Combinatorics of an exclusion process driven by an asymmetric tracer

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Plan of the Talk

1. Model definition and motivation
2. Stationary distribution
3. Stirling numbers and the partition function
4. Correlation functions and the tracer's point of view
5. Asymptotics

Model definition

- L sites with periodic boundary conditions ($\mathbb{Z}/L\mathbb{Z}$)
- n (ordinary) particles, denoted 1
- one tracer particle, denoted $\hat{1}$
- remaining vacancies/holes, denoted 0
- Dynamics:
  - All particles perform symmetric exclusion with rate 1

$$10 \underset{1}{\overset{1}{\rightleftharpoons}} 01.$$

  - The tracer performs asymmetric exclusion

$$\hat{1}0 \underset{q}{\overset{p}{\rightleftharpoons}} 0\hat{1}.$$

- Let $\Omega_{L,n}$ be the set of configurations and $M_{L,n}$ be the generator of the process.

Example: $L = 3, n = 1$

- Order the configurations as

$$\Omega_{3,1} = \{(0,1,\hat{1}),(0,\hat{1},1),(1,0,\hat{1}),(1,\hat{1},0),(\hat{1},0,1),(\hat{1},1,0)\}.$$

- The (column-stochastic) generator is then

$$M_{3,1} = \begin{pmatrix} -p-1 & 0 & 1 & 0 & 0 & q \\ 0 & -q-1 & 0 & 1 & p & 0 \\ 1 & 0 & -q-1 & p & 0 & 0 \\ 0 & 1 & q & -p-1 & 0 & 0 \\ 0 & q & 0 & 0 & -p-1 & 1 \\ p & 0 & 0 & 0 & 1 & -q-1 \end{pmatrix}.$$

Jump ahead

History

- First studied by Ferrari, Goldstein and Lebowitz (1985) to understand the validity of the Einstein relation in microscopic dynamics. (Yes!)
- A similar model on $\mathbb{Z}$ was studied by G. Oshanin's group (1992-99). They showed that the mean displacement of the tracer grows like $\sqrt{t}$ rather than t.
- When $p = q = 1$, the tracer is indistinguishable from other particles and is known as the tagged particle in the literature.
- For this model on $\mathbb{Z}$, a law of large numbers for the displacement of the tracer was proven by Landim, Olla and Volchan (1998) and a CLT was proven by Landim and Volchan (2000).
- For a similar process on $\mathbb{Z}^d$, Loulakis (2005) shows that the Einstein relation does not hold for $d \geq 3$.

Motivation

- Fix an edge e between two sites.
- Let $N_+(t)$ (resp. $N_-(t)$) be the number of times a particle crosses e in the forward (resp. backward) direction until time t.
- The current of a particle across e is given by

$$J = \lim_{t \to \infty} \frac{N_+(t) - N_-(t)}{t}.$$

- This turns out to be independent of e.
- The existence of a current is one of the basic signatures of a nonequilibrium system.
- One of our motivations was to see if one could obtain a nontrivial current by having a single tracer.

Long-term behaviour

- We are interested in looking at the system at large times.
- This is given by the stationary distribution.
- Note that this process is irreducible, i.e. one can start from any configuration and end up at any other.
- For a finite-state irreducible Markov process, general theorems guarantee that the stationary distribution is unique.
- Computationally, this is given by the right nullvector $\pi_{L,n}$ of $M_{L,n}$.
- For example, Back to example

$$\pi_{3,1} = \frac{1}{3(p+q+2)} \left(q+1, p+1, p+1, q+1, q+1, p+1\right)^{\mathrm{T}}.$$

Properties of the stationary distribution

Proposition (Translation invariance)

The steady state probabilities are invariant under translation, i.e.

$$\pi(\tau_1, \tau_2, \ldots, \tau_L) = \pi(\tau_2, \ldots, \tau_L, \tau_1).$$

Proposition (Reflection 'invariance')

The steady state probabilities are invariant under reflection and the interchange of p and q, i.e.

$$\pi(\tau_1, \tau_2, \ldots, \tau_L) = \pi(\tau_L, \ldots, \tau_2, \tau_1)\Big|_{p \leftrightarrow q}.$$

Main formula

- It suffices to consider the stationary probabilities of configurations that begin with $\hat{1}$.
- For a configuration τ with $\tau_1 = \hat{1}$, let

$$w(\tau) = \prod_{\substack{i=2 \\ \tau_i=0}}^{L} \left(1 + p\, m_i(\tau) + q\, n_i(\tau)\right),$$

where $m_i(\tau)$ (resp. $n_i(\tau)$) is the number of 1's to the left (resp. right) of i in τ.

Main formula

Theorem (A., 2020+)

In the system with L sites and n 1's, the steady state probability of $\tau \in \Omega_{L,n}$ with $\tau_1 = \hat{1}$ is given by

$$\pi(\tau) = \frac{w(\tau)}{Z_{L,n}},$$

where

$$Z_{L,n}(p,q) = \sum_{\tau \in \Omega_{L,n}} w(\tau)$$

is the (nonequilibrium) partition function or normalisation factor.

Example: $L = 5, n = 2$

τ	$w(\tau)$
$(\hat{1}, 0, 0, 1, 1)$	$(2q+1)^2$
$(\hat{1}, 0, 1, 0, 1)$	$(p+q+1)(2q+1)$
$(\hat{1}, 0, 1, 1, 0)$	$(2p+1)(2q+1)$
$(\hat{1}, 1, 0, 0, 1)$	$(p+q+1)^2$
$(\hat{1}, 1, 0, 1, 0)$	$(2p+1)(p+q+1)$
$(\hat{1}, 1, 1, 0, 0)$	$(2p+1)^2$

Proof idea

Proof.

- Since the stationary distribution is unique, it suffices to verify that $\pi(\tau)$ satisfies the master equation,

$$\sum_{\tau' \in \Omega_{L,n}} \text{rate}(\tau \to \tau')\pi(\tau) = \sum_{\tau' \in \Omega_{L,n}} \text{rate}(\tau' \to \tau)\pi(\tau').$$

- This can be done with some case analysis.
- The proof can also be explained by a standard mapping to the zero-range process, for which the factorisation is a well-established property.

□

Restricted partition function

- Since there is only one $\hat{1}$, there are no configurations which are fixed-points of arbitrary translations.
- Therefore, $Z_{L,n}$ is L times a polynomial in p and q with integer coefficients.
- We define the restricted partition function

$$\left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{p,q} = \sum_{\substack{\tau \in \Omega_{L,n} \\ \tau_1 = \hat{1}}} w(\tau) = \frac{Z_{L,n}(p,q)}{L}.$$

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- Why this notation?

Digression: Stirling numbers of the second kind

- Let $[n] := \{1, \dots, n\}$.
- Let $\left\{ {[n] \atop k} \right\}$ denote the collection of set partitions of $[n]$ into exactly k parts.
- For example,

$$\left\{ {[4] \atop 2} \right\} = \{123|4, 124|3, 134|2, 1|234, 12|34, 13|24, 14|23\}.$$

- The number of set partitions of $[n]$ into k parts is known as the Stirling number of the second kind, denoted $\left\{ {n \atop k} \right\}$. For example, $\left\{ {4 \atop 2} \right\} = 7$

Go ahead

Digression: Properties of Stirling numbers

- They satisfy the recurrence

$$\left\{ {n+1 \atop k} \right\} = \left\{ {n \atop k-1} \right\} + k \left\{ {n \atop k} \right\},$$

with $\left\{ {n \atop 1} \right\} = \left\{ {n \atop n} \right\} = 1.$

- The first few numbers are

$n \backslash k$	1	2	3	4	5
1	1				
2	1	1			
3	1	3	1		
4	1	7	6	1	
5	1	15	25	10	1

Digression: Properties of Stirling numbers

- As a side remark, the total number of set partitions of $[n]$ is called the Bell number, denoted B_n, $B_n = \sum_k \left\{ {n \atop k} \right\}$.
- Many formulae are known for the Stirling numbers of the second kind.
- The column generating function is given by the product formula,

$$\sum_{n \geq k} \left\{ {n \atop k} \right\} x^n = \frac{x^k}{(1-x)(1-2x)\cdots(1-kx)}.$$

Digression: Properties of Stirling numbers

- From this generating function, we get

$$\left\{ {n \atop k} \right\} = \sum_{r=1}^{k} (-1)^{k-1} \frac{r^n}{r!(k-r)!},$$

which holds true even when even when $n < k$.

- The mixed bivariate generating function is given by

$$\sum_{n \geq 0} \sum_{k=0}^{n} \left\{ {n \atop k} \right\} \frac{x^n}{n!} y^k = \exp(y(\exp(x) - 1)).$$

Explanation of the notation

Corollary

The restricted partition function when $p = 1$ and $q = 0$ is given by the Stirling number of the second kind,

$$\left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{1,0} = \left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}.$$

- There are many variants of the Stirling numbers in the literature.
- L. Carlitz (1958), H. Gould (1961), M. Wachs and D. White (1991), J. Cigler (1992), H. Park (1994) and A. Hennessy and P. Barry (2011), all have different p, q- or q-Stirling numbers.
- None of them seem to match $\left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{p,q}$.
- To prove this corollary, we will consider the more general case, $q = 0$.

Special case: $q = 0$

- Generalize the Stirling numbers by setting

$$\left\{ {n \atop k} \right\}_p = \sum_{\pi \in \left\{ {[n] \atop k} \right\}} p^{\#\{\text{parts in } \pi \text{ containing } 1\} - 1}.$$

- For example, $\left\{ {4 \atop 2} \right\}_p = 1 + 3p + 3p^2$.
- One can prove a similar recurrence,

$$\left\{ {n+1 \atop k} \right\}_p = \left\{ {n \atop k-1} \right\}_p + (k - 1 + p) \left\{ {n \atop k} \right\}_p,$$

with initial conditions $\left\{ {n \atop n} \right\}_p = 1$ and $\left\{ {n \atop 1} \right\}_p = p^{n-1}$.

Special case: $q = 0$

Theorem

The restricted partition function when $q = 0$ is given by

$$\left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{p,0} = p^{L-n-1} \left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{1/p}.$$

Setting $p = 1$ proves the corollary.

Properties of the restricted partition function

Corollary

The restricted partition function $\left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{p,q}$ *is a symmetric polynomial in* p *and* q *with integer coefficients.*

For generic values of p and q, this process is irreversible. That is to say,

$$\pi(\tau)\text{rate}(\tau \to \tau') \neq \pi(\tau')\text{rate}(\tau' \to \tau)$$

for all $\tau, \tau' \in \Omega_{L,n}$.

Corollary

When $p = q$*, the stationary distribution is uniform and the process is reversible.*

Properties of the restricted partition function

Proposition

The restricted partition function satisfies the recurrence

$$\left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{p,q} = (1+nq) \left\{ \begin{matrix} L-1 \\ n+1 \end{matrix} \right\}_{p,q} + (1+p)^{L-n-1} \left\{ \begin{matrix} L-1 \\ n \end{matrix} \right\}_{\frac{p}{1+p}, \frac{q}{1+p}},$$

for $L > n \geq 0$, *with the initial conditions* $\left\{ \begin{matrix} L \\ 1 \end{matrix} \right\}_{p,q} = \left\{ \begin{matrix} L \\ L \end{matrix} \right\}_{p,q} = 1.$

Column generating function

Now consider the generating function

$$F_n(x) = \sum_{L=n+1}^{\infty} \left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{p,q} x^{L-n-1}.$$

Theorem

The generating function $F_n(x)$ is given by

$$F_n(x) = \prod_{j=0}^{n} \frac{1}{1-(1+jp+(n-j)q)x}.$$

This generalises the column generating function of $\left\{ \begin{matrix} n \\ k \end{matrix} \right\}$.

An explicit formula

Corollary

The restricted partition function is given by

$$\left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\}_{p,q} = \sum_{j=0}^{n} \frac{(-1)^{n-j}}{j!(n-j)!} \frac{(1+jp+(n-j)q)^{L-1}}{(p-q)^n}.$$

- Although this result is nice, it is not useful for asymptotic computations because the summands are not all positive.
- However, it is very useful for fast exact computations on a computer for numerical values of p and q.

Bivariate generating function

Theorem (A., 2020+)

The mixed bivariate generating function of the restricted partition function is given by

$$\sum_{L=1}^{\infty}\sum_{n=0}^{L-1}\left\{ {L \atop n+1} \right\}_{p,q} x^n \frac{y^{L-1}}{(L-1)!} = \exp\left(y + x\frac{\exp(py)-\exp(qy)}{p-q} \right).$$

This generalises the bivariate generating function of $\left\{ {n \atop k} \right\}$.

Asymptotics

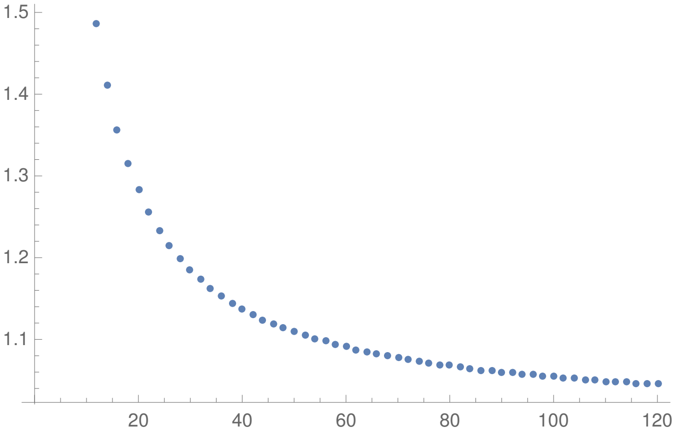
- Take $n, L \to \infty$ so that $n/L \to \rho$.
- Let y_0 be the unique real positive solution to

$$\exp((p-q)y) = \frac{\rho q y - 1}{\rho p y - 1},$$

- Then

$$\left\{ \begin{matrix} L \\ \rho L + 1 \end{matrix} \right\}_{p,q} \approx \frac{1}{\sqrt{2\pi L\left(\rho - (p\rho y_0 - 1)(q\rho y_0 - 1)\right)}} \frac{\exp(y_0 - 1)}{y_0^{L-1}} \times \left(\frac{L}{e}\right)^{L(1-\rho)-1} \left(\frac{\exp(py_0) - \exp(qy_0)}{\rho(p-q)}\right)^{\rho L}.$$

Comparison with data



A plot of the ratio of the asymptotic to the exact formula for the restricted partition function with $n = 0.5L$, $p = 0.55$ and $q = 0.78$ for even values of L ranging from 12 to 120.

Special case: $p = 1, q = 0$

- The Lambert W function is a family of functions defined by the inverse function of $f(z) = z\exp(z)$.
- It is multivalued since f is not injective, and so let W_0 be the principal branch.
- It turns out that $y_0 = 1/\rho - G$, where

$$G = -W_0\left(-\frac{\exp(-1/\rho)}{\rho}\right).$$

- Here we find a simpler formula, due to Temme (1993),

$$\left\{ \begin{matrix} L \\ n+1 \end{matrix} \right\} \approx \frac{1}{\sqrt{2\pi\rho L(1-G)}} \left(\frac{\rho L}{1-\rho G}\right)^{L-\rho L-1} e^{\rho L(1-G)+1/\rho-G}.$$

Free energy

- The partition function in this case grows faster than exponentially in L.
- The nonequilibrium free energy, defined by

$$\lim_{L\to\infty} \frac{\log Z_{L,\rho L}}{L}$$

  does not exist.
- Such behaviour is not expected to hold for reversible processes.
- This seems to be the first exactly solvable example.

Current

- Recall that the current of any particle across an edge is the amount per unit time it jumps across the bond in the forward direction minus that in the reverse direction.
- Let, for $1 \le i \le L$, $\sigma_i = 1$ (resp. $\tau_i = 1$) if and only if the i'th site is occupied by a $\hat{1}$ (resp. 1), and otherwise σ_i (resp. τ_i) is zero.
- Denote expectations in the stationary distribution by $\langle \cdot \rangle_{L,n}$.
- In the stationary distribution, the currents are given by

$$J_1 = \langle \tau_i (1 - \tau_{i+1} - \sigma_{i+1}) \rangle_{L,n} - \langle (1 - \tau_i - \sigma_i) \tau_{i+1} \rangle_{L,n},$$
$$J_{\hat{1}} = p \langle \sigma_i (1 - \tau_{i+1} - \sigma_{i+1}) \rangle_{L,n} - q \langle (1 - \tau_i - \sigma_i) \sigma_{i+1} \rangle_{L,n}.$$

Formula for the current

Theorem (A., 2020+)

In the lattice with L sites and n 1's, the currents are given by

$$J_{\hat{1}} = (p-q)\frac{\left\{ {L-1 \atop n+1} \right\}_{p,q}}{Z_{L,n}}, \quad J_1 = (p-q)\frac{n\left\{ {L-1 \atop n+1} \right\}_{p,q}}{Z_{L,n}}.$$

Proved directly using the definition of $w(\tau)$.

Asymptotics of the current

- Let $L, n \to \infty$ so that $n/L \to \rho$.
- We then find that

$$J_{\hat{1}} \approx \frac{(p-q)y_0 e^{\rho}}{L^2}, \quad J_1 \approx \frac{(p-q)y_0 \rho e^{\rho}}{L}.$$

- Thus, the current does not survive in the limit, as expected.

Densities

Proposition

In the system with L sites and n 1's,

$$\langle \sigma_i \rangle_{L,n} = \frac{1}{L}, \qquad \langle \tau_i \rangle_{L,n} = \frac{n}{L}.$$

This is an easy consequence of translation invariance.

From the point of view of the tracer

- Consider the profile of particles from the point of view of the tracer particle, known as the environment process.
- Let $\langle\langle \cdot \rangle\rangle_{L,n}$ denote the expectation in the environment process.
- By computing $\langle \sigma_1 \tau_i \rangle_{L,n}$, we can obtain $\langle\langle \tau_i \rangle\rangle_{L,n}$.
- For convenience, we will place the $\hat{1}$ at position 0.
- Label forward positions by $1, \dots, L-1$ and backward positions by $-1, \dots, -(L-1)$.

From the point of view of the tracer

Theorem (A., 2020+)

In the system with L sites and n 1's,

$$\langle\langle \tau_i \rangle\rangle_{L,n} = \sum_{j=0}^{L-n-1} \sum_{k=0}^{j} \binom{L-1-i}{k} \binom{i-1}{j-k} p^k q^{j-k} \frac{\left\{ {L-j-1 \atop n} \right\}_{p,q}}{\left\{ {L \atop n+1} \right\}_{p,q}},$$

$$\langle\langle \tau_{-i} \rangle\rangle_{L,n} = \sum_{j=0}^{L-n-1} \sum_{k=0}^{j} \binom{L-1-i}{k} \binom{i-1}{j-k} q^k p^{j-k} \frac{\left\{ {L-j-1 \atop n} \right\}_{p,q}}{\left\{ {L \atop n+1} \right\}_{p,q}},$$

for $1 \leq i \leq L-1$.

Special case: $p = 1, q = 0$

Corollary

When $p = 1$ *and* $q = 0$,

$$\langle\langle \tau_i \rangle\rangle_{L,n} = \sum_{j=0}^{L-n-1} \binom{L-i-1}{j} \frac{\left\{ {L-j-1 \atop n} \right\}}{\left\{ {L \atop n+1} \right\}},$$

$$\langle\langle \tau_{-i} \rangle\rangle_{L,n} = \sum_{j=0}^{L-n-1} \binom{i-1}{j} \frac{\left\{ {L-j-1 \atop n} \right\}}{\left\{ {L \atop n+1} \right\}},$$

for $1 \leq i \leq L-1$.

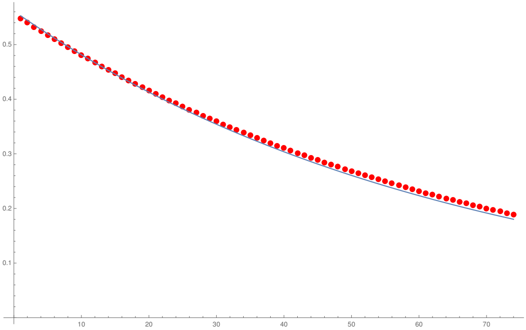
Asymptotic densities

- As usual, take $L, n \to \infty$ so that $n/L \to \rho$.
- Further, let $x \in [0,1]$ and focus on position $\pm\lfloor xL \rfloor$.
- Let $\langle\langle \cdot \rangle\rangle$ denote averages in this limiting distribution.
- Then

$$\langle\langle \tau_{xL} \rangle\rangle \approx \rho y_0 (p-q) \frac{\exp(-(p-q)y_0 x)}{1-\exp(-(p-q)y_0)},$$

$$\langle\langle \tau_{-xL} \rangle\rangle \approx \rho y_0 (p-q) \frac{\exp((p-q)y_0 x)}{\exp((p-q)y_0)-1}.$$

Comparison with data



A plot of the exact density of particles (red dots) ahead of the tracer particle in a system of size $L = 75$ with $n = 17$, $p = 0.75$ and $q = 0.4$, along with the expected curve in blue .

Special case: $p = 1, q = 0$

- Using properties of the Lambert function, we find that the prefactor becomes 1.
- In front of the tracer,

$$\langle\langle \tau_{xL} \rangle\rangle \approx (\rho G)^{-x}.$$

- Behind the tracer,

$$\langle\langle \tau_{-xL} \rangle\rangle \approx (\rho G)^{1-x}.$$

Heuristic picture

- Consider what happens when $x = 0+$.
- Then the density is 1, i.e., there is a particle ahead of the tracer with probability 1.
- But the same argument holds if we consider the density at any fixed position i (not scaling with L).

Heuristic picture

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- Infinite traffic jam!

Heuristic picture

- Consider what happens when $x = 0+$.
- Then the density is 1, i.e., there is a particle ahead of the tracer with probability 1.
- But the same argument holds if we consider the density at any fixed position i (not scaling with L).
- Infinite traffic jam!
- At $x = 0-$, i.e. immediately behind the tracer, the density is small.
- But infinitely far behind, the density becomes 1.

Stirling number asymptotics

- The asymptotics of $\left\{ {n \atop k} \right\}$ are well-studied.
- More than a dozen papers give asymptotic formulas in various regimes:
  - L. Hsu (1948): $k = o(n^{1/2})$.
  - L. Moser and M. Wyman (1958): $k = n - o(n^{1/2})$.
  - I. Good (1961): $c_1 < n/k < c_2$.
  - E. Bender (1973): $\epsilon < k/n < 1 - \epsilon$.
  - W. Bleick and P. Wang (1974): $k = o(n^{2/3})$.
  - E. Tsylova (1995): $k = tn + o(n^{2/3})$.
  - P. Erdős and G. Szekeres, in V. Sachkov (1997): $k < n/\ln n$.
  - R. Chelluri, L. Richmond and N. Temme (2000): $n - k = \Omega(n^{1/3})$ and $n - k = o(n^{1/3})$.
  - G. Louchard (2013): $k = n - n^{\alpha}, \alpha \in (1/2, 1)$.

Uniform bounds

- Temme (1993) gave the first uniform bounds for large n, k for Stirling numbers, both of the first and second kinds.
- This is the result stated in Wikipedia.
- Originally, the statement had an error and I had to fix it!
- His idea is to use the saddle point method starting with the generating function.
- However, he uses a clever change of variables trick, whose genesis is a complete mystery to me!
- Fortunately for us, this trick works for $\left\{ {L \atop n+1} \right\}_{p,q}$ with virtually no change.

Thank you!