Fractional Brownian motion and polymers: Learning from each other

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Self-avoiding or self-repelling random paths, with motivation from their use in polymer physics, have been widely studied using the tools of mathematics, physics, and computer simulations. We illustrate this by three recent examples.

1. Introduction

Self-avoiding or self-repelling random path models for polymer configurations have been studied extensively in mathematics using combinatorics, stochastic analysis, in statistical mechanics, and in computer physics using Monte Carlo methods. Classical texts are e.g.⁴ and¹², a recent review can be found in¹⁷. The field is highly interdisciplinary: the motivation came from chemistry, while physics provides structural intuition and far-reaching predictions, and computer simulations can check them out. The mathematical results are less far-reaching but provide the higher reliability characteristic of the mathematical approach; much remains to be done in the stochastic analysis setting.

Apart from self-avoiding random walks, a prominent realization is the Edwards model of self-repelling (or “weakly self-avoiding”) Brownian paths, an example of models where self-crossings are not strictly forbidden but where there is an exponential penalty on self-crossings.⁸

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Recently the Edwards model has been extended to fractional Brownian motion (fBm),¹³ allowing for models of stiffer or curlier polymers than those described by classical Brownian motion.

It is in this context that we shall present report on progress on three fronts, where methods from stochastic analysis, arguments from statistical physics, and numerical computation have been employed.

2. Recent developments

2.1. Varadhan's existence proof

In the Edwards model self-repelling paths are described via a “Boltzmann factor” to suppress self-intersections of Brownian motion B :

$$G = \frac{1}{Z} \exp \left(-g \int_0^N ds \int_0^N dt \delta(B(s) - B(t)) \right)$$

with

$$Z = E \left(\exp \left(-g \int_0^N ds \int_0^N dt \delta(B(s) - B(t)) \right) \right).$$

The mathematical problem here lies with the existence of this exponential, how to make sense of

$$L = \int_0^N ds \int_0^N dt \delta(B(s) - B(t))$$

One uses delta sequences to approximate the Dirac distribution

$$\delta_\varepsilon(x) := \frac{1}{(2\pi\varepsilon)^{d/2}} e^{-\frac{|x|^2}{2\varepsilon}}, \quad \varepsilon > 0,$$

$$L_\varepsilon := \int_0^l dt \int_0^t ds \delta_\varepsilon(B(t) - B(s)). \quad (1)$$

Removing the regularization depends on the dimension of the Brownian paths, it is straightforward for $d = 1$ but for $d \geq 2$ the expectation diverges

$$\lim_{\varepsilon \searrow 0} \mathbb{E}(L_\varepsilon) = \infty.$$

In $d = 2$ one needs to subtract the expectation, setting

$$L_\varepsilon^c = L_\varepsilon - \mathbb{E}(L_\varepsilon),$$

and will define the centered self-intersection local time as

$$L^c = \lim_{\varepsilon \searrow 0} L_\varepsilon^c.$$

In $d = 3$ a further, multiplicative renormalization is required,²⁰ but for $d = 2$ one is thus led to consider

$$\exp(-gL^c).$$

However, after centering L^c is unbounded below, and

$$\exp(-gL^c) \rightarrow \infty \text{ when } L^c \rightarrow -\infty.$$

So one needs to show that large values occur only with small probability such that the expectation is nevertheless finite. Varadhan¹⁹ shows that

$$\mathbb{E}(\exp(-gL^c)) < \infty$$

and a bona fide probability distribution for planar self-repelling Brownian paths exists if $g > 0$ is sufficiently small. By a further scaling argument this existence result can be extended to all $g > 0$.

Varadhan's famous proof is based on a clever use of the Chebyshev inequality, using the logarithmic divergence of the expectation and an estimate of the rate of convergence

$$\|L^c - L_\varepsilon^c\|_{L^2(\mu)}^2 \leq \text{const.} \varepsilon^a \text{ for all } a < 1/2.$$

Concerning this rate of convergence, in his words, “...this is the most difficult step of all and requires considerable estimation”. Hence an alternate proof may be of interest.

Using the tools of White Noise Analysis, in the particular multiple Wiener integral or “chaos” decomposition of the self-intersection local time⁹ it is straightforward to show²

Theorem 2.1. *Let $T > 0$ be given. Then*

$$\|L_\varepsilon^c(T) - L^c(T)\|^2 \leq C\varepsilon^\alpha \quad \forall \alpha < 1.$$

Apart from a simplified proof one notes the doubling of the convergence rate α .

Remark 2.1. While a generalisation of the Varadhan existence proof to fBm is now available,¹³ its extension to arbitrary coupling constants g remains an open challenge.

2.2. The Flory index

Contrary to the above, the scaling behavior of self-repelling paths is not (yet) accessible to strict mathematical arguments, with the exception of the unphysical one-dimensional case.¹⁴

The question, in physical terms, is about the “end-to-end-length” R of polymer, and how it grows as one increases the number N of monomers in the chain. Mathematically, for a (fractional) Brownian path $x = B^H$, one has

$$\mathbb{E}(x(N) - x(0))^2 = N^{2\nu}$$

with ν equal to the “Hurst index” H which characterizes the fBm. The suppression of self-intersections, “excluded volume effect” in physics terminology, will make the paths swell and one expects $\nu > H$.

Flory's famous formula¹⁰

$$\nu = \frac{3}{d+2}$$

for spatial dimensions $d = 1, 2, 3$ was based on a flawed mean field argument¹² but is remarkably accurate.¹⁷ Recently it was extended to the fractional case,¹ with

$$\nu_H = \frac{2H+2}{d+2}.$$

Computer simulations appear to support this formula at least for $d = 1$. In Refs. ⁵ and ⁶ the original self-avoiding Brownian model has been extended to the case where k -fold intersections are tolerated, and only higher order ones penalized. Informally this would correspond to the use of higher order self-intersection local times

$$L^{(k)}(N) \equiv \int_0^N dt \int_0^N d^k s \prod_{l=1}^k \delta(x(t) - x(s_l)).$$

For a rigorous mathematical discussion of such higher order intersection local times and the necessary renormalizations to make them well-defined see e.g.⁷.

Putting aside the problems of a rigorous definition, one can invoke, simple, dimensional arguments would lead to

$$\nu_{H,k}(d) = \frac{2H+k+1}{kd+2} \quad (2)$$

which now covers all values of the dimension d , the Hurst index H , and the tolerance level k , up to the limiting dimensions where there are no more self-intersections, see formula (3) below.

The singularity of higher order self-intersection local times and the non-Markovian nature of fBm complicate the mathematical analysis of scaling even beyond the classical Brownian case. In this light it is remarkable that for

$$Hd = \frac{k+1}{k}$$

the formula (2) produces

$$\nu_{H,k}(d) = H \quad (3)$$

i.e. there is no swelling from the suppression of self-intersections. This coincides in fact with a rigorous mathematical result: Talagrand¹⁸ proves that indeed with probability 1 fBm has no $(k+1)$ -tuple points whenever

$$Hd \geq \frac{k+1}{k}.$$

On the other hand one notes that for $d = 1$ the formula (2) would predict increased swelling for $k > 1$; also in the Bm case one expects Wilson type renormalization to induce a $k = 1$ term in the renormalized interaction,¹⁶ hence the usual Flory scaling also for k -tolerant models.

2.3. Computational results

In view of the difficulties confronting a mathematical investigation computer simulations suggest themselves.

Results in this direction are based on a discretized version of the k -tolerant model, with monomer positions

$$x_k = B^H(k), k = 0, 1, 2, \dots, N - 1.$$

As for the self-intersection local time $L^{(k)}$, one notes that, informally, we can express it in terms of the local time $L(N, u)$, given informally by

$$L(N, u) = \int_0^N dt \delta(x(t) - u).$$

Indeed one has

$$\begin{aligned} L^{(k)}(N) &= \int_0^N dt \int_0^N d^k s \prod_{l=1}^k \delta(x(t) - x(s_l)) \\ &= \int_0^N du \left(\int_0^N dt \delta(x(t) - u) \right)^{k+1} \\ &= \int_0^N du L^{k+1}(N, u) \end{aligned}$$

and the latter is straightforward to discretize. Monte Carlo computations with importance sampling¹⁵ are then based on a conformation energy

Fig. 1.

$$E(x) = E_0(x) + gE_1(x)$$

where E_0 is obtained by inverting the fBm covariance matrix, and the excluded volume energy is given by a discretized version of $L^{(k)}$.

Preliminary results for $d = 1$, $k = 1$, and $0 < H < 1/2$ give encouraging results, see Fig. 1. The straight line corresponds to formula (2) for $k = 1$; extensive precision calculations are under way³.

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