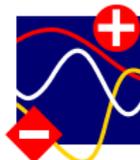


Efficient simulation of Fractional Brownian Motion for several values of the Hurst exponent

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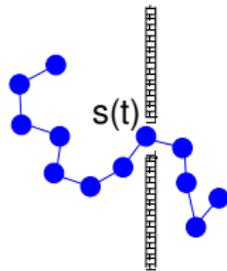


Outline

- 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

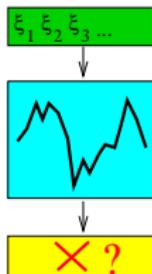


- Proposal [Zoia, Rosso, Majumdar, PRL 2009]:
Described by fractional Brownian motion = Gaussian process with $\langle s(t_1)s(t_2) \rangle \sim t_1^{2H} + t_2^{2H} - |t_1 - t_2|^{2H}$
 $\Rightarrow C(t_1 - t_2) = \langle [s(t_1) - s(t_2)]^2 \rangle \sim |t_1 - t_2|^{2H}$
- H : Hurst exponent: $H = 1/2$: 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 $y \rightarrow 0$: $P(y) \sim y^\phi$ with $\phi = (1 - H)/H$

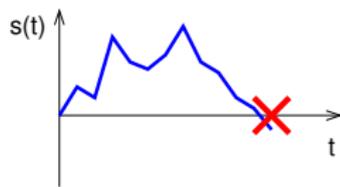
Random Walks

- 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*) $\sim t^{-\theta}$ ($\theta = 1 - H$)

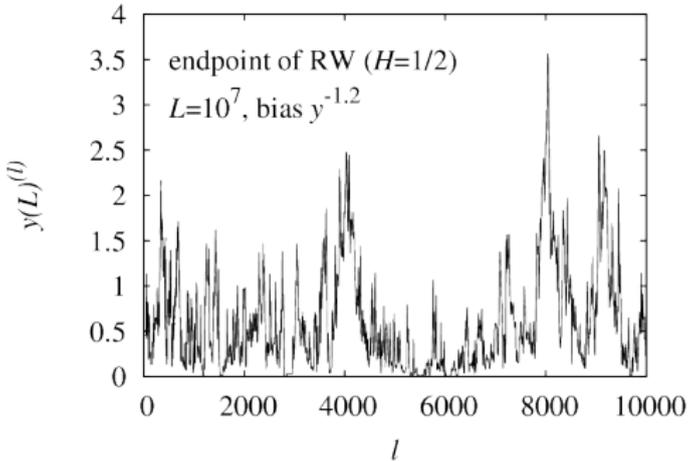
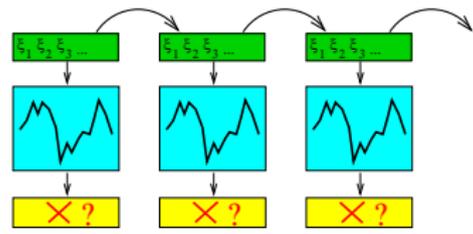


$L =$	10^1	10^3	10^5	10^7
$H = 2/3 \theta = 1/3$	0.5	0.1	$2 \cdot 10^{-2}$	$5 \cdot 10^{-3}$
$H = 1/2 \theta = 1/2$	0.3	0.03	$3 \cdot 10^{-3}$	$3 \cdot 10^{-4}$
$H = 1/4 \theta = 3/4$	0.2	0.006	$2 \cdot 10^{-4}$	$6 \cdot 10^{-6}$

→ becomes unefficient

Monte Carlo approach

- Basic idea:
 - Markov chain of vectors
 - $\xi^{(0)} \rightarrow \xi^{(1)} \rightarrow \xi^{(2)} \rightarrow \dots$
 - step: change fraction of $\xi^{(l)}$
 - accept if walk not absorbed
- Possible: additional reweighting $w \sim y^\kappa$ ($\kappa = -\phi \rightarrow$ "flat" sampling near $y = 0$)



Distribution of Endpoints

- Raw result \rightarrow
(simple $\leftrightarrow \kappa = 0$)
at low κ :
small endpoints preferred

- MC moves: $\xi \rightarrow \xi'$
change of displacement
 \rightarrow original probability

$P_0(\xi)$, additionally:

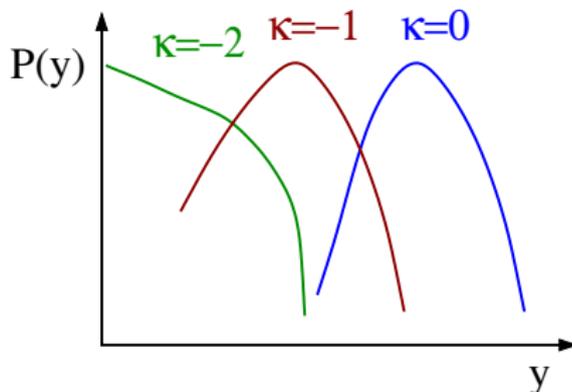
$\text{Pr}(\text{acceptance}) = \min\{1, (y(\xi')/y(\xi))^\kappa\}$

- \Rightarrow equilibrium distribution $Q_\kappa(\xi) = P_0(\xi)y(\xi)^\kappa / Z(\kappa)$
with $P_0(\xi) = \text{Gaussian etc}$, $Z(\kappa) = \sum_\xi P_0(\xi)y(\xi)^\kappa$

$\Rightarrow p_\kappa(y) = \sum_{\xi, y(\xi)=y} Q_\kappa(\xi) = \frac{y^\kappa}{Z(\kappa)} \sum_{\xi, y(\xi)=y} P_0(\xi)$

$\Rightarrow P(y) = p_\kappa(y)Z(\kappa)y^{-\kappa}$

[AKH, PRE 2001]

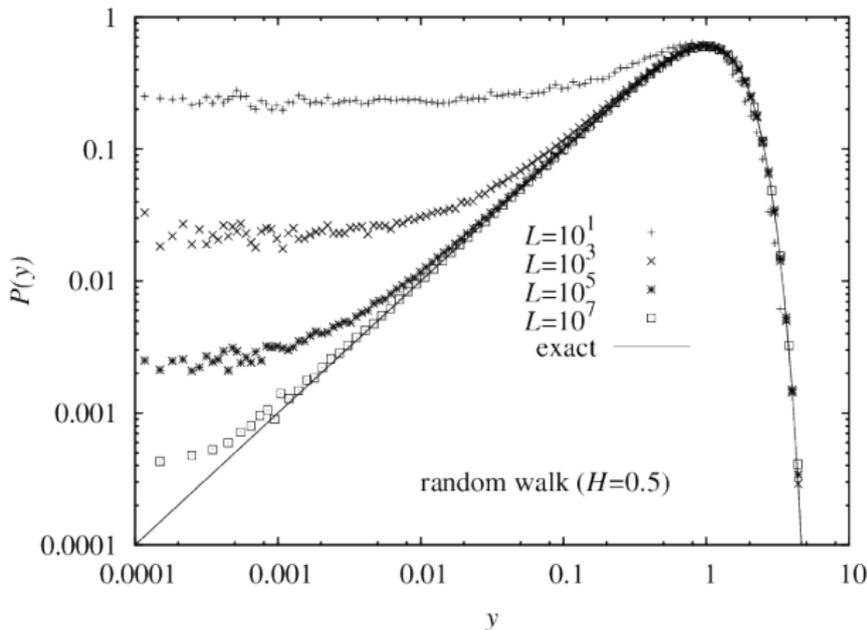


Results

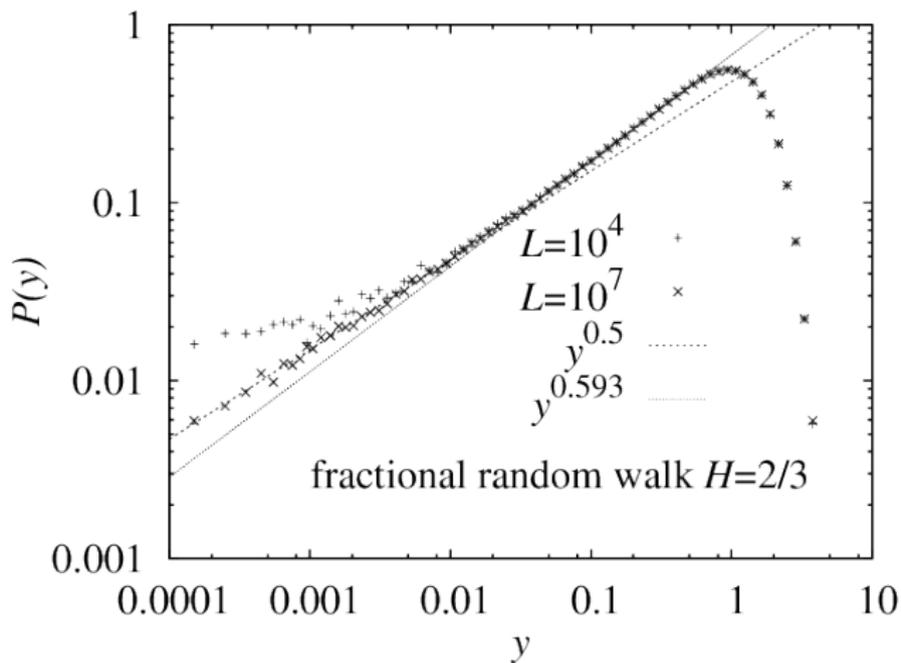
Testcase pure Brownian motion ($H = 0.5$)

Distribution exactly known [Zoja, Rosso, Majumdar, PRL 2009]

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

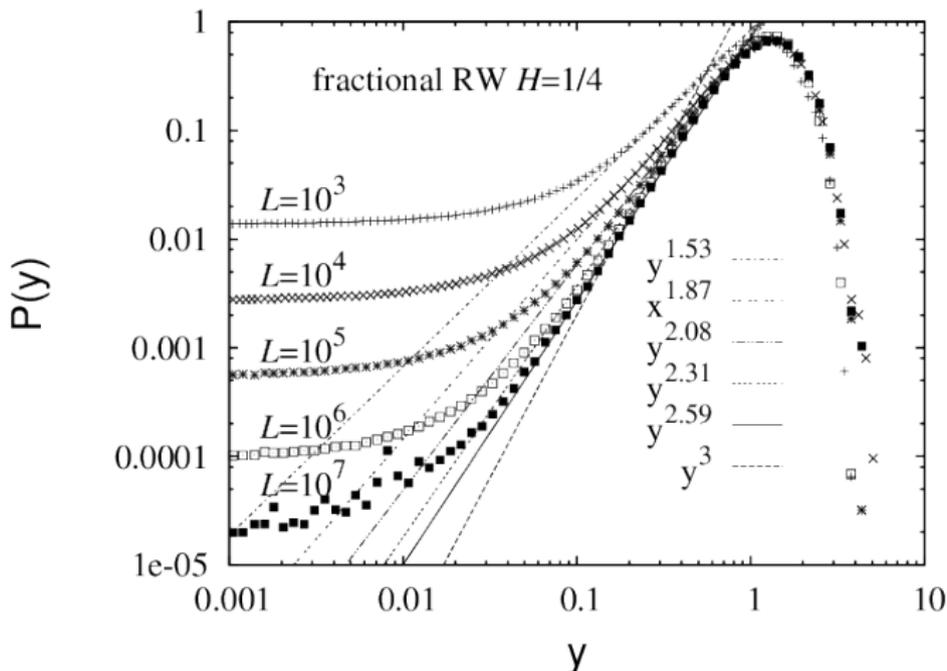


Superdiffusive case ($H = 2/3$)



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

Subdiffusive case ($H = 1/4$)



→ strong finite-length effects

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

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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A.K. Hartmann, [Practical Guide to Computer Simulations](#) (World Scientific, Singapore 2009)

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