

Randonnée aléatoire le long des solénoïdes d'un tore

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Who am I? In spite of the multiple geometrical concepts presented on the pictures, I am not a geometer. I work in numerical analysis, a field that oscillates between mathematics and computer science, which is concerned with the creation and study of computer algorithms to solve mathematical problems. In my research, I create numerical methods to solve equations mixing derivatives and randomness called *stochastic differential equations*.

Context of the algorithm used. The numerical method used here has its origin in a completely different context: molecular dynamics. If one looks at a gas containing a large number of particles under a high temperature, it can be shown that the particles follow the following equation, called *Langevin overdamped equation*,

$$dX(t) = -\nabla V(X(t))dt + \sigma dW(t).$$

Here, V is a potential that forces particles to prefer certain places to others, and W is Brownian motion, a random process that accounts for the collisions of particles with their environment. Very often, the particles do not evolve freely. For example, in a water molecule H_2O , the three atoms form a fixed angle and therefore do not evolve freely. This is called a constraint, and it amounts to making our particles evolve on a *differential variety*, like a curve or a surface. The random walk represented on the image is in fact a particle walking on a torus (a mathematical doughnut), and undergoing a potential V which constrains the particle close to the solenoids of this torus.

But what is it useful for? Knowing how to approximate the trajectory of particles is extremely useful in chemistry as well as in quantum physics, especially if we can take into account different constraints. For example, simulating the interaction of proteins with their environment allows to choose good candidates for vaccines. Nevertheless for the picture on the poster, I chose a trajectory close to the solenoids of a torus for the only reason that I find it pretty!

I want more details ! Under constraints, we can rewrite the Langevin overdamped equation on a variety as

$$dX(t) = -\nabla V(X(t))dt + \sigma dW(t) + \nabla \zeta(X(t))d\lambda_t, \quad \zeta(X(t)) = 0,$$

where the solution is constrained on the variety $\mathcal{M} = \{x \in \mathbb{R}^d, \zeta(x) = 0\}$ and λ is to be interpreted as a *Lagrange multiplier*. This equation can be discretized into an *Runge-Kutta*

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method of the form

$$Y_i = X_n + h \sum_{j=1}^s a_{ij} f(Y_j) + \sigma \sqrt{h} \sum_{k=1}^l d_i^{(k)} \xi_n^{(k)} + \lambda_i \sum_{j=1}^s \hat{a}_{ij} g(Y_j), \quad i = 1, \dots, s,$$

$$\zeta(Y_i) = 0 \quad \text{si} \quad \delta_i = 1, \quad i = 1, \dots, s,$$

$$X_{n+1} = Y_s,$$

where $\xi_n^{(k)}$ are independent Gaussian vectors, and $A = (a_{ij})$, $\hat{A} = (\hat{a}_{ij}) \in \mathbb{R}^{s \times s}$, $b = (b_i) \in \mathbb{R}^s$, $d^{(k)} = (d_i^{(k)}) \in \mathbb{R}^s$, $\delta_i = \sum_{j=1}^s \hat{a}_{ij} \in \{0, 1\}$ are the coefficients of the Runge-Kutta method. An example of method of this form is the Euler method with implicit direction

$$X_{n+1} = X_n + hf(X_n) + \sigma \sqrt{h} \xi_n + \lambda g(X_{n+1}), \quad \zeta(X_{n+1}) = 0.$$

A new method of this form was used for the image, but of second order. If you are really very interested, you can find the method in the article [1].

References

- [1] A. Laurent and G. Vilmart. *Order conditions for sampling the invariant measure of ergodic stochastic differential equations on manifolds*. Submitted, 2020.