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Coarse-graining of Fokker–Planck equations
Upanshu Sharma

On 12 January 2017 Upanshu Sharma successfully defended his Ph.D. thesis *Coarse-graining of Fokker-Planck equations*, written under guidance of prof. dr. Mark Peletier (TU/e) and dr. M. Hong Duong (Warwick). He worked in the group CASA, a rich and vibrant environment, both academically and socially. He may be biased, but thinks that this vibrance is a reflection of the general outlook towards research in the Netherlands: informal, communicative and inclusive. Anyway, his years in Eindhoven were a great and fruitful experience and he absolutely enjoyed being a PhD student in the Netherlands.

When asked to tell about his research, Sharma first explains the title of his thesis: what has he been studying, and why? Next, he discusses how his results were obtained.

Coarse-graining

Coarse-graining is an umbrella term for procedures and techniques used to approximate a system by a simpler and lower dimensional one: a system is represented with fewer degrees of freedom than those actually present in the system. Most real-life applications and problems are fairly complex and higher dimensional, making their analysis difficult. As a result coarse-graining has gained tremendous importance in various fields of science. In particular, the questions raised and studied in Sharma's thesis were inspired from statistical mechanics, molecular dynamics and thermodynamics.

Fokker–Planck equations

The focus of his study was a class of evolution equations called the *Fokker–Planck* equations. These are partial differential equations which describe the collective behaviour of (infinitely many) microscopic particles which feel the effect of *deterministic* and *random* forces. As an example, Sharma describes a simple case where the position of each of these microscopic particles follows a Brownian motion, written informally as

$$\frac{dx}{dt} = \sqrt{2}\,\dot{B}_t.$$

Here $x(t)$ is the position of each individual particle at time t, which evolves randomly as modelled by the Brownian motion $\dot{B}_t$. Since each of the particles is moving randomly, the mean of the positions of these particles is also random. A very classical result then states that as the number of particles goes to infinity, this random mean converges to a *deterministic* macroscopic time-dependent density ρ which solves the well-known 'diffusion equation'

$$\frac{\partial \rho}{\partial t} = \Delta \rho,$$

where Δ is the Laplace operator. (Formally the quantity considered is the *empirical measure* instead of the mean.) The important point here is that the diffusion equation can be viewed as *arising from random particles*. Like the diffusion equation, many related linear and nonlinear equations share this feature and thus fall under the category of Fokker–Planck equations. It should be noted that Fokker–Planck equations are widely employed in both natural and social sciences.

Eliminating 'uninteresting' fast variables

Having discussed coarse-graining and Fokker–Planck equations, Sharma now links the two. Coarse-graining in the context of evolution equations typically arises in the presence of temporal and/or spatial *scale separation* which is indicated by the presence of a small or large parameter in the system. As a result of this parameter, the system has fast and slow variables. As the ratio of 'fast' to 'slow' increases, some form of averaging allows one to remove the fast variables, thereby producing a reduced dynamics on the slow variables. In other words, by coarse-graining, one eliminates the fast variables and keeps the coarse-grained variables with time or length scales much larger than typical particle scales.

A classical example helps to make these ideas more concrete: a randomly perturbed Hamiltonian system, which is for $\varepsilon = 0$ a classical Hamiltonian system. Consider the following random evolution of a particle in $\mathbb{R}^2$:

$$\frac{dX}{dt} = J\nabla H(x) + \sqrt{2\varepsilon}\,\dot{B}_t.$$

Here $X(t) \in \mathbb{R}^2$ is a variable in the phase space, $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ is the canonical symplectic matrix and $H : \mathbb{R}^2 \to \mathbb{R}$ is a Hamiltonian. As before, $\dot{B}_t$ is the Brownian motion. The small parameter $0 < \varepsilon \ll 1$ intuitively controls the amplitude of the noise. Repeating the same procedure as before, the random mean of infinitely many such particles converges to a deterministic macroscopic time-dependent density ρ which satisfies the following Fokker–Planck equation:

$$\frac{\partial \rho}{\partial t} = \mathrm{div}(\rho J \nabla H(x)) + \varepsilon \Delta \rho. \tag{1}$$

Here ρ can also be interpreted as the probability density function of the random variable X. The central question in this context is: "What is the behaviour of (1) in the limit of $\varepsilon \to 0$?" Under appropriate rescaling (which allows to see the effect of the noise), a scale separation arises in this system as $\varepsilon \to 0$: there is a faster Hamiltonian motion around the level sets and a slower diffusive motion from one level set to another. Following the discussion above, as this ratio of fast to slow increases it becomes possible to derive a simpler model.

In fact, this classical coarse-graining question has received wide attention in the dynamical systems and probability communities since it models a commonly encountered issue: the effect of noise in observation data in dynamical systems. Sharma does not give a solution to this problem here, but interested readers are welcome to have a look at his thesis for a solution to this simple, yet fascinating, question. Another interesting question from a numerical perspective would be to derive quantitative estimates which relate the behaviour in the limit $\varepsilon \to 0$ to the behaviour $\varepsilon > 0$.

Main results

While the Fokker–Planck equations in the examples above are linear, these equations can be nonlinear as well. An abstract Fokker–Planck equation can be written as

$$\partial_t \rho = (\mathcal{N}^\varepsilon)\,\rho, \tag{2}$$

where $\mathcal{N}$ is in general a nonlinear operator and $0 < \varepsilon \ll 1$ indicates the presence of scale separation in the system. The main results of Sharma's thesis are towards addressing two facets of coarse-graining:

1. Qualitative coarse-graining: understand the behaviour of (2) as $\varepsilon \to 0$.
2. Quantitative coarse-graining: derive quantitative estimates for the solution of (2) for $\varepsilon > 0$.

While these questions are about the behaviour of the *macroscopic* Fokker–Planck equations, the crucial ingredient in the analysis, is the behaviour of the *microscopic* random particles underlying these equations. Specifically, Sharma uses the so-called 'large deviations' of the underlying stochastic process or random particles. Large deviations is a theory that analyses the rates of convergence of the underlying microscopic particles to the corresponding macroscopic equations. In addition to providing various insights, in the current context, the theory of large deviations can also be used to reformulate the Fokker–Planck equations as a solution to a *variational problem*. It turns out that this variational problem reveals the *geometrical structure* underlying the Fokker–Planck equations and also meshes well with coarse-graining questions. As a result this variational formulation of the Fokker–Planck equations is the central ingredient in Sharma's thesis.

In light of this very fascinating and interesting micro–macro connection, the main message and novelty of Sharma's thesis is that "studying underlying microscopic systems gives us structure and tools to understand Fokker–Planck equations".

Significant moments

When asked about significant moments that had stood out for him, Sharma says that ironically the best period during his PhD time was also the hardest one: the last few months before the thesis submission. There was a palpable sense of pressure, which any PhD student will recognise. However, in his case this really helped since suddenly interesting ideas and connections kicked in. As a result he was doing some very interesting mathematics untill the last day before his submission deadline, as opposed to the oft-heard dictum "All I do is write". Additionally, the process of the thesis writing opened Sharma's eyes to closely-related literature and helped him connect with some very interesting people. Hard but fun, the last few months were definitely his favourite.

In March, Sharma joined the École des Ponts ParisTech in France as a postdoc. Since Paris is a great city, both for mathematics and for life in general, he has really been looking forward to the experience. Hopefully he can continue to combine hard and fun work.