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Feynman-Kac Interpretation Models

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– Brief introduction to Feynman-Kac and evolutionary particle models.
– Mean field particle interpretation models $\simeq$ stochastic linearization Methods.
– Feynman-Kac interpretations of directed polymer measures
– Some asympt. analysis $\oplus$ propagations of chaos expansions

Evolutionary type models

Simple Genetic Branching Algo.	*Mutation*	‖	*Selection/Branching*
Metropolis-Hastings Algo.	*Proposal*	‖	*Acceptance/Rejection*
Sequential Monte Carlo methods	*Sampling*	‖	*Resampling (SIR)*
Filtering/Smoothing	*Prediction*	‖	*Updating/Correction*
Particle $\in$ Absorbing Medium	*Evolution*	‖	*Killing/Creation/Anhiling*

Other Botanical Names : multi-level splitting (Khan-Harris 51), prune enrichment (Rosenbluth 1955), switching algo. (Magill 65), matrix reconfiguration (Hetherington 84), restart (Villen-Altamirano 91), particle filters (Rigal-Salut-DM 92), SIR filters (Gordon-Salmon-Smith 93, Kitagawa 96), go-with-the-winner (Vazirani-Aldous 94), ensemble Kalman-filters (Evensen 1994), quantum Monte Carlo methods (Melik-Nightingale 1999), sequential Monte Carlo Methods (Arnaud Doucet 2001), spawning filters (Fisher-Maybeck 2002), SIR Pilot Exploration Resampling (Liu-Zhang 2002),...

$\Longleftrightarrow$ Particle Interpretations of Feynman-Kac models

Since R. Feynman's phD. on path integrals 1942

Physics $\longleftrightarrow$ Biology $\longleftrightarrow$ Engineering Sciences $\longleftrightarrow$ Probability/Statistics

- **Physics** :
  - $FKS \in$ nonlinear integro-diff. éq. ($\sim$ generalized Boltzmann models).
  - Spectral analysis of Schrödinger operators and large matrices with nonnegative entries. (particle evolutions in disordered/absorbing media)
  - Multiplicative Dirichlet problems with boundary conditions.
  - Microscopic and macroscopic interacting particle interpretations.

- **Biology** :
  - Self-avoiding walks, macromolecular polymerizations.
  - Branching and genetic population models.
  - Coalescent and Genealogical evolutions.

- **Rare events analysis** :
  - Multisplitting and branching particle models (Restart).
  - Importance sampling and twisted probability measures.
  - Genealogical tree based simulation methods.

- **Advanced Signal processing** :
  - Optimal filtering/smoothing/regulation, open loop optimal control.
  - Interacting Kalman-Bucy filters.
  - Stochastic and adaptative grid approximation-models

- **Statistics/Probability** :
  - Restricted Markov chains (w.r.t terminal values, visiting regions,...)
  - Analysis of Boltzmann-Gibbs type distributions (simulation, partition functions,...).
  - Random search evolutionary algorithms, interacting Metropolis/simulated annealing algo.
  - Bayesian methodology.

Mean field particle models=Non Linear Monte Carlo Methods

η_t Non linear PDE $\sim (L_{t,\eta})_{(t,\eta)\in(\mathbb{R}_+\times\mathcal{P}(E))}$ infinitesimal generators

$$\frac{d}{dt}\eta_t(f) = \eta_t L_{t,\eta_t}(f) =_{\text{def.}} \int_E \eta_t(dx)\ L_{t,\eta_t}(f)(x)$$

$$\downarrow$$

Interacting Particle Approximation Model $\xi_t = (\xi_t^i)_{1\leq i\leq N}$ infinitesimal generator $\mathcal{L}_t$

$$\mathcal{L}_t(F)(x^1,\ldots,x^N) =_{\text{def.}} \sum_{i=1}^N L^{(i)}_{t,m(x)} F(x^1,\ldots,x^i,\ldots,x^N) \quad \text{with} \quad m(x) = \frac{1}{N}\sum_{i=1}^N \delta_{x^i}$$

$$\downarrow \quad \left(\eta_t^N := m(\xi_t)\right)$$

$$d\eta_t^N(f) = \eta_t^N L_{t,\eta_t^N}(f)dt + dM_t^N(f) \quad \text{with} \quad \langle M^N(f)\rangle_t = \frac{1}{N}\int_0^t\ \eta_s^N \Gamma_{L_{s,\eta_s^N}}(f,f)\ ds$$

Example : (L. Miclo & P. DM SPA 2000**)**

$(X_t \simeq L_t -$ motion on $E), (V_t : E \to \mathbb{R}_+) \rightsquigarrow$ **F.K. norm. model** $\eta_t(f) := \gamma_t(f)/\gamma_t(1)$

$$\text{with} \quad \gamma_t(f) = \mathbb{E}\left(f(X_t)\,\text{exp}\left\{-\int_0^t V_s(X_s)ds\right\}\right)\left(= \eta_t(f)\ \ \text{exp}\left\{-\int_0^t \eta_s(V_s)ds\right\}\right)$$

$$\downarrow$$

$$\begin{aligned}
\frac{d}{dt}\gamma_t(f) &= \gamma_t(L_t^V(f)) \quad \text{with the Schrödinger operator} \quad L_t^V := L_t - V_t \\
\frac{d}{dt}\eta_t(f) &= \eta_t L_{\eta_t}(f) := \int \eta_t(dx)\ \left\{L_t(f)(x) + V_t(x)\ \int\ (f(y) - f(x))\ \eta_t(dy)\right\}
\end{aligned}$$

Moran's type IPS Model $(\xi_t^i)_{1 \leq i \leq N}$ = L-motions $\oplus$ interacting jumps (V-intensity)

$$\begin{aligned}
\mathcal{L}_t(F)(x^1, \ldots, x^N) &= \sum_{i=1}^N L_t^{(i)} F(x^1, \ldots, x^i, \ldots, x^N) + \sum_{i=1}^N V_t(x^i) \\
&\quad \times \int\ \left(F(x^1, \ldots, y^i, \ldots, x^N) - F(x^1, \ldots, x^i, \ldots, x^N)\right)\ m(x)(dy^i)
\end{aligned}$$

Particle approximation measures :

$$\eta_t^N(f) := \frac{1}{N}\sum_{i=1}^{N} f(\xi_t^i) \quad \rightarrow_{N\to\infty} \quad \eta_t(f)$$

$$\gamma_t^N(f) := \eta_t^N(f) \;\; \mathsf{exp}\left\{-\int_0^t \eta_s^N(V)ds\right\} \quad \rightarrow_{N\to\infty} \quad \gamma_t(f) := \mathbb{E}\left(f(X_t)\,\mathsf{exp}\left\{-\int_0^t V(X_s)ds\right\}\right)$$

Propagation of chaos property :

$$\mathsf{Law}(\xi_t^1,\ldots,\xi_t^q) \rightarrow_{N\to\infty} \eta_t^{\otimes q}$$

Discrete generation models

$$\eta_n = \eta_{n-1} K_{n,\eta_{n-1}} =_{\text{def.}} \int_{E_{n-1}} \eta_{n-1}(dx) \quad \underbrace{K_{n,\eta_{n-1}}(x, \centerdot)}_{Markov\ transitions}$$

$$\downarrow$$

Interacting Particle Approximation Model

$$\forall 1 \leq i \leq N \qquad \xi^i_{n-1} \longrightarrow \xi^i_n \sim K_{n,\eta^N_{n-1}}(\xi^i_{n-1}, \centerdot) \quad \text{with} \quad \eta^N_{n-1} = \frac{1}{N}\sum_{i=1}^N \delta_{\xi^i_{n-1}}$$

$$\downarrow$$

$$\eta^N_n = \eta^N_{n-1} K_{n,\eta^N_{n-1}} + \frac{1}{\sqrt{N}}\, W^N_n \quad \text{with} \quad W^N_n \simeq \text{centered Gauss field}$$

$\rightsquigarrow$ adaptive dynamics, genetic and branching population model, etc.

Example : Feynman-Kac & Genetic interpretation models

(Discrete time parameter $n \in \mathbb{N} = \{0, 1, 2, ...\}$, state spaces E_n ($\in \{\mathbb{Z}^d, \mathbb{R}^d, \underbrace{\mathbb{R}^d \times \ldots \times \mathbb{R}^d}_{(n+1)-times}\}$)

– *Reference Markov chain/Mutation/exploration/prediction/proposal* :

$\longrightarrow$ Markov transitions $M_n(x_{n-1}, dx_n)$ from E_{n-1} into E_n.

– *Environment/Selection/absorption/updating/acceptance* :

$\longrightarrow$ Potential functions G_n from E_n into $[0, 1]$.

Random environment/medium impurities :

$\hookrightarrow$ $(G_n(x_n))_{n,x_n}$ independent r.v. (Ex. : X_n r.w. $\in \mathbb{Z} \oplus$ Bernoulli $\in \{1, e^{-\beta}\}$)

Feynman-Kac models $\rightarrow$ weighted random paths $\rightarrow$ directed polymers

Directed Polymer measure :

$$d\mathbb{Q}_n = \frac{1}{Z_n} \left\{ \prod_{0 \le p < n} G_p(X_p) \right\} d\mathbb{P}_n \quad \text{with} \quad \mathbb{P}_n = \text{Law}(X_0, \ldots, X_n)$$

$$\begin{aligned} 0 = G_n(x_n) &\iff \text{hard obstacle} \\ 0 < G_n(x_n) < 1 &\iff \text{repulsive point/soft obstacle} \\ G_n(x_n) \ge 1 &\iff \text{attractive point} \end{aligned}$$

n-th marginals :

$$\eta_n(f_n) = \gamma_n(f_n)/\gamma_n(1) \quad \text{with} \quad \gamma_n(f_n) := \mathbb{E}\left(f_n(X_n) \prod_{0 \le p < n} G_p(X_p) \right) \qquad (Z_n = \gamma_n(1))$$

Path models, Markov monomial $X'_n \in E'_n$:

$$[\ X_n = (X'_0, \ldots, X'_n) \text{ and } G_n(X_n) = G'_n(X'_n)\ ] \hookrightarrow \text{Same Math. Model!!}$$

Examples :

– *Self avoiding walks* $X'_n \in \mathbb{Z}^d$

$$X_n = (X'_0, \ldots, X'_n) \quad \text{and} \quad G_n(X_n) = 1_{\not\in \{X'_0, \ldots, X'_{n-1}\}}(X'_n)$$

FK model :

$$\gamma_n(1) = \text{Proba}(\forall 0 \leq p \neq q \leq n, \quad X'_p \neq X'_q)$$

and

$$\eta_n = \text{Law}(X'_0, \ldots, X'_n \mid \forall 0 \leq p \neq q \leq n, \quad X'_p \neq X'_q)$$

Ex. : (*Connectivity constants*)

$$\gamma_n(1) = \frac{1}{(2d)^n} \times \#\{\text{non intersecting walks with length n}\} \simeq \frac{\exp(\mathbf{c}\ n)}{(2d)^n}$$

– *Edwards' model*

$$X_n = (X'_0, \ldots, X'_n) \quad \text{and} \quad G_n(X_n) = \exp\{-\beta \sum_{0 \leq p < n} 1_{X'_p}(X'_n)\}$$

- Random medium $(G_n(x))_{n,x}$ i.i.d random variables

  $G_n(x) \in \{0,1\} \Rightarrow \eta_n = \text{Law}(X_n \mid X \in \text{percolation clusters})$

- Weak-Strong disorder : $(\mathbb{E}(G_n(x)) = 1)$ (Subadditivity $\oplus$ concentration)

  $$W_n := \frac{1}{n} \log Z_n = \frac{1}{n} \log \gamma_n(1) = \frac{1}{n} \sum_{0 \le p < n} \log \eta_p(G_p) \to_{n\to\infty} W_\infty = \begin{cases} 0 & \text{Strong disorder} \\ < 0 & \text{Weak disorder} \end{cases}$$

  Random Walk $\in \mathbb{Z}^d$, $G_n = e^{-\beta V_n}$ regular medium :
  - strong disorder $(d = 1, 2)$; weak disorder ($d \geq 3$, small β)
    [Ref. : Bolthausen, Carmona-Hu, Comets-Yoshida-Shiga, Imbrie-Spencer]
  - $d \geq 3$ and small $\beta \Rightarrow$ Diffusive regime [Comets, Bolthausen, Sinai]
  - Strong disorder $\Longleftrightarrow$ Replica localisation [Comets, Derrida, Spohn, Vargas]
  - Conjectures : (Under $\mathbb{Q}_n$) [Universal constants, small β]

  $$|X_n| \simeq n^{a(d)} \quad \text{and} \quad \log \gamma_n(1) - \mathbb{E}(\gamma_n(1)) \simeq n^{b(d)} \quad (b(d) \leq 1/2)$$

  $$(a(1), b(1)) = (2/3, 1/3) \quad \text{and} \quad b(d) = 2a(d) - 1$$

  [Comets, large deviations arguments] $b(d) \geq 2a(d) - 1 (\Rightarrow a(d) \leq 3/4)$

Feynman-Kac and Particle Interpretation Models

I-Nonlinear equation $(G_n \leq 1)$

$$\eta_{n+1} = \eta_n K_{n+1,\eta_n}$$

with the composition transition

$$K_{n+1,\eta_n} = S_{n,\eta_n} M_{n+1}$$

the selection type Markov transition

$$S_{n,\eta}(x, dy) = G_n(x)\ \delta_x(dy) + (1 - G_n(x))\ \Psi_n(\eta)(dy)$$

and the Boltzman transformation

$$\Psi_n(\eta)(dy) = \frac{1}{\eta(G_n)}\ G_n(y)\ \eta(dy)$$

II-Particle interpretation=Genetic Model $\Rightarrow$ Markov $\xi_n = (\xi_n^1, \ldots, \xi_n^N) \in E_n^N = E_n \times \ldots \times E_n$

$$\xi_n \in E_n^N \xrightarrow{\text{selection}} \widehat{\xi}_n \in E_n^N \xrightarrow{\text{mutation}} \xi_{n+1} \in E_{n+1}^N$$

- **Selection transition** ($\exists \neq$ types $\rightarrow$ Ex. : accept/reject)

$$\xi_n^i \rightsquigarrow \widehat{\xi}_n^i = \xi_n^i \quad \text{with proba. } G_n(\xi_n^i) \quad \textbf{[Acceptance]}$$

> Otherwise we select a better fitted individual in the current configuration
>
> $$\widehat{\xi}_n^i = \xi_n^j \quad \text{with proba. } G_n(\xi_n^j)/\sum_{k=1}^N G_n(\xi_n^k) \quad \textbf{[Rejection + Selection]}$$

- **Mutation transition**

$$\widehat{\xi}_n^i \rightsquigarrow \xi_{n+1}^i \sim M_{n+1}(\widehat{\xi}_n^i, \,\centerdot\,)$$

Genetic Evolution Model on Path Spaces=Genealogical tree model

Occupation/Empirical measures ($\forall f_n$ test function on E_n)

$$\eta_n^N(f_n) = \frac{1}{N}\sum_{i=1}^{N} f_n(\xi_n^i) = \frac{1}{N}\sum_{i=1}^{N} f_n \underbrace{(\xi_{0,n}^i, \xi_{1,n}^i, \ldots, \xi_{n,n}^i)}_{i\text{-th ancestral lines}} \longrightarrow_{N\to\infty} \eta_n(f_n)$$

$$\downarrow$$

Unbias-particle measures & Unnormalized Feynman-Kac measures :

$$\gamma_n^N(f_n) \quad = \quad \eta_n^N(f_n) \ \times \prod_{0\leq p<n} \eta_p^N(G_p) \longrightarrow_{N\to\infty} \gamma_n(f_n) = \eta_n(f_n) \ \times \prod_{0\leq p<n} \eta_p(G_p)$$

Asymptotic theory $(n, N) \to \infty$ (usual LLN, CLT, LDP,...)

Example : [$p \geq 1$ + $\mathcal{F}_n$ not too large + regular mutations]

(JTP 2000, joint work with M. Ledoux+ FK Formulae Springer 2004)

$$\sup_{n\geq 0} \mathbb{E}(\sup_{f_n\in\mathcal{F}_n} |\eta_n^N(f_n) - \eta_n(f_n)|^p)^{1/p} \leq c(p)/\sqrt{N}$$

and

$$\sup_{n\geq 0} \mathbb{P}(|\eta_n^N(f_n) - \eta_n(f_n)| > \epsilon) \leq (1 + \epsilon\sqrt{N/2}) \ \exp -\frac{N\epsilon^2}{\sigma^2}$$

Functional representation at any order : $(\mathbb{Q}_{n,q}^N(F) := \mathbb{E}((\gamma_n^N)^{\otimes q}(F)))$

$\hookrightarrow$ `Coalescent tree based functional representations for some Feynman-Kac particle models.`

(joint work with F. Patras and S. Rubenthaler)

thm :

$$\mathbb{Q}_{n,q}^N = \gamma_n^{\otimes q} + \sum_{1 \leq k \leq (q-1)(n+1)} \frac{1}{N^k} \, \partial^k \mathbb{Q}_{n,q}$$

and

$$\mathbb{P}_{n,q}^N \simeq \eta_n^{\otimes q} + \sum_{1l \leq l \leq k} \frac{1}{N^l} \, \partial^l \mathbb{P}_{n,q} + \frac{1}{N^{k+1}} \, \partial^{k+1} \mathbb{P}_{n,q}^N \quad \text{with} \quad \sup_{N \geq 1} \|\partial^{k+1} \mathbb{P}_{n,q}^N\|_{\text{tv}} < \infty$$

Consequences : Sharp + strong propagations of chaos estimates at any order, Wick product formulae on forests, sharp $\mathbb{L}_p$-mean error bounds, law of large numbers for U-statistics for interacting processes,. . . .

Rare events : Adaptive Algorithm

Parameters

N the number of particles.
K the number of succeeding particles at each step.

Initialization

Draw an i.i.d. N-sample $\xi_j, j = 1, \dots, N$ of the trajectory of X until stopping time T_j^0 when it hits A_0, compute $S_j = \sup_{0 \le t \le T_j^0} \Phi(\xi_j(t))$.

Sort the S_j, $j = 1, \dots, N$ in decreasing order, and reorder the ξ_j, T_j^0 accordingly.

Take S_K, the K^{th} sorted value, and for $j = 1, \dots, K$ compute $T_j^S = \inf\{0 \le t \le T_j^0, \Phi(\xi_j(t)) \ge S_K\}$.

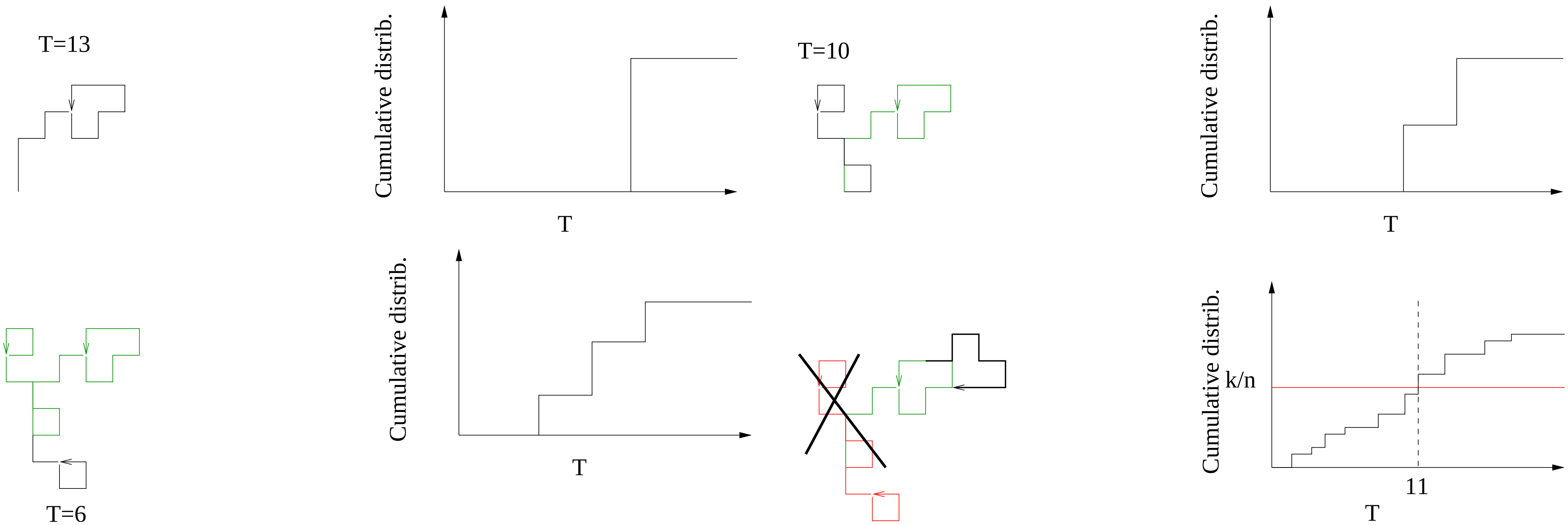
$m \leftarrow 0$.

Iterations

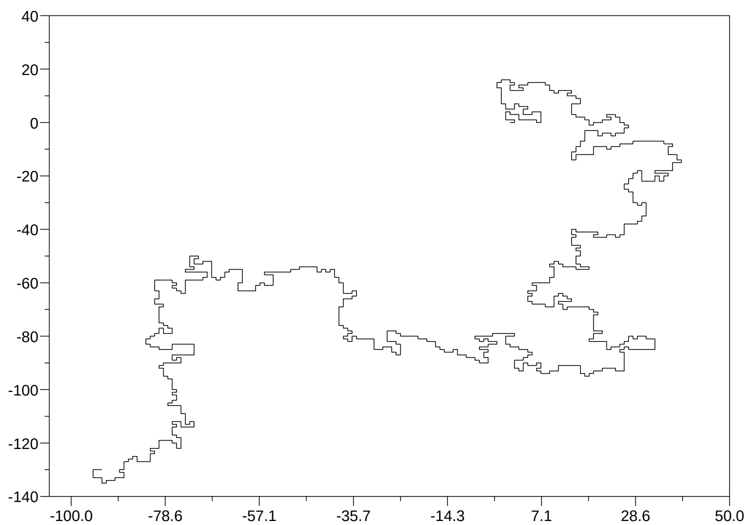
while $S_K < \lambda_R$ do
  $m \leftarrow m + 1$.
  for $j = K + 1, \dots, N$
    Choose at random an index ℓ in $1, \dots, K$ with uniform probability.
    Let $\xi_j = \xi_\ell$ until time T_ℓ^S, and extend the trajectory by simulation until new T_j^0 when it hits A_0, re-compute $S_j = \sup_{0 \le t \le T_j^0} \Phi(\xi_j(t))$.
  endfor
  Sort the S_j, $j = 1, \dots, N$ in decreasing order, and reorder the ξ_j, T_j^0 accordingly.
  Take S_K, the K^{th} sorted value, and for $j = 1, \dots, K$ re-compute $T_j^S = \inf\{0 \le t \le T_j^0, \Phi(\xi_j(t)) \ge S_K\}$.
endwhile
let $\tilde{P}$ be the proportion of trajectories that actually hit R.

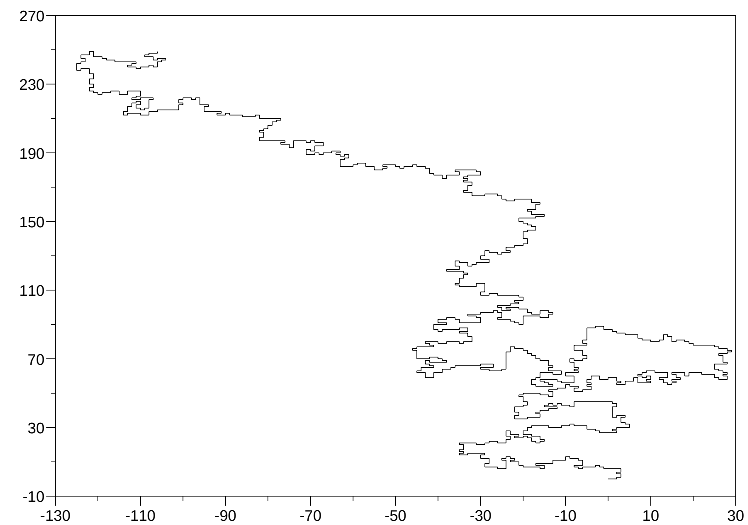
Output

estimate the probability of the rare event by $\hat{P}_2 = \tilde{P}.(\frac{K}{N})^m$.

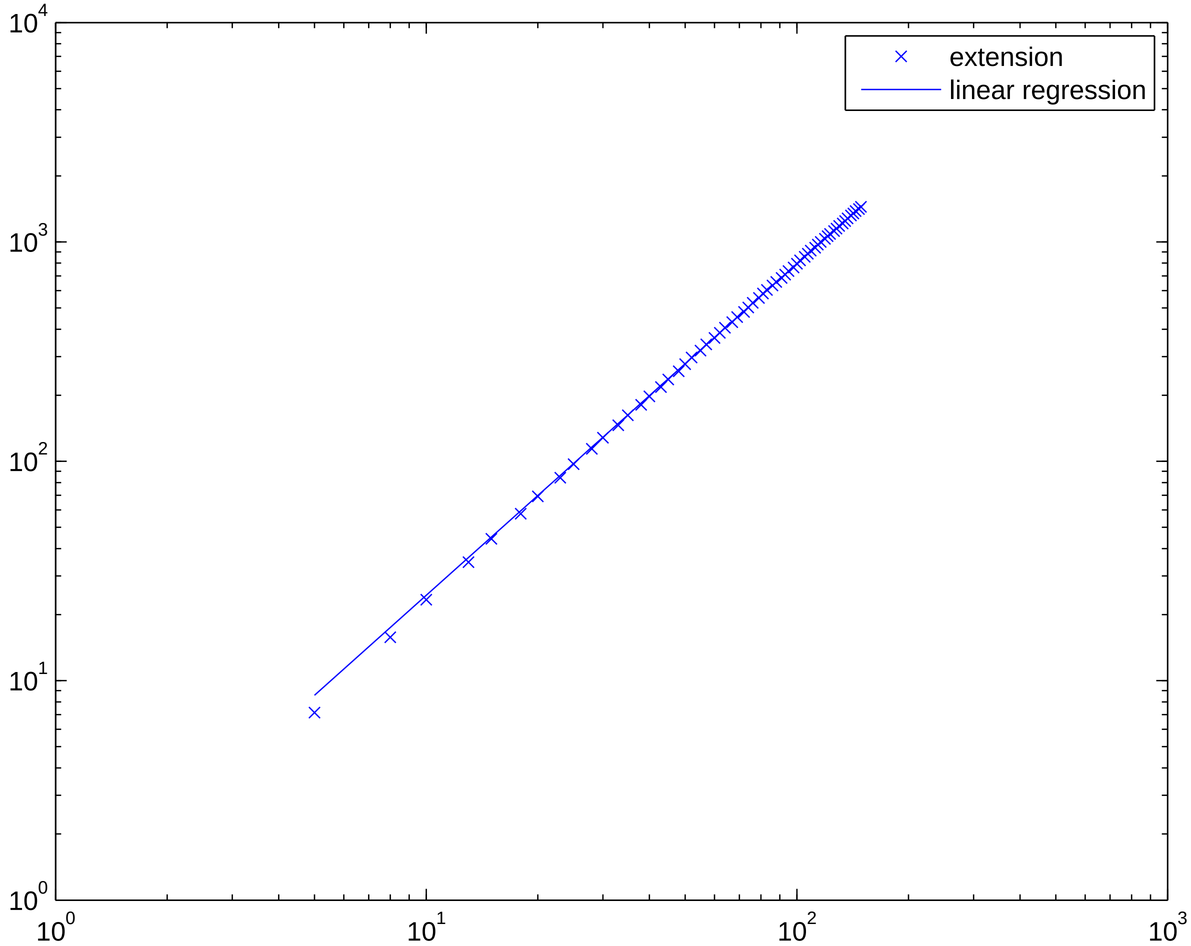


Adaptive algorithm applied to self avoiding walks on the 2 dimensional lattice.

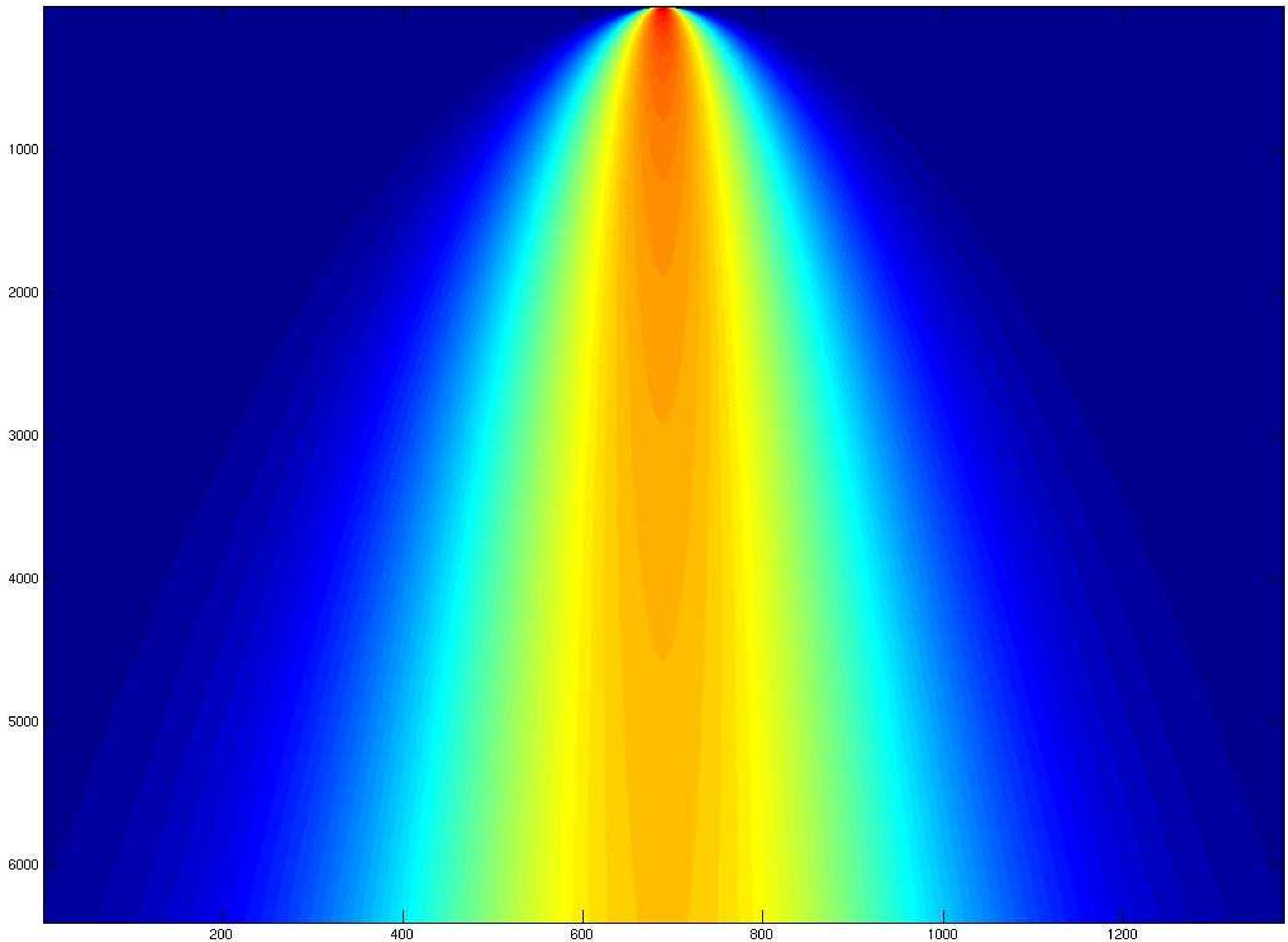




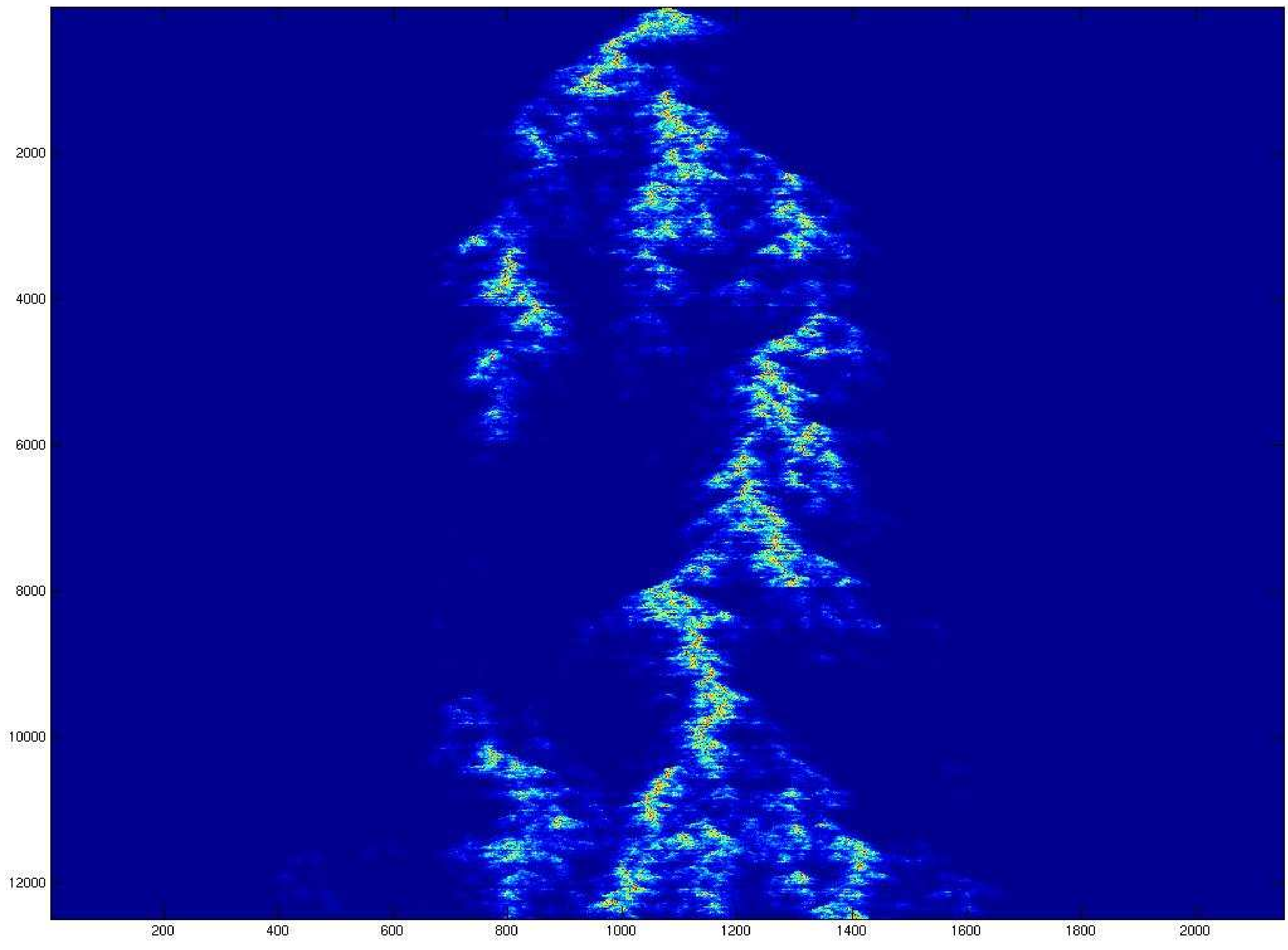
Examples of **saw**.



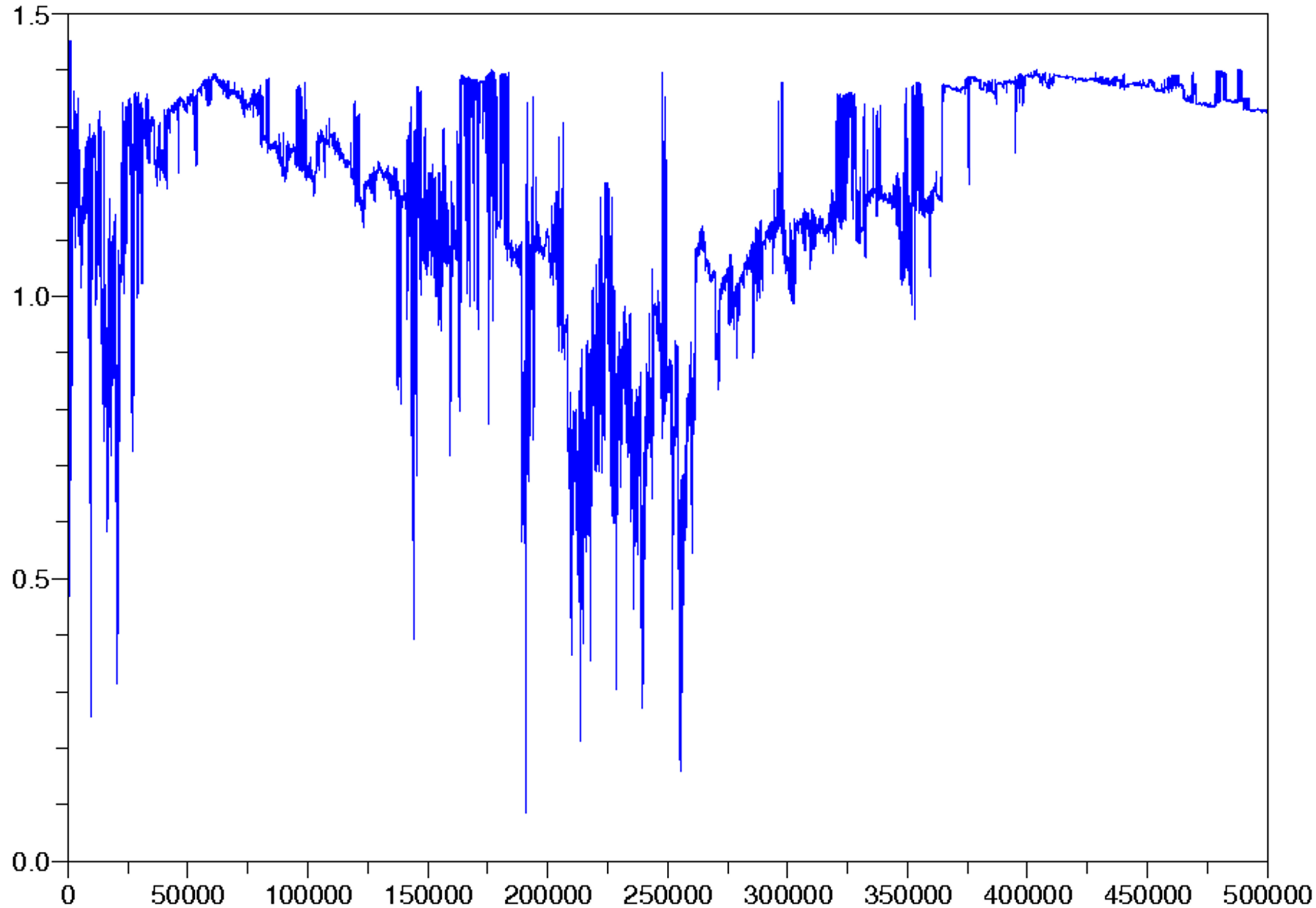
Extension exponent $\gamma \simeq 1.511$ (conjecture : 1.5).



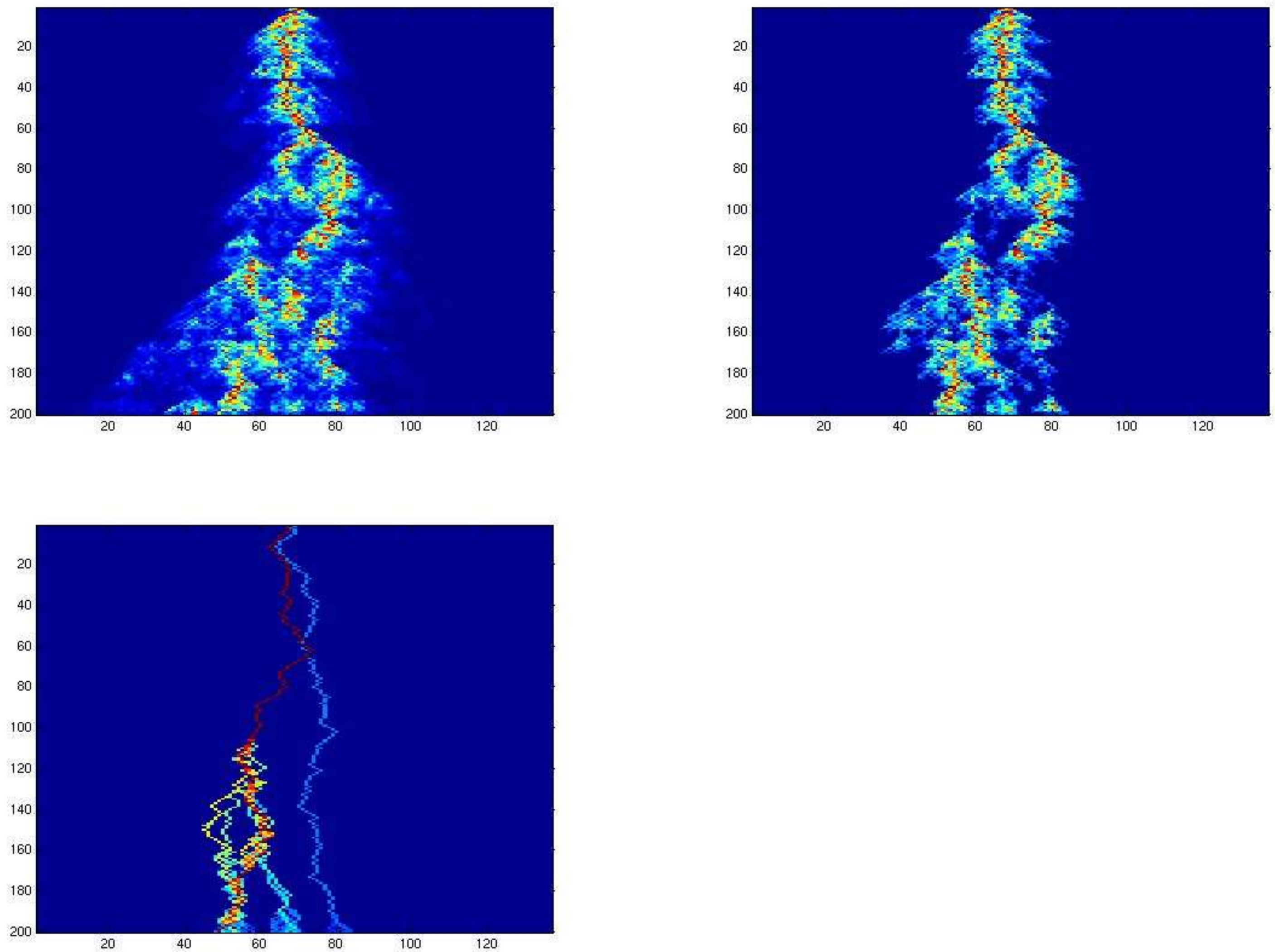
Standard random walk



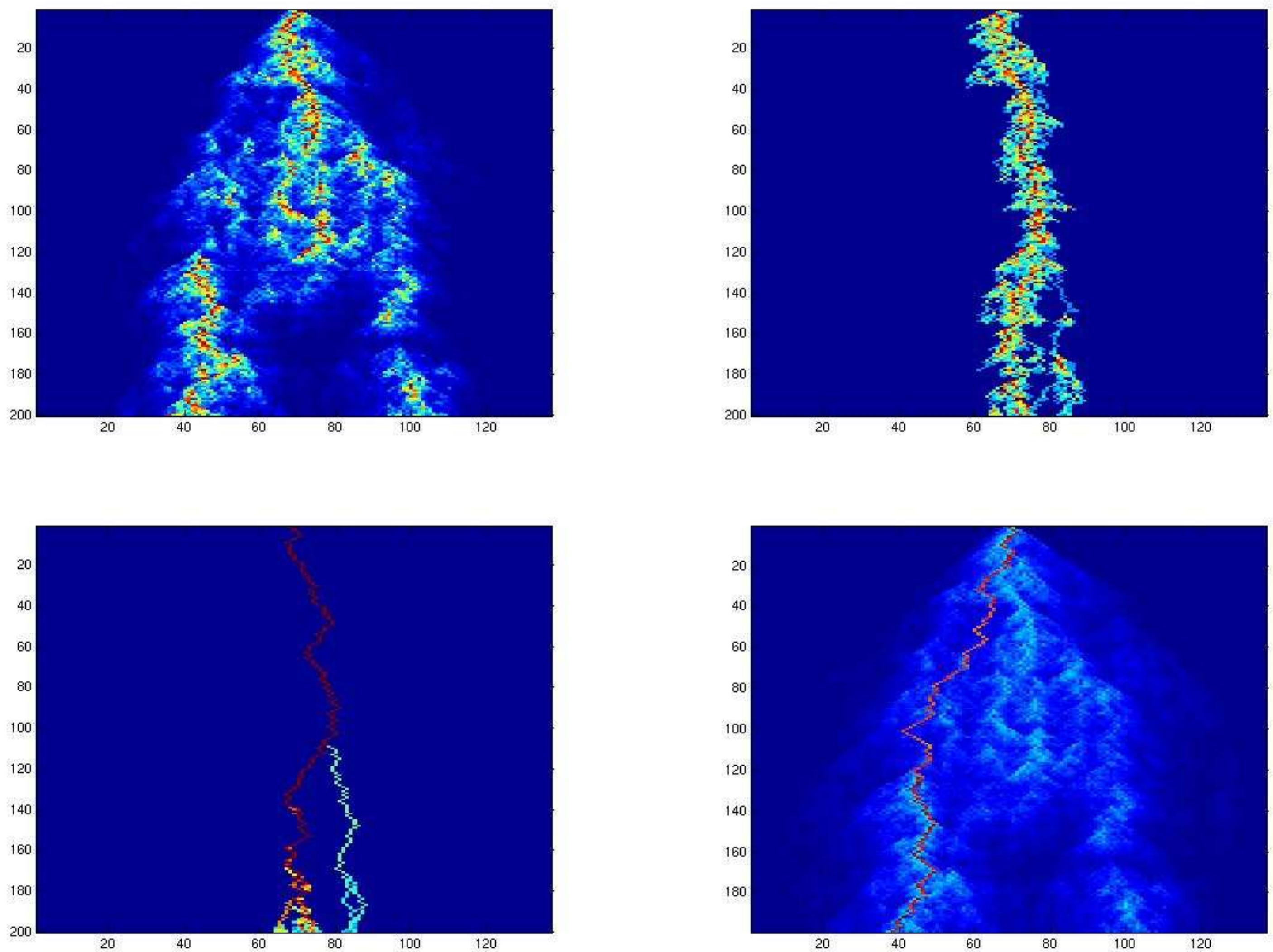
Random walk in strongly disordered medium.



Strongly disordered medium, $\log E(X_t^2)/\log t$ (conjecture : 4/3).



5000 particles, the law is well approximated.



1000 particles, the particles cannot track the path with maximum likelihood.