u,v}(Y'_{u,j_u}))_{u\in\mathcal{I}(v)}). \tag{6.5}$$

This definition generalises the derivation of (6.3).

We now study the consistency of the estimator $\widehat{\mathrm{QI}}_{n_\mathcal{V}}$, defined in (6.1), with weights $w_{j_\mathcal{V}}(\mathbf{S}_\mathcal{V})$ given by (6.5). We shall state a rather weak form of consistency, in which the limits $n_v \to +\infty$, $v \in \mathcal{V}$ must be taken in the reverse order induced by $\mathcal{G}$, see Theorem 6.2.7 below. We believe that stronger conditions on the model and the WLAMs may be imposed in order to make the consistency hold in the joint limit $(n_v)_{v\in\mathcal{V}} \to +\infty$, but stick to this simple statement as a first theoretical justification of the approximation of QI by $\widehat{\mathrm{QI}}_{n_\mathcal{V}}$. From now on, we denote by N the cardinality of $\mathcal{V}$.

Definition 6.2.6 ($\mathcal{G}$-coherent enumeration of $\mathcal{V}$)**.** *An enumeration $v_1, \dots, v_N$ of $\mathcal{V}$ is* $\mathcal{G}$-coherent *if, for any pair of indices (k, l) such that $k < l$, there is no oriented path from v_l to v_k in $\mathcal{G}$.*

Given such an enumeration, to any measurable and bounded function $\Phi : \prod_{v\in\mathcal{V}} \mathsf{F}_v \to \mathbb{R}$ we associate the family of measurable and bounded functions $\Phi_l : \prod_{k=1}^{l} \mathsf{F}_{v_k} \to \mathbb{R}$, $l \in \{0, \dots, N\}$, defined by $\Phi_N := \Phi$ and, for $l \in \{0, \dots, N-1\}$,

$$\Phi_l\left((y_{v_k})_{1\le k\le l}\right) := \int_{y_{v_{l+1}}\in\mathsf{F}_{v_{l+1}}} \Phi_{l+1}\left(y_{v_1}, \dots, y_{v_l}, y_{v_{l+1}}\right) \ell_{v_{l+1}}\left(x_{v_{l+1}}, \mathrm{d}y_{v_{l+1}}\right),$$

with $x_{v_{l+1}} = (g_{u,v_{l+1}}(y_u))_{u\in\mathcal{I}(v_{l+1})}$, and $\ell_{v_{l+1}}(x_{v_{l+1}}, \mathrm{d}y_{v_{l+1}})$ replaced with $\ell_{v_{l+1}}(\mathrm{d}y_{v_{l+1}})$ if $v_{l+1} \in \mathcal{R}$. This expression is well defined because $x_{v_{l+1}}$ can only depend on the values of $y_{v_1}, \dots, y_{v_l}$; besides, $\Phi_0 = \mathrm{QI}$.

Theorem 6.2.7 ($\mathcal{G}$-consistency of $\widehat{\mathrm{QI}}_{n_\mathcal{V}}$)**.** *Assume that for each $v \in \mathcal{V}$, the WLAM $(\mathbf{W}_{v,n_v}, \mathbf{X}'_{v,n_v})$ is $\mathfrak{B}_v$-consistent, for some linear subspace $\mathfrak{B}_v$ of the space of bounded and measurable functions $\mathfrak{B}_{\mathsf{F}_v}$ on F_v. Let $v_1, \dots, v_N$ be a $\mathcal{G}$-coherent enumeration of $\mathcal{V}$. Let $\Phi : \prod_{v\in\mathcal{V}} \mathsf{F}_v \to \mathbb{R}$ be a measurable and bounded function, and assume that for any $l \in \{1, \dots, N\}$, for all $(y_{v_k})_{1\le k\le l-1}$, the function $y_{v_l} \mapsto \Phi_l(y_{v_1}, \dots, y_{v_{l-1}}, y_{v_l})$ belongs to $\mathfrak{B}_{v_l}$. Then we have*

$$\lim_{n_{v_1}\to+\infty} \cdots \lim_{n_{v_N}\to+\infty} \widehat{\mathrm{QI}}_{n_\mathcal{V}} = \mathrm{QI}, \qquad \textit{in probability on } (\Omega^*_\mathcal{V}, \mathcal{F}^*_\mathcal{V}, \mathbb{P}^*_\mathcal{V}).$$

Proof. Let us define the family of functions $\widehat{\Phi}_l$, $l \in \{0, \dots, N\}$ by the same formulæ as Φ_l but replacing each ℓ_v with $\widehat{\ell}_{v,n_v}$, so that in particular $\widehat{\Phi}_0 = \widehat{\mathrm{QI}}_{n_\mathcal{V}}$. It follows from a backward inductive argument over $l \in \{0, \dots, N\}$, the consistency of each WLAM and the dominated convergence theorem that for any $(y_{v_k})_{1 \le k \le l}$,

$$\lim_{n_{v_{l+1}} \to +\infty} \cdots \lim_{n_{v_N} \to +\infty} \widehat{\Phi}_l \left((y_{v_k})_{1 \le k \le l} \right) = \Phi_l \left((y_{v_k})_{1 \le k \le l} \right),$$

in probability. For $l = 0$, this yields the claimed identity. □

Let us assume that all roots $v \in \mathcal{R}$ are provided with the WLAM described in Example 6.2.3. On the one hand, if all spaces E_v, $v \in \mathcal{V} \setminus \mathcal{R}$ are discrete, and provided with a WLAM as described in Example 6.2.4, then the assumptions of Theorem 6.2.7 hold for any measurable and bounded function $\Phi : \prod_{v \in \mathcal{V}} \mathsf{F}_v \to \mathbb{R}$, without any more condition over the functions f_v and $g_{u,v}$ than mere measurability. On the other hand, if some spaces E_v, $v \in \mathcal{V} \setminus \mathcal{R}$ are continuous and provided with the Nadaraya–Watson WLAM from Example 6.2.5, then more intricate uniform continuity conditions must be imposed over Φ and the functions f_v and $g_{u,v}$ for the assumptions of Theorem 6.2.7 to hold.

Algorithmic remarks

From a computational point of view, the formulæ (6.1) and (6.5) defining $\widehat{\mathrm{QI}}_{n_\mathcal{V}}$ are severely demanding, since in order to evaluate the latter quantity, the simulation architect has to compute the $\prod_{v \in \mathcal{V}} n_v$ weights $w_{j_\mathcal{V}}(\mathbf{S}_\mathcal{V})$. It is therefore likely that the combinatorics of the problem become prohibitive quickly. However, if Φ only depends on a few of the random variables Y_v, $v \in \mathcal{V}$, then the formula (6.5) can be marginalised so as to display fewer terms. We treat a somehow extreme case in the next example.

Example 6.2.8 (Composition of WLAMs on the line graph)**.** *Let us consider the case of the line graph $\mathcal{V} = \{v_1, \dots, v_N\}$, $\mathcal{E} = \{(v_l, v_{l+1}), 1 \le l \le N-1\}$, and assume that the quantity of interest writes*

$$\mathrm{QI} = \mathbb{E}[\phi(Y_{v_N})].$$

The estimator $\widehat{\mathrm{QI}}_{n_\mathcal{V}}$ then writes

$$\widehat{\mathrm{QI}}_{n_\mathcal{V}} = \sum_{j_{v_N}=1}^{n_{v_N}} w_{v_N, j_{v_N}} \phi(Y'_{v_N, j_{v_N}}),$$

with weights given by

$$w_{v_N, j_{v_N}} = (\mathrm{W}_{v_1} \mathrm{W}_{v_2} \cdots \mathrm{W}_{v_N})_{j_{v_N}}, \tag{6.6}$$

where W_{v_1} is the (row) vector with coordinates $(W_{v_1, j_{v_1}})_{1 \le j_{v_1} \le n_{v_1}}$ while, for $l \ge 2$, W_{v_l} is the $n_{v_{l-1}} \times n_{v_l}$ matrix with coordinates $(W_{v_l, j_{v_l}}(\mathbf{S}_{v_l, n_{v_l}}, g_{v_{l-1}, v_l}(Y'_{v_{l-1}, j_{v_{l-1}}})))_{1 \le j_{v_{l-1}} \le n_{v_{l-1}}, 1 \le j_{v_l} \le n_{v_l}}$. Computing the matrix product $\mathrm{W}_{v_1} \mathrm{W}_{v_2} \cdots \mathrm{W}_{v_N}$ from the left to the right requires $n_{v_1} n_{v_2} + n_{v_2} n_{v_3} + \cdots + n_{v_{N-1}} n_{v_N}$ operations. Assume for simplicity that all samples have the same size n, then the computational cost of the method reduces from computing the n^N weights $w_{j_\mathcal{V}}(\mathbf{S}_\mathcal{V})$ to simply $(N-1)n^2$ operations for this chain matrix product.

In the general case, such a marginalisation procedure can still be implemented, with the matrix product appearing in (6.6) replaced with tensor contraction, but it becomes a combinatorial optimisation problem. The theory of *Bayesian networks* provides algorithms for this task. Indeed, let us still denote by W_v the $(\prod_{u \in \mathcal{I}(v)} n_u) \times n_v$ array with coefficients

$$W_{v, j_v} \left(\mathbf{S}_{v, n_v}, (g_{u,v}(Y'_{u, j_u}))_{u \in \mathcal{I}(v)} \right), \qquad \forall u \in \mathcal{I}(v), \quad 1 \le j_u \le n_u, \qquad 1 \le j_v \le n_v.$$

Then, for each $v \in \mathcal{R}$, the vector W_v can be interpreted as the probability mass function of a random variable $\mathcal{Y}_v$ which takes its values in the set $\{Y'_{v, j_v}, 1 \le j_v \le n_v\}$, while for each $v \in \mathcal{V} \setminus \mathcal{R}$, the array W_v can be interpreted as the conditional probability table of a random variable $\mathcal{Y}_v$, which takes its values

in the set $\{Y'_{v,j_v}, 1 \leq j_v \leq n_v\}$, given all possible values of the variables $\mathcal{Y}_u$, $u \in \mathcal{I}(v)$. The joint law of $(\mathcal{Y}_v)_{v\in\mathcal{V}}$ is then given by the factorisation formula (6.5), which makes the pair $(\mathcal{G}, (\mathcal{Y}_v)_{v\in\mathcal{V}})$ a *Bayesian network* [KF09, Definition 3.5, p. 62]. In this context, the marginalisation procedure described above amounts to computing the joint law of a subset of all variables $(\mathcal{Y}_v)_{v\in\mathcal{V}}$. This task is called *exact inference* in Bayesian networks [KF09, Chapter 9], and therefore dedicated algorithmic tools can be readily employed in our context to compute $\widehat{\mathrm{QI}}_{n_\mathcal{V}}$ as efficiently as possible.

6.3 Nearest Neighbour WLAM

In this section, we first describe in Subsection 6.3.1 the results of [A11] where a simplified version of the uncertainty propagation problem from Section 6.2, with a single numerical model involved, was studied. An estimator of the quantity of interest, based on the Nearest Neighbour nonparametric regression method, is introduced and rates of convergence are derived. In Subsection 6.3.2, these results are employed to construct and study the consistency of a Nearest Neighbour-based WLAM.

6.3.1 Nearest Neighbour approach to covariate shift

Let us consider the reweighting procedure for one numerical model. The quantity of interest is

$$\mathrm{QI} = \mathbb{E}[\phi(Y)],$$

with $Y = f(X, \Theta) \in \mathbb{R}^e$ the output of the numerical model, $X \in \mathbb{R}^d$ the input and $\Theta \in \mathsf{T}$ the parameter. Both X and Θ are random, with respective distributions μ_X and μ_Θ, and they are independent. In order to reproduce the offline/online phases of Section 6.2, we assume that:

- in an offline phase, a synthetic iid sample $\mathbf{X}'_n = (X'_1, \ldots, X'_n)$ is generated from some user-chosen probability measure $\mu_{X'}$, together with an independent sample $\Theta_1, \ldots, \Theta_n$ from μ_Θ, and the numerical model f is used to compute $Y'_1, \ldots, Y'_n$ defined by $Y'_j = f(X'_j, \Theta_j)$;
- in an online phase, an independent sample $\mathbf{X}_m = (X_1, \ldots, X_m)$ from μ_X becomes available, but evaluations of the numerical model f are no longer allowed.

In this subsection, we describe an estimator of QI based on the so-called *Nearest Neighbour method* in nonparametric statistics [BD15].

Remark 6.3.1 (Covariate shift)**.** *From a statistical learning point of view, we are in a situation where the regression function $\psi(x) = \mathbb{E}[Y|X = x]$ is learned on a* training set $\mathbf{X}'_n$ *and must then be applied on an* evaluation set $\mathbf{X}_m$ *with a different law. This situation is called* covariate shift*, or* domain adaptation*, in the litterature.*

Density ratio estimation

A natural importance sampling estimator of QI is

$$\frac{1}{n}\sum_{j=1}^{n} \rho(X'_j)\phi(Y'_j), \qquad \rho_{X,X'} := \frac{\mathrm{d}\mu_X}{\mathrm{d}\mu_{X'}}.$$

However, in the Computer Experiments context which motivates our study, the measure $\mu_{X'}$ is user-chosen, but the true law μ_X of the input variable X is not known, hence neither is $\rho_{X,X'}$. The problem of estimating the latter function based on the samples $\mathbf{X}'_n$ and $\mathbf{X}_m$ is known in the statistical learning litterature as *density ratio estimation* [SSK12]. A rather generic procedure to proceed consists in fixing a distance-like function d on the set of probability measures on $\mathbb{R}^d$, writing

$$\rho_{X,X'} = \arg\min_{\rho} \mathsf{d}\left(\rho\mu_{X'}, \mu_X\right),$$

and estimating $\rho_{X,X'}$ by

$$\widehat{\rho}_{\mathbf{X}_m,\mathbf{X}'_n} := \arg\min_{\rho} \mathsf{d}\left(\rho\widehat{\mu}_{\mathbf{X}'_n}, \widehat{\mu}_{\mathbf{X}_m}\right), \qquad \widehat{\mu}_{\mathbf{X}'_n} := \frac{1}{n}\sum_{j=1}^{n}\delta_{X'_j}, \quad \widehat{\mu}_{\mathbf{X}_m} := \frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}. \tag{6.7}$$

This approach has been applied with several choices of distance-like functions d, such as moment/kernel matching, L^2 distance between densities, Kullback–Leibler divergences; we refer to [SSK12] for an extensive review supplemented with a detailed list of references. Since the primary purpose of these methods is the approximation of the density ratio $\rho_{X,X'}$, the existence of this ratio (and often the existence of positive densities for μ_X and $\mu_{X'}$ with respect to the Lebesgue measure, at least on some bounded subset of $\mathbb{R}^d$) is almost always a necessary condition for their theoretical analysis. In our context, this ratio need not exist: indeed, while some prior information on the law μ_X may be known, such as bounds on its support, mean or dispersion, it may happen for example that some components of the vector X be tied to each other by deterministic relations of the form $h(X) = 0$, so that the actual support of μ_X might be contained in a low-dimensional manifold and difficult to determine precisely. Therefore, designing a synthetic probability distribution $\mu_{X'}$ with respect to which μ_X is absolutely continuous may actually turn out to be impossible.

Wasserstein distance minimisation and Nearest Neighbour estimation

Since the quantity which is minimised in (6.7) only depends on ρ through the measure $\rho\widehat{\mu}_{X'}$, and thus through the values $\rho(X'_1), \dots, \rho(X'_n)$, the actual output is a vector of *weights* $\widehat{\mathbf{w}}_n := (\widehat{w}_1, \dots, \widehat{w}_n)$ which approximate the values of $\rho_{X,X'}$ at the points $X'_1, \dots, X'_n$, and (6.7) rewrites

$$\widehat{\mathbf{w}}_n := \arg\min_{\mathbf{w}_n} \mathsf{d}\left(\frac{1}{n}\sum_{j=1}^{n} w_j\delta_{X'_j}, \frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}\right). \tag{6.8}$$

In Proposition 6.3.2 below, we solve this problem for $\mathsf{d} = W_q$, the Wasserstein distance of order q on $\mathbb{R}^d$. A practical advantage of this distance with respect to the L^2 distance between densities or the Kullback–Leibler divergence is that it is not sensitive to whether the measures are absolutely continuous with respect to each other or with respect to the Lebesgue measure, which makes it quite robust with respect to the choice of μ_X and $\mu_{X'}$. Before proceeding, we note that, in the minimisation problem (6.8), the first argument of $\mathsf{d}(\cdot,\cdot)$ is a probability measure if and only if the vector $\mathbf{w}_n = (w_1, \dots, w_n)$ satisfies

$$\forall j \in \{1, \dots, n\}, \quad w_j \geq 0, \qquad \text{and} \qquad \sum_{j=1}^{n} w_j = n. \tag{6.9}$$

The resolution of (6.8) for the Wasserstein distance involves the notion of *Nearest Neighbour*. For $x \in \mathbb{R}^d$ and $k \in \{1, \dots, n\}$, we denote by $\mathrm{NN}^{(k)}_{\mathbf{X}'_n}(x)$ the *k-th Nearest Neighbour* (k-NN) of x, that is to say the k-th closest point to x, among the sample $\mathbf{X}'_n$ (for a given norm $|\cdot|$ on $\mathbb{R}^d$). If there are several such points, we define $\mathrm{NN}^{(k)}_{\mathbf{X}'_n}(x)$ to be the point X'_j with lowest index j. Last, for any $x \in \mathbb{R}^d$ and $l \in \{1, \dots, n\}$, we denote by $j^{(l)}(x)$ the (lowest) index j such that $X'_j = \mathrm{NN}^{(l)}_{\mathbf{X}'_n}(x)$. The next statement is the first main result from [A11].

Proposition 6.3.2 (Optimal vector of weights for Wasserstein distance)**.** *Let the NN vector of weights $\mathbf{w}_n^{(1)} = (w_1^{(1)}, \dots, w_n^{(1)})$ be defined by, for all $j \in \{1, \dots, n\}$,*

$$w_j^{(1)} := \frac{n}{m}\sum_{i=1}^{m} \mathbb{1}_{\{j = j^{(1)}(X_i)\}}.$$

The vector $\mathbf{w}_n^{(1)}$ *is optimal for the problem* (6.8)–(6.9) *with Wasserstein distances of any order, in the sense that for any* $q \in [1, +\infty)$,

$$W_q^q\left(\frac{1}{n}\sum_{j=1}^n w_j^{(1)}\delta_{X'_j}, \frac{1}{m}\sum_{i=1}^m \delta_{X_i}\right) = \inf W_q^q\left(\frac{1}{n}\sum_{j=1}^n w_j\delta_{X'_j}, \frac{1}{m}\sum_{i=1}^m \delta_{X_i}\right),$$
$$\mathbf{w}_n = (w_1, \ldots, w_n) \text{ satisfies (6.9)}.$$

In the sequel we shall consider more generally the k-NN vector of weights $\mathbf{w}_n^{(k)} = (w_1^{(k)}, \ldots, w_n^{(k)})$ be defined by, for all $j \in \{1, \ldots, n\}$,

$$w_j^{(k)} := \frac{n}{km}\sum_{i=1}^m \sum_{l=1}^k \mathbb{1}_{\{j=j^{(l)}(X_i)\}}, \tag{6.10}$$

which although suboptimal for the problem (6.8)–(6.9), will prove to induce better convergence properties, in the regime $k = k_n \to +\infty$ when $n \to +\infty$, for the estimation of QI.

Convergence analysis

The estimator of QI based on the k-NN vector of weights (6.10) writes

$$\widehat{\mathrm{QI}}_{n,m}^{(k)} := \frac{1}{n}\sum_{j=1}^n w_j^{(k)}\phi(Y'_j) = \frac{1}{m}\sum_{i=1}^m \frac{1}{k}\sum_{l=1}^k \phi\left(Y'_{j^{(l)}(X_i)}\right).$$

We now discuss the convergence of $\widehat{\mathrm{QI}}_{n,m}^{(k)}$, in the $n, m \to +\infty$ limit, toward QI. As an intermediary step, we first study the convergence of the reweighted measure

$$\widehat{\mu}_{\mathbf{X}'_n}^{(k)} := \frac{1}{n}\sum_{j=1}^n w_j^{(k)}\delta_{X'_j}$$

to μ_X. To this aim, we use Jensen's inequality to write, for $q \in [1, +\infty)$,

$$\mathbb{E}\left[W_q^q\left(\widehat{\mu}_{\mathbf{X}'_n}^{(k)}, \mu_X\right)\right] \le 2^{q-1}\left(\mathbb{E}\left[W_q^q\left(\widehat{\mu}_{\mathbf{X}'_n}^{(k)}, \widehat{\mu}_{\mathbf{X}_m}\right)\right] + \mathbb{E}\left[W_q^q\left(\widehat{\mu}_{\mathbf{X}_m}, \mu_X\right)\right]\right).$$

The second term in the right-hand depends on m but not on n, and under suitable moment conditions over μ_X, it is known to converge to 0 when $m \to +\infty$, with explicit rates [FG15]. The asymptotic behaviour of the first term is described by the next result, from [A11]. For any probability measure ν on $\mathbb{R}^d$, we define the support of ν by

$$\mathrm{supp}(\nu) := \{x \in \mathbb{R}^d : \forall r > 0, \nu(B(x, r)) > 0\}.$$

Proposition 6.3.3 (Consistency of $\widehat{\mu}_{\mathbf{X}'_n}^{(k)}$)**.** *Assume that* $\mathrm{supp}(\mu_X) \subset \mathrm{supp}(\mu_{X'})$ *and that there exists an integer* $m_0 \ge 1$ *such that* $\mathbb{E}[\min_{1\le j\le m_0} |X'_j|] < +\infty$. *Then, for any* $q \in [1, +\infty)$ *such that* μ_X *has a finite* q*-th order moment, and for any sequence of positive integers* $(k_n)_{n\ge1}$ *such that* $k_n/n \to 0$, *we have*

$$\lim_{n\to+\infty} \mathbb{E}\left[W_q^q\left(\widehat{\mu}_{\mathbf{X}'_n}^{(k_n)}, \widehat{\mu}_{\mathbf{X}_m}\right)\right] = 0,$$

uniformly in m.

Under various assumptions on μ_X and $\mu_{X'}$, rates of convergence for $\mathbb{E}[W_q^q(\widehat{\mu}_{\mathbf{X}'_n}^{(k_n)}, \widehat{\mu}_{\mathbf{X}_m})]$ are also obtained in [A11]. We do not detail these results, and turn our attention to the convergence of $\widehat{\mathrm{QI}}_{n,m}^{(k)}$.

A first striking result is that under the assumptions of Proposition 6.3.3, the estimator $\widehat{\mathrm{QI}}^{(1)}_{n,m}$ need not be consistent. Indeed, consider the case where X is actually deterministic and always equal to some $x_0 \in \mathbb{R}^d$. Then we have

$$\widehat{\mathrm{QI}}^{(1)}_{n,m} = \frac{1}{m}\sum_{i=1}^{m} \phi\left(Y'_{j^{(1)}(X_i)}\right),$$

where we recall that $j^{(1)}(X_i)$ is the index of the closest X'_j to X_i. But since $X_i = x_0$ for all i, all indices $j^{(1)}(X_i)$ are equal to some $j^{(1)}$ and the estimator rewrites

$$\widehat{\mathrm{QI}}^{(1)}_{n,m} = \phi\left(Y'_{j^{(1)}}\right) = \phi\left(f(X'_{j^{(1)}}, \Theta_{j^{(1)}})\right).$$

While the support assumption from Proposition 6.3.3 ensures that $X'_{j^{(1)}}$ converges to x_0 when $n \to +\infty$, in general $\Theta_{j^{(1)}}$ remains random and thus $\widehat{\mathrm{QI}}^{(1)}_{n,m}$ does not converge to a deterministic limit.

As is evidenced on this example, the presence of an atom in the law of X makes the estimator $\widehat{\mathrm{QI}}^{(1)}_{n,m}$ depend on a single realisation of Θ and therefore prevents this estimator from displaying an averaging behaviour with respect to the law of Θ. In Proposition 6.3.4 below, adapted from the results of [A11], we clarify this point by exhibiting a necessary and sufficient condition for the estimator $\widehat{\mathrm{QI}}^{(1)}_{n,m}$ to be consistent, and then we show that replacing $\widehat{\mathrm{QI}}^{(1)}_{n,m}$ with $\widehat{\mathrm{QI}}^{(k_n)}_{n,m}$, for $k_n \to +\infty$, allows to recover such an averaging behaviour and make the estimator consistent, even when μ_X has atoms.

In the next statement, we denote $\psi(x) := \mathbb{E}[\phi(f(x,\Theta))]$ and $\vartheta(x) := \mathrm{Var}(\phi(f(x,\Theta)))$. We also denote by $\mathcal{A}_X$ the set of atoms of μ_X, that is to say the set of $x \in \mathbb{R}^d$ such that $\mu_X(\{x\}) > 0$.

Proposition 6.3.4 (Consistency of $\widehat{\mathrm{QI}}^{(k)}_{n,m}$)**.** *Let the assumptions of Proposition 6.3.3 hold, and assume that:*

- *the function ϕ is bounded;*
- *the function ψ is Lipschitz continuous.*

(i) Case $k = 1$: assume in addition that the function ϑ is continuous. Then $\widehat{\mathrm{QI}}^{(1)}_{n,m}$ converges to QI *in probability if and only if $\vartheta(x) = 0$ for all $x \in \mathcal{A}_X$.*

(ii) Case $k_n \to +\infty$: for any sequence of positive integers $(k_n)_{n\geq 1}$ such that $k_n \to +\infty$ and $k_n/n \to 0$, $\widehat{\mathrm{QI}}^{(k_n)}_{n,m}$ converges to QI *in probability.*

6.3.2 The Nearest Neighbour WLAM

From the results of Subsection 6.3.1, we naturally infer the construction of the following WLAM: $\mathbf{X}'_n$ is the synthetic sample $X'_1, \dots, X'_n$, taken iid according to $\mu_{X'}$, and for any $\mathbf{s}_n = (\mathbf{x}'_n, \mathbf{y}_n)$ and $x \in \mathbb{R}^d$, we let $\mathbf{W}^{(k)}_n = (W^{(k)}_j)_{1\leq j\leq n}$ be defined by

$$W^{(k)}_j(\mathbf{s}_n, x) = \frac{1}{k}\sum_{l=1}^{k} \mathbb{1}_{\{j=j^{(l)}(x)\}},$$

with $j^{(l)}(x)$ the (lowest) index j such that x'_j is the l-th closest point to x, among the sample $\mathbf{x}'_n$. The consistency of this WLAM follows from the results from Subsection 6.3.1 with $\mu_X = \delta_x$.

Proposition 6.3.5 (Consistency of the Nearest Neighbour WLAM)**.** *Assume that the synthetic sample $\mathbf{X}'_n$ is drawn according to a probability measure $\mu_{X'}$ with support $\mathbb{R}^d$ and such that there exists $m_0 \geq 1$ for which $\mathbb{E}[\min_{1\leq j\leq m_0} |X'_j|] < +\infty$. Then for any sequence of positive integers $(k_n)_{n\geq 1}$ such that $k_n \to +\infty$ and $k_n/n \to 0$, the WLAM $(\mathbf{X}'_n, \mathbf{W}^{(k_n)}_n)$ is $\mathfrak{B}$-consistent, for any class $\mathfrak{B}$ of measurable and bounded functions ϕ for which the mapping $x \mapsto \mathbb{E}[\phi(f(x,\Theta))]$ is Lipschitz continuous.*

More explicitly, if the mapping $x \mapsto f(x, \theta)$ is assumed to be Lipschitz continuous, uniformly in θ, then under the assumptions of Proposition 6.3.5, the WLAM $(\mathbf{X}'_n, \mathbf{W}_n^{(k_n)})$ is $\mathfrak{B}$-consistent with $\mathfrak{B}$ the class of bounded and Lipschitz continuous functions.

6.4 Summary

The whole reweighting method presented in Sections 6.2 and 6.3, using Nearest Neighbour WLAMs at each node and Bayesian network algorithms to compute global weights, was implemented on an industrial test case, provided by Airbus, by Adrien Touboul in his PhD thesis [Tou21]. While the method is currently only designed to approximate quantities of interest of the form $\mathrm{QI} = \mathbb{E}[\Phi(Y_{\mathcal{V}})]$, we believe that it may be combined with sensitivity analysis numerical techniques in order to approximate such quantities as $\mathrm{Var}(\mathbb{E}[\Phi(Y_{\mathcal{V}})|U])$, where U is a subset of the variables $\Theta_v, X_{u,v}, Y_v, \ldots$ involved in the numerical design phase. This would allow to screen which of those quantities are actually influential in the variability of $\Phi(Y_{\mathcal{V}})$ and would hopefully help to reduce the computational complexity of this phase by neglecting the variability of those variables which are not deemed influential. This task is a natural perspective for the continuation of the works presented in this chapter.

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