Dynamics of Maximal Entropy Random Walk: Solvable Cases

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Introduction

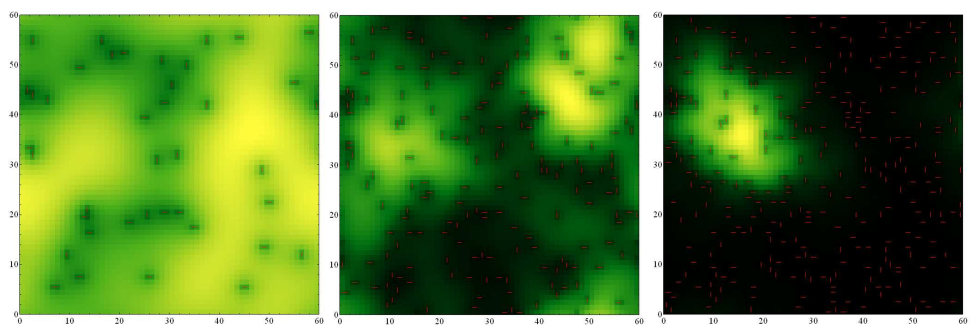

Figure 1: *Localisation of Maximal Entropy Random Walk's stationary probability on a 2D square defected lattice.*
Interactive demonstration at: HTTP://DEMONSTRATIONS.WOLFRAM.COM/GENERICRANDOMWALKANDMAXIMALENTROPYRANDOMWALK/

BROWNIAN MOTION has been proposed in the seminal works by Einstein and Smoluchowski as a microscopic theory for diffusive transport. Random walk (RW) models stemming from its discretization have been used across the whole realm of sciences, including diffusion processes in physical and biological contexts or information spread.

While Generic Random Walk (GRW) relies on locally equiprobable random moves, **Maximal Entropy Random Walk (MERW)**[1, 2] utilises equiprobable paths (a natural choice in the path-integral formalism of quantum mechanics) and is derived from the principle of maximal entropy. We present curious features of MERW:**localisation**, extremely fast **dynamics** (on Cayley tree) or quantum **tunnelling**-like behaviour (on ladder graphs with defects).

It has been shown that networks selected according to this principle are more robust against mutation[4] and might model biological evolution[5]. The unique features of MERW offer also the prospect of modelling spin glasses or information engineering.

Definitions

	GENERIC RW	MAXIMAL ENTROPY RW
TRANSITION MATRIX	$P_{ba} = \frac{A_{ba}}{k_a}$	$P_{ba} = \frac{A_{ba}}{\lambda_1}\frac{\psi_{1b}}{\psi_{1a}}$
PATH PROBABILITY	$P\left(\gamma_{a_t a_0}\right) = \prod_{i=0}^{t-1}\frac{1}{k_i}$	$P\left(\gamma_{a_t a_0}\right) = \frac{1}{\lambda_1{}^t}\frac{\psi_{1a_t}}{\psi_{1a_0}}$
STATIONARY STATE	$\pi_a = \frac{k_a}{2L}$	$\pi_a = \psi_{1a}{}^2$
ENTROPY PRODUCTION	$h = \frac{1}{2L}\sum_a k_a \ln k_a$	$h = \ln\lambda_1$

DISCRETE-TIME RANDOM WALK ON A GRAPH (undirected finite connected) is a Markov chain.

A_{ba} adjacency matrix of the graph

λ_i, ψ_i eigenvalues and eigenvectors of adjacency matrix $\sum_b A_{ba}\psi_{ib} = \lambda_i\psi_{ia}, \sum_b \psi_{ib}{}^2 = 1$

P_{ba} transition probability of a particle hopping from node a to node b, symmetric, constant w.r.t. time. Transition matrix obeys $P_{ba} \geq 0, \sum_b P_{ba} = 1$

$p_{ba}(t)$ probability that a particle starting from a is found at b after time t. $p_{ba}(t+1) = \sum_c P_{bc}p_{ca}(t)$

$P\left(\gamma_{a_t a_0}\right) = P_{a_t a_{t-1}} \ldots P_{a_2 a_1} P_{a_1 a_0}$ for fixed endpoints a_0, a_t is the probability of a given path

For the initial condition $p_{ba}(0) = \delta_{ba}$ one obtains:

$$p_{ba}(t) = \left(P^t\right)_{ba}$$

We assume that $p_{ba}(t)$ goes to a limiting (stationary) distribution $\lim_{t\to\infty} p_{ba}(t) = \pi_b$ independently of the initial point a, hence:

$$\pi_b = \sum_a P_{ba}\pi_a, \quad \sum_a \pi_a = 1$$

References

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[4] L. Demetrius, V.M. Gundlach and G. Ochs, *Theor. Popul. Biol.* **65** (2004) 211225.

[5] L. Demetrius, T. Manke, *Physica A* **346** (2005) 682696.

Acknowledgments

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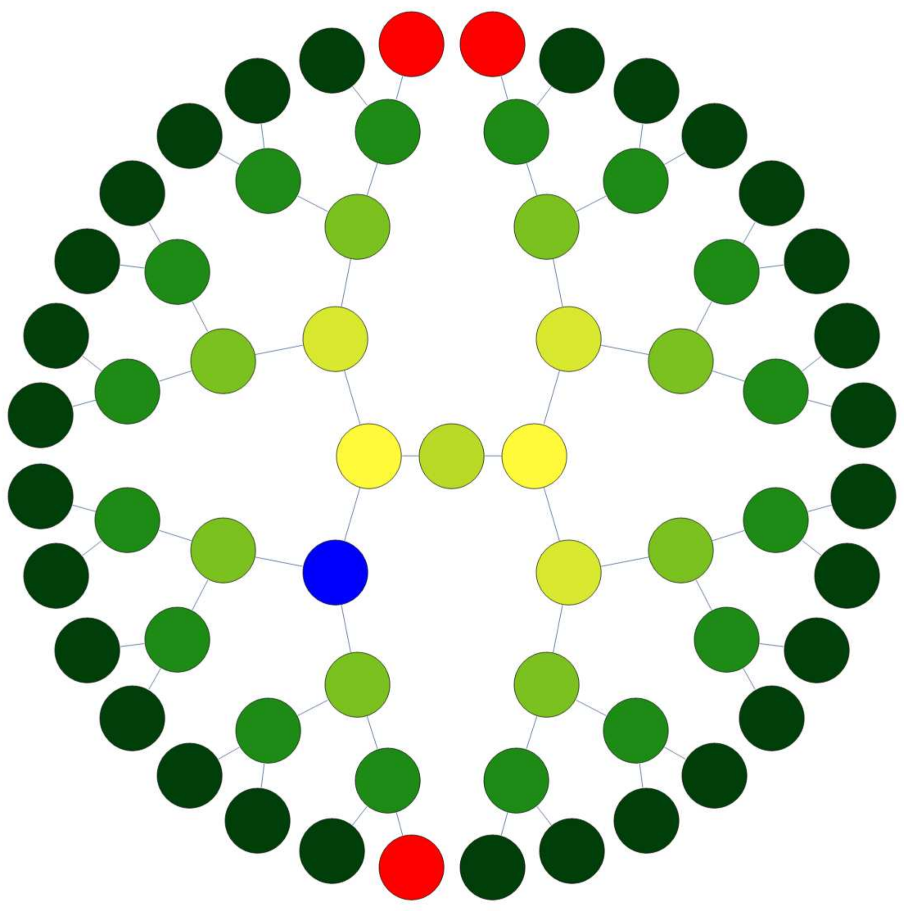


Cayley tree

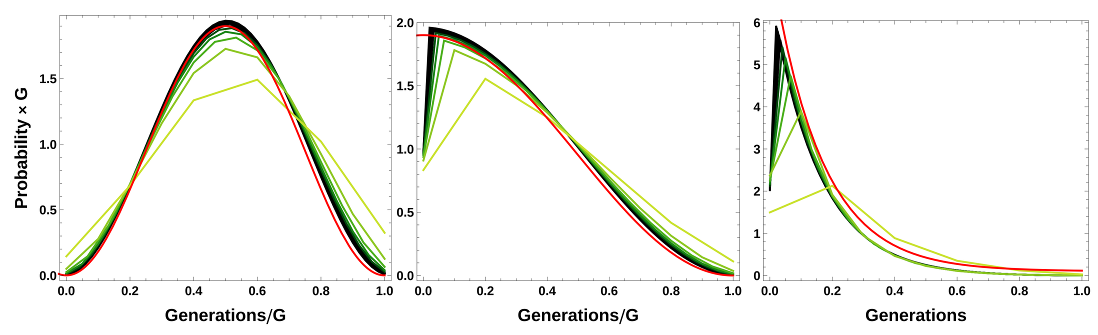
RELAXATION	GRW	MERW
GENERIC	$\tau \simeq \frac{2k}{k^2+1}\frac{\left(2+k^G\right)^2}{1+k^G} \sim \boldsymbol{k^G}$	$\tau \simeq \frac{2k-k_r}{k_r}\boldsymbol{G^3}$
FAST	$\tau \simeq a - \frac{a^2\pi^2}{2}\frac{1}{G^2} \to$ **const.**	$\tau \simeq \frac{2}{3\pi^2}\boldsymbol{G^2}$
ON A CHAIN	$\tau \sim G^2$	$\tau \sim G^3$

G number of generations of a Cayley tree

k branching number (ratio of nodes of the next generation and the given one)

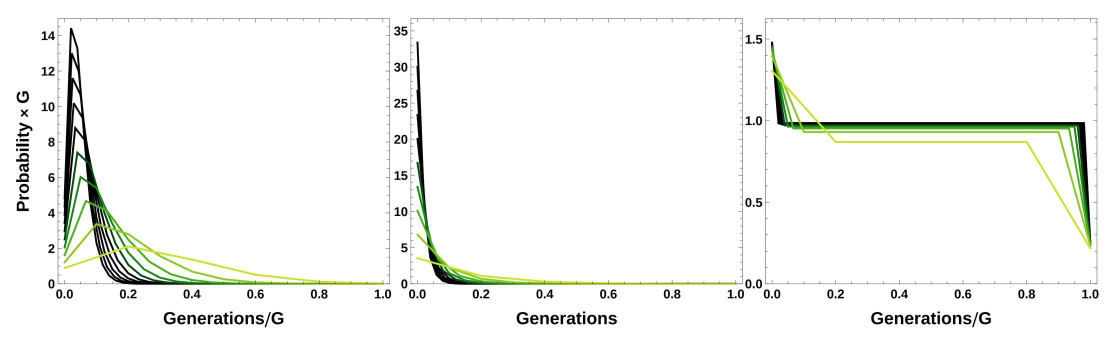
k_r the degree of the root

τ relaxation time (characteristic time scale of an exponential approach to the stationary state)



(a) (b) (c)

Figure 2: ***Stationary state probability per generation*** *for MERW, $k = 3$. (a) $k_r = 2$, distribution approaches $\sim \sin(\pi G)^2$ (red line) (b) $k_r = 6$, distribution approaches $\sim \cos(\pi/2G)^2$ (c) $k_r = 10$, distribution approaches $\sim \exp(-G)$. The darker the line, the more generations the tree has (5-50, the number has been normalised).*



(a) (b) (c)

Figure 3: ***Stationary state probabilities per node*** *for MERW (a)-(b) and GRW (c) for $k = 3$. (a) $k_r = 2$, (b) $k_r = 6$, (c) $k_r = 6$ for GRW. Note the difference between flat distribution of a diffusion and one concentrated around highest degree nodes for MERW.*

ADJACENCY MATRIX of a Cayley tree has a **hierarchy of eigenvalues** [3]:

$$\lambda(l, r) = 2\sqrt{k}\cos\left(\frac{r\pi}{l+2}\right), r = 1, ..., l+1;\ l = 0, ..., G-1.$$

The largest eigenvalue:

$$\lambda(G, 1) \simeq 2\sqrt{k}\cos\left(\pi \Big/ \left(G + \frac{2k}{2k-k_r}\right)\right).$$

The elements of eigenvector to the largest eigenvalue $\psi_{1l}^2, l = 1, \ldots, G$ give stationary state of MERW.

RELAXATION TIME τ is associated with **second largest eigenvalue** λ_2, which can be seen upon spectral decomposition of A_{ba}:

$$\left(P^t\right)_{ba} = \frac{(A^t)_{ba}}{\lambda_{\max}^t}\frac{\psi_{1b}}{\psi_{1a}} = \frac{\psi_{1b}}{\psi_{1a}}\sum_{i=1}^n\left(\frac{\lambda_i}{\lambda_1}\right)^t\psi_{ib}\psi_{ia},$$

where t denotes time (number of steps of a random walk).

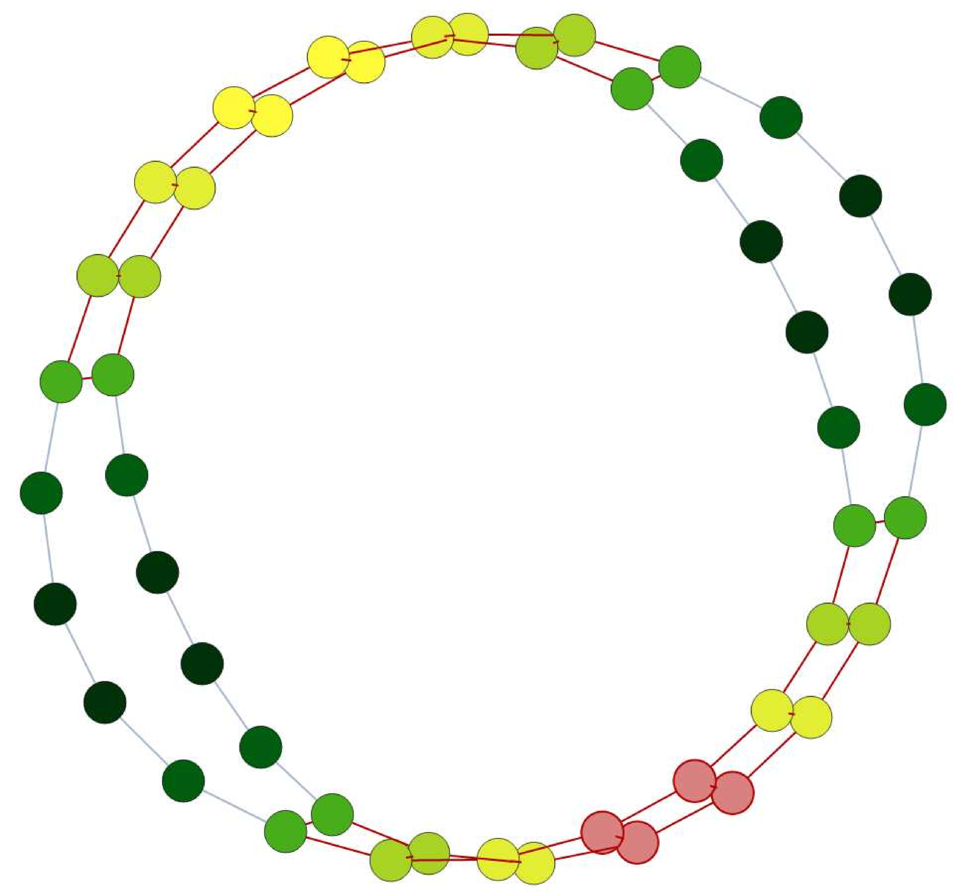
MERW $\lambda_2 = \lambda(G-1, r) = 2\sqrt{k}\cos\left(\frac{\pi}{G+1}\right)$

GRW $\lambda_2 = 2\sqrt{\frac{k}{(k+1)^2}}\left(1 - \frac{(k-1)^2}{(k+1)^2(1+2k^{-G})}\right)^{-1/2}$

There is also a faster relaxation! (If we measure probability at the central vertex or take symmetric initial conditions.)

MERW $\lambda(G, 2) = 2\sqrt{k}\cos\left(\frac{2\pi}{G+2}\right)$ for $k_r \neq 2k, k > 1, k_r > 1$

GRW $\lambda(G, 2) = 2\sqrt{\frac{k}{(k+1)^2}}\cos\left(\frac{\pi}{G}\right)$



Ladder graph

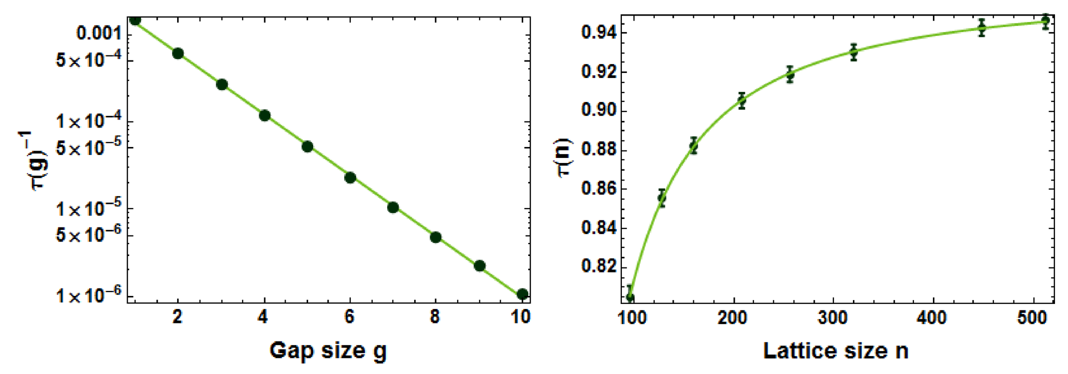
GRW	$\tau(n, g) = c \cdot \boldsymbol{n^d}, d =$ const. $= 2$
MERW	$\tau(n, g) = \exp\left(\left(cn^{-1/\nu} - c_\infty\right) \cdot \boldsymbol{g}\right)$

n number of nodes in a ladder (48-512)

g gap size (number of deleted rungs, 1-10)

τ relaxation time (characteristic time scale of an exponential approach to the stationary state)

c, c_∞, d constants



(a) (b)

Figure 4: ***Maximal Entropy Random Walk**: (a) Logarithmic plot of shows an **exponential dependence of the relaxation time on the gap size** (an exemplary system size, $n = 96$) reminding of quantum tunneling, (b) the dependence of the relaxation time on the system size.*

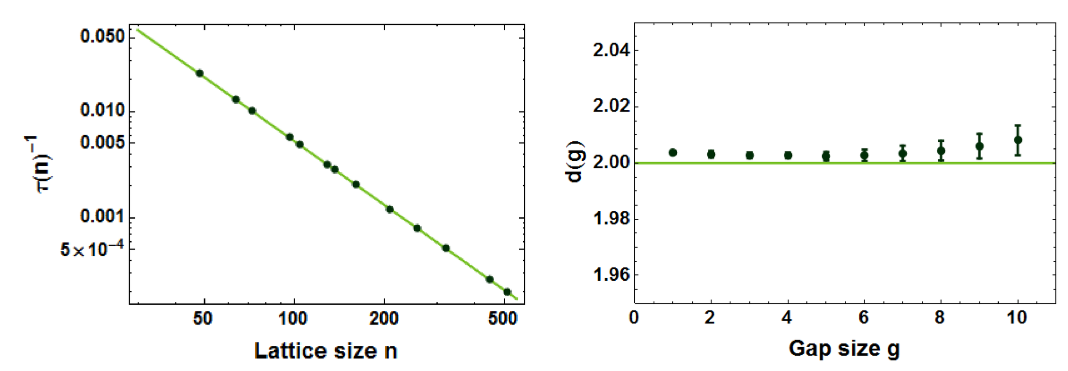


Figure 5: ***Generic Random Walk**:(a) log-log plot shows power law dependence of relaxation time, expected for a diffusion process, (b) the exponent of the power law is independent of the gap size.*

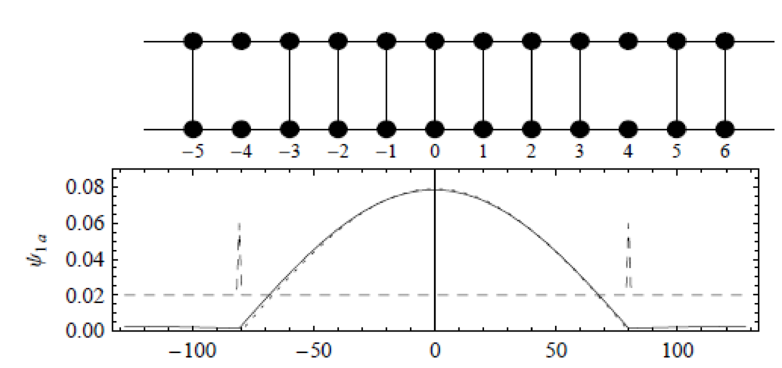


Figure 6: ***Stationary probability** for intact regions of uneven size shows **localisation** in the larger region.*

SYMMETRIC CASE is considered: two equal regions intact, two equal gaps. Initial probability 1 at the centre of one region. We measure the probability P_Σ summed over the whole region. We fit the numerical results to exponential dependence on time t: $P_\Sigma(t) \sim \exp(-a(t-b))$.

THE STATIONARY SOLUTION for MERW is obtained by solving the tight-binding equation:

$$(H\psi_1)_a = (-\Delta\psi_1)_a + V_a\psi_{1a} = E_1\psi_{1a},$$

with $V_a = k_{\max} - k_a, E_1 = k_{\max} - \lambda_1$.

For ladder graph with defects:

$$2\psi_{1a} - \psi_{1a-1} - \psi_{1a+1} + V_a\psi_{1a} = E_1\psi_{1a},$$

where $E_1 = 3 - \lambda_{max}$ and $V_a = 0$ or 1 (rung present or absent).