The one-transit walk model

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A Tour of Combinatorics and Statistical Mechanics
In Memory of Richard Brak

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Hugging the Airey's Inlet lighthouse

Motivation

- Describe the stationary state of a Markov chain
- Perron-Frobenius: elements are positive polynomials in the rates
- Give a combinatorial description of these polynomials
- Can equilibrium stat-mech describe stationary non-equilibrium processes?

Markov chain

$P_t(a)$: probability to find a process in configuration a at time t.

The Markov chain equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t} P_t(a) = \sum_{b \neq a} \left(r_{ab} P_t(b) - r_{ba} P_t(a) \right)$$

In matrix form:

$$\frac{\mathrm{d}}{\mathrm{d}t} |P_t\rangle = M |P_t\rangle, \qquad |P_t\rangle = \sum_a P_t(a) |a\rangle,$$

where M is the *transition matrix* with off-diagonal elements $M_{ab} = r_{ab} > 0$ and whose columns add up to zero.

Stationary state

Stationary state

$$|P_\infty\rangle = \lim_{t\to\infty} |P_t\rangle \quad \text{satisfies} \quad M|P_\infty\rangle = 0.$$

The eigenvalue equation is solved by the cofactors $X(b,b)$ of M,

$$M|P\rangle = 0 \quad \Leftrightarrow \quad P(b) = X(b,b).$$

Proof:

$$0 = \det M = \sum_b M_{ab} X(a,b) = \sum_b M_{ab} X(b,b),$$

This solution fixes a particular normalisation of the eigenvector. Probability $P(b)$ is written as

$$P_\infty(b) = \frac{X(b,b)}{Z_n}, \qquad Z_n = \sum_{b=1}^{\#(n)} X(b,b).$$

where n is the size of the system.

Normalisation vs Partition function

[Matrix tree theorem] Z_n is a homogeneous polynomial in the rates r_{ab} with *positive coefficients*

Generalized Boltzmann weights $r_{ab} = z_{ab}$: think of $Z_n(\{z_{ab}\})$ as a generalised partition sum for nonequilibrium systems.

The "free energy"

$$F_n = -\log Z_n$$

is a convex function in all its arguments z_{ab} with "particle numbers" N_{ab},

$$N_{ab} = -z_{ab}\frac{\partial F_n}{\partial z_{ab}}, \qquad N_{ab} \sim V(n)\rho_{ab} \quad \text{as } n \to \infty,$$

$V(n)$ is the "volume" and ρ_{ab} are the "densities".

The "particle numbers" are not necessarily extensive quantities. This implies that in the parameter space the ρ_{ab} might diverge and we have to change the definition of the factor $V(n)$ (special surface transitions).

Asymmetric exclusion process

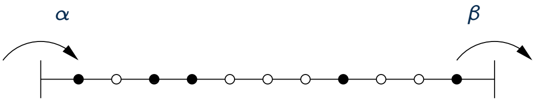


Figure: TASEP configuration. Particles enter the system from the left with rate α and leave from the right with rate β. Particles hop in the bulk from left to right with rate 1.

TASEP stationary probabilities are given by

$$P_\infty(\tau_1, \ldots, \tau_n) = \frac{1}{Z_n} \langle W| \prod_{i=1}^{n} (\tau_i D + (1-\tau_i)E) |V\rangle,$$

with Z_n is given by

$$Z_n = \langle W|(D+E)^n|V\rangle,$$

and the matrices D and E, and the vectors $\langle W|$ and $|V\rangle$ are a representation of the so-called DEHP algebra,

$$DE = D + E, \qquad D|V\rangle = \frac{1}{\beta}|V\rangle \qquad \langle W|E = \frac{1}{\alpha}\langle W|$$

Reformulation as walks model

The matrices D and E can be interpreted as transfer matrices (Brak and Essam).

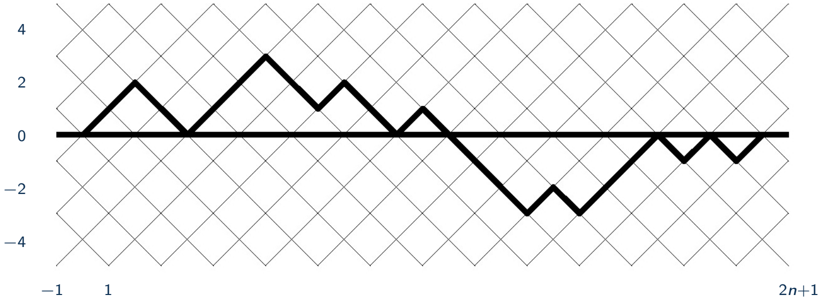


Figure: An example of an RSOS path starting at $(0,0)$ and ending at $(2n,0)$ crossing the x-axis only once.

- Paths start at $(0,0)$ and end at $(2n,0)$, can only move in the North-East (NE) or in the South-East (SE) direction and *cross the x-axis exactly once*.
- Associate weights α^{-1} and β^{-1} to the returns (or contact points) of the path above and below the x-axis respectively.

Partition function

The partition function of the one-transit model is simply given by

$$Z_n(\alpha,\beta) = (\alpha,\beta)^n \tilde{Z}_n(\alpha,\beta),$$

where

$$\tilde{Z}_n(\alpha,\beta) = \sum_{p=0}^{n} B_{n,p} \sum_{q=0}^{p} \alpha^{-q}\beta^{-p+q}.$$

and $B_{n,p}$ are Ballot numbers,

$$B_{n,p} = \frac{p}{n}\binom{2n-p-1}{n-1} = \frac{p(2n-p-1)!}{n!(n-p)!}.$$

Alternatively

$$Z_n(\alpha,\beta) = (\alpha,\beta)^n \sum_{p=0}^{n} \tilde{Z}_p(\alpha,\infty)\tilde{Z}_{n-p}(\infty,\beta).$$

This formula shows that we can also interpret the model as the combination of two contact models with a movable but impenetrable wall in between them at a random position, each position being equally probable.

Thermodynamics

Asymptotically

$$\tilde{Z}_n(z,\infty) \approx \begin{cases} \dfrac{z}{(1-2z)^2}\dfrac{4^n}{\sqrt{\pi}n^{3/2}} & z > 1/2 \\ \dfrac{4^n}{\sqrt{\pi}n^{1/2}} & z = 1/2 \\ \dfrac{1-2z}{1-z}\dfrac{1}{z^n(1-z)^n} & z < 1/2. \end{cases}$$

The grand canonical partition function

$$\omega = -\lim_{n\to\infty}\frac{1}{n}\log Z_n.$$

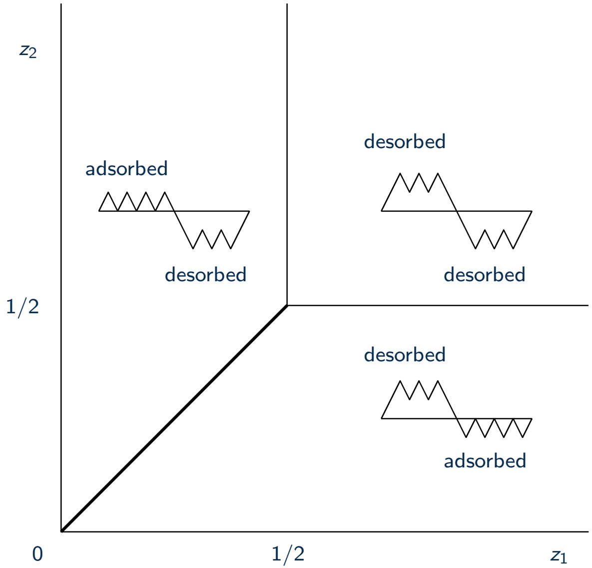
and contact averages are given by

$$a = 1 + \alpha\frac{\partial\omega}{\partial\alpha}, \qquad b = 1 + \beta\frac{\partial\omega}{\partial\beta}.$$

Relationship to TASEP curren J and density ρ

$$\frac{2\rho-1}{J} = \frac{b}{\beta} - \frac{a}{\alpha},$$

Phase diagram



Canonical free energy

The canonical free energy per site for given values of a and b can be calculated from the grand potential $\omega(\alpha, \beta)$,

$$f(a, b) = \sup_{\alpha,\beta}((1-a)\log\alpha + (1-b)\log\beta + \omega(\alpha, \beta)),$$

from which we find, using $r = a + b$ and $d = a - b$,

$$f(a, b) = (1-r)\log\left(1 - \frac{r+|d|}{2}\right) - (2-r)\log\left(2 - \frac{r+|d|}{2}\right).$$

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Farewell Richard