Reinforced random walks and statistical physics

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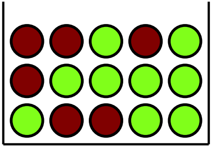
Outline

Pólya urn: definition

- Introduced by Eggenberger and Pólya in 1923: "Über die Statistik verketteter Vorgänge", i.e. "On statistics of linked behaviors".
- Urn with balls of two colors: green and red.
- Initially a, resp. $b > 0$ balls of green, red color.
- G_n, R_n numbers of balls of green, red color added until n-th draw, $G_0 = R_0 = 0$.
- Reinforcement rule: pick one ball at random and put it back together with another ball of same color:

$$\mathbb{P}(G_{n+1} = G_n + 1 \mid G_k, R_k \; k \leqslant n) = \frac{a + G_n}{a + G_n + b + R_n} =: \alpha_n.$$



Pólya urn: results and statistical view

Theorem

- *$(\alpha_n)_{n\in\mathbb{N}}$ converges a.s. to a random variable $\alpha \in (0,1)$.*
- *$\alpha \sim Beta(a,b)$.*
- *(de Finetti, by exchangeability) Conditionally on α, $(G_{n+1} - G_n)_{n\in\mathbb{N}}$ is an i.i.d. sequence of Bernoulli random variables with success probability α.*

Statistical view

- Given sequence of i.i.d. Bernoulli random variables with unknown random success probability α, how can we estimate α?
- Bayesian approach: choose prior distribution on random variable α.
- If prior on α is $Beta(a,b)$, then

$$\mathcal{L}((\mathbf{1}_{\text{success at time } n})_{n\in\mathbb{N}}) = \mathcal{L}((G_n)_{n\in\mathbb{N}}),$$

where $(G_n)_{n\in\mathbb{N}}$ defined from Pólya urn above.

Statistical view of Pólya urn: consequences

- Hence, if the prior on α is $Beta(a, b)$, then the posterior distribution after p successes and q failures is $Beta(a + p, b + q)$.
- The prior and posterior are in the same family of probability (beta) distributions, and are thus called conjuguate priors.
- (G_n, R_n) is a sufficient statistic for α at time n:
  - Informally: no other statistic that can be calculated from the sequences $(G_k)_{k \leqslant n}$ and $(R_k)_{k \leqslant n}$ provides any additional information as to the value of the parameter α.
  - Formally: given statistical model $\{P_\alpha : \alpha \in (0, 1)\}$, where P_α is the law of i.i.d. sequences with success probability α, $P_\alpha((G_k, R_k)_{k \leqslant n} | (G_n, R_n))$ does not depend on α.
  - It is a minimal sufficient statistics: there is no sufficient statistics that needs less information.

Edge-Reinforced Random Walk (Coppersmith and Diaconis, 1986)

- $G = (V, E)$ non-oriented locally finite graph
- $a_e > 0$, $e \in E$, initial weights

• Edge-Reinforced Random Walk (ERRW) (X_n) on V : $X_0 = i_0$ and, if $X_n = i$, then

$$\mathbb{P}(X_{n+1} = j \,|\, X_k,\, k \leqslant n) = \mathbb{1}_{\{j \sim i\}} \frac{Z_n(\{i,j\}))}{\sum_{k \sim X_n} Z_n(\{i,k\})}$$

where

$$Z_n(\{i,j\}) = a_{i,j} + \sum_{k=1}^{n} \mathbb{1}_{\{X_{k-1}, X_k\} = \{i,j\}}.$$

- a_e small: strong reinforcement
- a_e large: small reinforcement

First results on Edge-Reinforced random walk ('86-'09)

- Partially exchangeable: probability of path only depends on numbers of crossings of edges
- Diaconis and Freedman'80: partial exchangeability $\Longrightarrow$ ERRW is a Random Walk in Random Environment (RWRE)
- Explicit computation of mixing measure: Coppersmith-Diaconis '86, Keane-Rolles '00
- Pemantle '88: recurrence/transience phase transition on trees
- Merkl Rolles '09: recurrence on a $2d$ graph (but not $\mathbb{Z}^2$)

Edge Reinforced Random Walks (ERRW): Limit measure (Diaconis and Coppersmith, 1986, Keane and Rolles, 2000)

Theorem

- $(Z_n(e)/n)_{n\in\mathbb{N}}$ *converges a.s. to a random vector* $X = (X_e)_{e\in E}$
- *Conditionally on* x, *ERRW is a reversible Markov chain* P_x *with jump probability* x_{ij}/x_i *from* i *to* j, $x_i = \sum_{k\sim i} x_{ik}$.
- X *has the following density w.r.t to surface measure on the simplex* $\{\forall e \in E,\ x_e > 0\ \sum_{e\in E} x_e = 1\}$

$$\gamma(i_0,\alpha)\sqrt{x_{i_0}}\frac{\prod_{e\in E} x_e^{a_e-1}}{\prod_{i\in V} x_i^{\frac{1}{2}a_i}}\sqrt{D(x)}$$

Edge Reinforced Random Walks (ERRW): Limit measure (Diaconis and Coppersmith, 1986, Keane and Rolles, 2000)

We have

$$\gamma(i_0, \alpha) = \frac{2^{1-|V|+\sum_{e\in E} a_e}}{\sqrt{\pi}^{|V|-1}\Gamma(|V|)} \frac{\prod_{i\in V} \Gamma(\frac{1}{2}(a_i + 1 - \mathbb{1}_{i=i_0}))}{\prod_{e\in E} \Gamma(a_e)},$$

and

$$D(y) = \sum_{T\in\mathcal{T}} \prod_{e\in T} y_e,$$

where $\mathcal{T}$ is the set of (non-oriented) spanning trees of G.

Edge-Reinforced random walk (ERRW): statistical view

- Given reversible Markov Chain P_x with unknown random vector x, how can we estimate x?
- Bayesian approach: assume prior on x is $\mathbb{P}_{i_0,a}$, then law is the one of ERRW by definition
- Hence, the posterior distribution after n first steps is given by $\mathbb{P}_{X_n,(Z_n(e))_{e\in E}}$.
- Thus prior and posterior are conjuguate priors.
- (Diaconis and Rolles, 2006) $(Z_n(e) - Z_0(e))_{e\in E}$ is a minimal sufficient statistic for the model, also provide method of simulation of the posterior.

ERRW and statistical physics: ERRW $\longleftrightarrow$ VRJP (I)

Let $(W_e)_{e\in E}$ be conductances on edges, $W_e > 0$.
VRJP $(Y_s)_{s\geqslant 0}$ is a continuous-time process defined by $Y_0 = i_0$ and, if $Y_s = i$, then, conditionally to the past,

$$Y \text{ jumps to } j \sim i \text{ at rate } W_{i,j} L_j(s),$$

with

$$L_j(s) = 1 + \int_0^s \mathbb{1}_{\{Y_u = j\}} du.$$

Proposed by Werner and first studied **on trees** by Davis, Volkov ('02,'04).

ERRW and statistical physics: ERRW $\longleftrightarrow$ VRJP (II)
Random conductances $(W_e)_{e \in E}$

Theorem (T. '11, Sabot-T. '15)

$$\text{ERRW } (X_n)_{n\in\mathbb{N}} \text{ with weights } (a_e)_{e\in E} \overset{\text{"law"}}{=} \text{VRJP } (Y_t)_{t\geqslant 0} \text{ with conductances } W_e \sim \Gamma(a_e) \text{ indep. (at jump times)}$$

- Similar equivalence applies to any linearly reinforced RW on its continuous time version (initially proved for VRRW, T'. 11)

VRJP $\longleftrightarrow$ SuSy hyperbolic sigma model in QFT (I)
Fixed conductances $(W_e)_{e\in E}$, G finite

- $G=(V,E)$ finite, $N:=|V|$
- $\mathbb{P}_{i_0}$ law of $(Y_s)_{s\geqslant 0}$ starting from $i_0\in V$
- Change time at vertices $\ell_i=L_i^2-1$, $i\in V \longrightarrow (Z_t)_{t\geqslant 0}$

$$B(s)=\sum_{i\in V}(L_i(s)^2-1),\quad Z_t=Y_{B^{-1}(t)}.$$

Theorem (ST '15)

Under $\mathbb{P}_{i_0}$, $(Z_t)_{t\geqslant 0}$ is a mixture of Markov jump processes (MJPs) starting from i_0 with jump rate from i to j

$$\frac{1}{2}W_{i,j}e^{U_j-U_i}.$$

Let $\mathcal{Q}^{i_0,W}$ be the mixing measure on $U=(U_i)_{i\in V}$.

VRJP $\longleftrightarrow$ SuSy hyperbolic sigma model in QFT (II) Fixed conductances $(W_e)_{e\in E}$, G finite (ST '15 continued)

The measure $\mathcal{Q}^{i_0,W}(du)$ has density on $\mathcal{H}_0=\{(u_i),\ \sum u_i=0\}$

$$\frac{N}{(2\pi)^{(N-1)/2}}e^{u_{i_0}}e^{-H(W,u)}\sqrt{D(W,u)},$$

where

$$H(W,u)=2\sum_{\{i,j\}\in E}W_{i,j}\sinh^2((u_i-u_j)/2)$$

and

$$D(W,u)=\sum_{T\in\mathcal{T}}\prod_{\{i,j\}\in T}W_{\{i,j\}}e^{u_i+u_j},$$

$\mathcal{T}$ is the set of (non-oriented) spanning trees of G.

VRJP $\longleftrightarrow$ SuSy hyperbolic sigma model in QFT (III)
Fixed conductances $(W_e)_{e \in E}$, G finite (Merkl-Rolles-T.'19)

- $\mathcal{Q}^{i_0,W}(du)$ marginal of Gibbs "measure" on supermanifold extension $H^{2|2}$ of hyperbolic plane with action $A_W(v,v) = \sum_{i,j} W_{ij}(v_i - v_j, v_i - v_j)$, taken in horospherical coordinates after integration over fermionic variables.

- Merkl-Rolles-T.'19: Other variables in extension SuSy model arise on two different time scales as limits of
  - local times on logarithmic scale
  - rescaled fluctuations of local times
  - rescaled crossing numbers
  - last exit trees of the walk (tree version of fermionic variables)
- Bauerschmidt-Helmuth-Swan '19 (AP and AIHP): very nice interpretation of in terms of Brydges-Fröhlich-Spencer-Dynkin isomorphism for the supersymmetric field

Linear ERRW and statistical physics: other links
Fixed conductances $(W_e)_{e\in E}$, G finite

- Random Schrödinger operator (Sabot-T.-Zeng '17): let

$$\beta_i = \frac{1}{2}\sum_{j\sim i} W_{ij} e^{u_j - u_i} + \mathbf{1}_{i_0}\gamma,$$

  $\gamma \sim \Gamma(1/2)$ indep. of u: β field 1-dependent on $\{H_\beta > 0\}$,
  $H_\beta = -\Delta^W + 2\beta$, Δ^W discrete Laplacian
  $\longrightarrow e^{u_\cdot}$ proportional to **Green function** $H_\beta^{-1}(i_0, .)$.
- Ray-Knight second generalised Theorem (Sabot-T.'16, Lupu-Sabot-T'19): reversed VRJP $\tilde{Y}$, with jump rate $W_{ij}L_j(t)$ from i to j

$$L_i(t) = \varphi_i - \int_0^s \mathbb{1}_{\{\tilde{Y}_u = j\}} du$$

  enables to invert Ray-Knight identity in a magnetized version.

ERRW/VRJP and statistical physics: implications

Using link with QFT and localisation/delocalisation results of Disertori, Spencer, Zirnbauer '10 :

Theorem (ST'15, Angel-Crawford-Kozma'14, G bded degree)

ERRW (resp.VRJP) is positive recurrent at strong reinforcement, i.e. for a_e (resp. W_e) uniformly small in $e \in E$.

Theorem (ST'15, Disertori-ST'15, $G = \mathbb{Z}^d$, $d \geqslant 3$)

ERRW (resp. VRJP) is transient at weak reinforcement, i.e. for a_e (resp. W_e) uniformly large in $e \in E$.

Using link with Random Schrödinger operator:

Theorem (Sabot-Zeng '19, Sabot -19, Merkl-Rolles '09)

ERRW with constant weights $a_e = a$ (resp. $W_e = W$) is recurrent in dimension 2.

*-Edge-Reinforced Random Walk motivation : Reversible k-dependent Markov chains

- (Y_i) k-dependent Markov chain on S finite (i.e. law of Y_{n+1} depends only on $(Y_{n-k+1}, \ldots, Y_n)$).
- Equivalent to Markov chain (X_n) on the (directed) de Bruijn graph $G = (V = S^k, E)$ with

$$\omega = (i_1, \ldots, i_k) \to \tilde{\omega} = (i_2, \ldots, i_{k+1})$$

  with transition rate $p(\omega, \tilde{\omega})$, and invariant measure $\pi(\omega)$.

The k-dependent Markov chain is called reversible if

$$(Y_1, \ldots, Y_n) \stackrel{law}{=} (Y_n, \ldots, Y_1).$$

as soon as $(Y_1, \ldots, Y_k) \sim \pi$. This is equivalent to the "modified" balance condition

$$\pi(\omega) p(\omega, \tilde{\omega}) = \pi(\tilde{\omega}^*) p(\tilde{\omega}^*, \omega^*),$$

where ω^* is the flipped k-string $\omega^* = (i_k, \ldots, i_1)$.

General framework

- $G = (V, E)$ directed graph with involution $*$ on V s.t.

$$(i,j) \in E \Rightarrow (j^*, i^*) \in E$$

- $\alpha_{i,j} > 0$, $(i,j) \in E$ such that $\alpha_{i,j} = \alpha_{j^*,i^*}$.

We call $\star$-ERRW with initial weights (α_e), the discrete time process (X_n) defined by

$$\mathbb{P}(X_{n+1} = j \,|\, X_k,\ k \leqslant n) = \mathbb{1}_{\{X_n \to j\}} \frac{Z_n((X_n, j))}{\sum_{l, X_n \to l} Z_n((X_n, l))}$$

where

$$Z_n((i,j)) = \alpha_{i,j} + N_{i,j}(n) + N_{j^*,i^*}(n)$$

$$N_{i,j}(n) = \sum_{k=1}^{n} \mathbb{1}_{\{(X_{k-1}, X_k) = (i,j)\}}.$$

Let div be the divergence operator div : $\mathbb{R}^E \mapsto \mathbb{R}^V$

$$\mathrm{div}(z)(i) = \sum_{j, i \to j} z_{i,j} - \sum_{j, j \to i} z_{j,i}.$$

Proposition (Bacallado '11, Baccalado, Sabot and T. '21)

i) Let $i_0 \in V$. If div(α) $= \delta_{i_0^*} - \delta_{i_0}$, then the $\star$-ERRW starting from i_0 is partially exchangeable.

Proof.

Let σ be a path. We prove that

$$\mathbb{P}^{\star-ERRW}(X \text{ follows } \sigma) = \frac{\text{function } (N_e(\sigma))}{\text{function } (N_i(\sigma))},$$

where as usual $N_{i,j}(\sigma)$ is the number of crossings of the (directed) edge (i,j) and

$$N_i(\sigma) = \sum_{i \to j} N_{i,j}(\sigma).$$

Numerator : trivial
Denominator : needs condition (1).

-Edge Reinforced Random Walks (-ERRW): statistical view

- Statistical analysis of molecular dynamics simulations with microscopically reversible laws.
- Two other applications, beyond Bayesian analysis of higher-order Markov chains (Bacallado, 2006):
  - Variable-order Markov chains with context set $\mathcal{C} \subseteq S \cup S^2 \cup \cdots \cup S^k$ on de Bruijn graph: $\forall (i_1, \ldots, i_\ell) \in \mathcal{C}$, transition probabilities out of x and y are the same whenever x and y both end in $(i_1, \ldots, i_\ell)$. Can define a prior with full support on the space of variable-order, reversible Markov chains with a specific context set.
  - Reinforced random walk with amnesia: RW on $G = (V, E)$ defined by $V = S \cup S^2 \cup \ldots S^k$ with two types of edges: "forgetting" ones $(i_1, \ldots, i_m) \to (i_2, \ldots, i_m)$, if $m > 1$, "appending" ones $(i_1, \ldots, i_m) \to ((i_1, \ldots, i_m, j)$, for each $j \in V$, if $m < k$. Generalization of the above.

-Edge Reinforced Random Walks (-ERRW): results

Theorem (Bacallado, Sabot and T., 2021)

- $(Z_n(e)/n)_{n\in\mathbb{N}}$ *converges a.s. to a random vector* $X = (X_e)_{e\in E}$ *in*

$$\mathcal{L}_1 = \left\{ (x_e) \in (0,\infty)^E : x_{i,j} = x_{j^*,i^*},\ div(x) = 0,\ \sum_{e\in E} x_e = 1 \right\}.$$

- *Conditionally on* x, *ERRW is a reversible Markov chain* P_x *with jump probability* x_{ij}/x_i *from* i *to* j, $x_i = \sum_{i\to k} x_{ik}$.
- *The random variable* X *has the following density on* $\mathcal{L}_1$, *w.r.t pullback of Lebesgue measure on* $\mathbb{R}^B$ *by the projection* $(x_e) \in \mathcal{L}_0 \mapsto (x_e)_{e\in B}$, B *basis of* $\mathcal{L}_1$:

$$C\gamma(i_0,\alpha)\sqrt{x_{i_0}} \left(\frac{\prod_{(i,j)\in\tilde{E}} x_{i,j}^{\alpha_{i,j}-1}}{\prod_{i\in V} x_i^{\frac{1}{2}\alpha_i}} \right) \frac{1}{\prod_{i\in V_0}\sqrt{x_i}} \sqrt{D(x)}\, dx_{\mathcal{L}_1},$$

-Edge Reinforced Random Walks (-ERRW): results

We have

$$\gamma(i_0,\alpha) = \frac{\left(\prod_{i\in V_0}\Gamma(\frac{1}{2}(\alpha_i+1-\mathbb{1}_{i=i_0})2^{\frac{1}{2}(\alpha_i-\mathbb{1}_{i=i_0})}\right)\left(\prod_{i\in V_1}\Gamma(\inf(\alpha_i,\alpha_{i^*}))\right.}{\prod_{(i,j)\in\tilde{E}}\Gamma(\alpha_{i,j})}$$

$$C = \frac{2}{\sqrt{2\pi}^{|V_0|-1}\sqrt{2}^{|V_0|+|V_1|}},$$

and

$$D(y) = \sum_T \prod_{(i,j)\in T} y_{i,j}.$$

The last sum runs on spanning trees directed towards a root $j_0 \in V$ (value does not depend on the choice of the root j_0.