Efficient simulation of Fractional Brownian Motion for several values of the Hurst exponent

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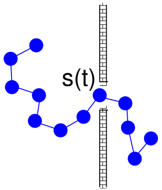
Outline

- Fractional Brownian motion
- Efficient algorithm for long walks
- Distribution of endpoints

Fractional Brownian Motion

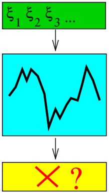
- Translocation of polymer through pore:
  viral injection of DNA
  DNA sequencing with engineered channels
  $s(t)$: position of chain at time t
  $s(t > 0) = 0$: absorbing boundary



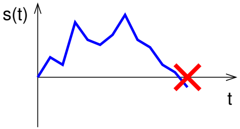
- Proposal [Zoia, Rosso, Majumdar, PRL 2009]:
  Described by fractional Brownian motion = Gaussian process with $\langle s(t_1)s(t_2)\rangle \sim t_1^{2H} + t_2^{2H} - |t_1 - t_2|^{2H}$
  $\Rightarrow \quad C(t_1 - t_2) = \langle [s(t_1) - s(t_2)]^2 \rangle \sim |t_1 - t_2|^{2H}$
  H: Hurst exponent: $H = 1/2$: Brownian motion,
  $H > 1/2$: correlation, $H < 1/2$: anticorrelation
  ($H = 1/(1 - \nu)$, where $R_g \sim N^{\nu}$ [Chuang, Kantor, Kadar 2001])
  Rescaled variable: $y(t) = s(t)/t^H$
  Prediction for $y \to 0$: $P(y) \sim y^{\phi}$ with $\phi = (1 - H)/H$

Random Walks

- Traditional method for (non-absorbed) walks of length L
  1. Vector ξ of $\tilde{L} \geq L$ Gaussian random numbers ξ_i
  2. For (approximate) correlation: Fourier transform
  3. Create walk $s(t) = \sum_{i<t} \xi_i$
  4. Accept if $s(t) \geq 0$ for all t (non absorbed)



- Problem:
  Success probability of non absorbance (*persistence*) $\sim t^{-\phi}$

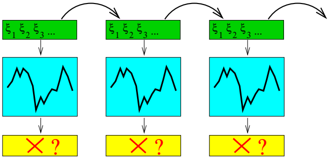


$L =$	10^1	10^3	10^5	10^7
$H = 2/3$ $\phi = 1/2$	0.3	0.03	0.003	0.0003
$H = 1/2$ $\phi = 1$	0.1	10^{-3}	10^{-5}	10^{-7}
$H = 1/4$ $\phi = 3$	10^{-3}	10^{-9}	10^{-15}	10^{-21}

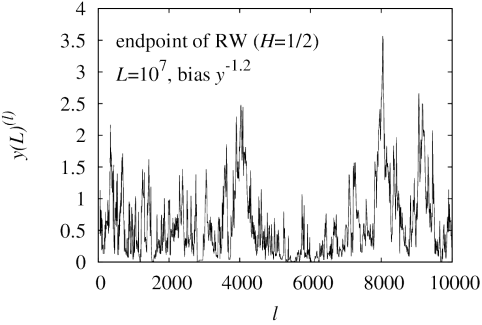
$\rightarrow$ becomes unefficient

Monte Carlo approach

- Basic idea:
  Markov chain of vectors
  $\xi^{(0)} \to \xi^{(1)} \to \xi^{(2)} \to \ldots$
  step: change fraction of $\xi^{(l)}$
  accept if walk not absorbed



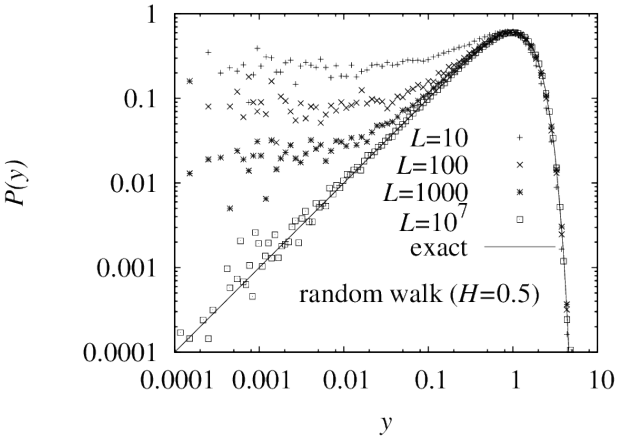
- Possible: additional reweighting $w \sim y^{\kappa}$ ($\kappa = -\phi \to$ "flat" sampling near $y = 0$)



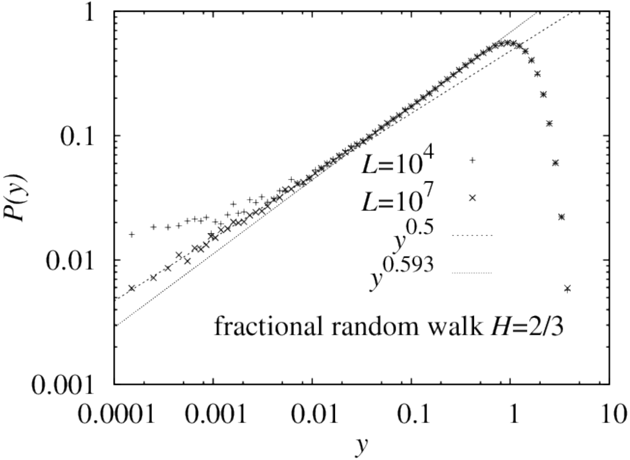
Results

Testcase pure Brownian motion ($H = 0.5$)
Distribution exactly known [Zoia, Rosso, Majumdar, PRL 2009]

$$P(y) = y \exp(-y^2/2)$$

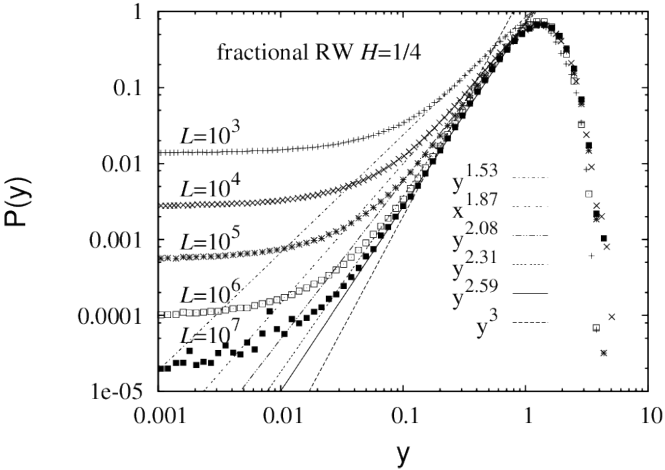


Superdiffusive case ($H = 2/3$)



$\longrightarrow$ prediction $\phi = (1 - H)/H = 1/2$ well found ($y \to 0$)
confirmed medium-scale behavior y^γ ($\gamma > \phi$)
predicted by [Wiese, Rosso, Majumdar, PRE 2012]

Subdiffusive case ($H = 1/4$)



$\longrightarrow$ strong finite-length effects

converges towards prediction $\phi = (1 - H)/H = 3$ ($y \to 0$)

in contrast to prediction $\phi = 2$ [Amitai, Kantor, Kadar, PRE 2010]

(simulation of effective model for $N = 257$ coupled particles)

Summary

- Fractional Brownian motion: translocation of polymers
- Using large-deviation/MC approach: walks $L = 10^7$ feasible
- (Angti-)correlations readily included
- Reweighting: focus to region of interest $\rightarrow$ better statistics
- $\phi(H = 0.25) \gg 2$: in favor of Zoia et al prediction

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