Mixing of Diffusing Particles

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Talk, paper available from: http://cnls.lanl.gov/~ebn

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Diffusion in One Dimension

- **Mixing:** well-studied in fluids, granular media, not in diffusion.
- **System:** $N$ independent random walks in one dimension.

- **Strong Mixing:** trajectories cross many times
- **Poor Mixing:** trajectories rarely cross

How to quantify mixing of diffusing particles?
The Inversion Number

• Measures how “scrambled” a list of numbers is

• Used for ranking, sorting, recommending (books, songs, movies)
  - I rank: 1234, you rank 3142
  - There are three inversions: \{1,3\}, \{2,3\}, \{2,4\}

• Definition: The inversion number $m$ equals the number of pairs that are inverted = out of sort

• Bounds:

$$0 \leq m \leq \frac{N(N - 1)}{2}$$

McMahon 1913
Random Walks and Inversion Number

- **Initial conditions:** particles are ordered
  \[ x_1(0) < x_2(0) < \cdots < x_{N-1}(0) < x_N(0) \]
- **Each particle is an independent random walk**
  \[ x \rightarrow \begin{cases} 
    x - 1 & \text{with probability } 1/2 \\
    x + 1 & \text{with probability } 1/2 
  \end{cases} \]
- **Inversion number**
  \[ m(t) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \Theta(x_i(t) - x_j(t)) \]
- **Strong mixing:** large inversion number
- **Weak mixing:** small inversion number persists

Inversion number is a natural measure of mixing
Equilibrium Distribution

- Diffusion is ergodic, order is completely random when $t \to \infty$
- Every permutation occurs with the same weight $1/N!$
- Probability $P_m(N)$ of inversion number $m$ for $N$ particles
  \[
  \begin{aligned}
  (P_0, P_1, \ldots, P_M) &= \frac{1}{N!} \times \\
  &\begin{cases}
  (1) & N = 1, \\
  (1, 1) & N = 2, \\
  (1, 2, 2, 1) & N = 3, \\
  (1, 3, 5, 6, 5, 3, 1) & N = 4.
  \end{cases}
  \end{aligned}
  \]

- Recursion equation
  \[
  P_m(N) = \frac{1}{N} \sum_{l=0}^{N-1} P_{m-l}(N-1)
  \]

- Generating Function
  \[
  \sum_{m=0}^{M} P_m(N)s^m = \frac{1}{N!} \prod_{n=1}^{N} (1 + s + s^2 + \cdots + s^{n-1})
  \]

Knuth 1998
Equilibrium Properties

- Average inversion number scales quadratically with $N$
  \[ \langle m \rangle = \frac{N(N - 1)}{4} \]

- Variance scales cubically with $N$
  \[ \sigma^2 = \frac{N(N - 1)(2N + 5)}{72} \]

- Asymptotic distribution is Gaussian
  \[ P_m(N) \sim \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[ -\frac{(m - \langle m \rangle)^2}{2\sigma^2} \right] \]

- Large fluctuations
  \[ m - N^2/4 \sim N^{3/2} \]
Transient Behavior

- Assume particles well mixed on a growing length scale
- Use equilibrium result for the sub-system $\langle m \rangle / N \sim \ell$
- Length scale must be diffusive $\ell \sim \sqrt{t}$
  $$\langle m(t) \rangle \sim N \sqrt{t} \quad \text{when} \quad t \ll N^2$$
- Equilibrium behavior reached after a transient regime
- Nonequilibrium distribution is Gaussian as well
First-Passage Kinetics

• Survival probability $S_m(t)$ that inversion number $< m$ until time $t$

1. Probability there are no crossing

   \[ S_1(t) \sim t^{-N(N-1)/4} \]

   Fisher 1984

2. Two-particles: coordinate $x_1 - x_2$ performs a random walk

   \[ S_1(t) \sim t^{-1/2} \]

• Map $N$ 1-dimensional walks to 1 walk in $N$ dimensions
  - Allowed region: inversion number $< m$
  - Forbidden region: inversion number $\geq m$

• Absorbing boundary condition

Problem reduces to diffusion in $N$ dimensions in presence of complex absorbing boundary
Three particles

- Diffusion in three dimensions; Allowed regions are wedges

\[
S(t) \sim t^{-1/(4V)}
\]

- Survival probability in wedge with “fractional volume” \(0 < V < 1\)

\[
S_1 \sim t^{-3/2}, \quad S_2 \sim t^{-1/2}, \quad S_3 \sim t^{-3/10}
\]

- In general, the survival probabilities decay as power-law

\[
S_m \sim t^{-\beta_m} \quad \text{with} \quad \beta_1 > \beta_2 > \cdots > \beta_{N(N-1)/2}
\]

Huge spectrum of first-passage exponents

Redner 2001
Cone approximation

- Fractional volume of allowed region given by equilibrium distribution of inversion number
  \[ V_m(N) = \sum_{l=0}^{m-1} P_l(N) \]

- Replace allowed region with cone with same fractional volume
  \[ V(\alpha) = \frac{\int_0^\alpha d\theta (\sin \theta)^{N-3}}{\int_0^\pi d\theta (\sin \theta)^{N-3}} \]

- Use analytically known exponent for first-passage in cone
  \[ Q_{2\beta+\gamma}^\gamma(\cos \alpha) = 0 \quad N \text{ odd}, \quad \gamma = \frac{N - 4}{2} \]
  \[ P_{2\beta+\gamma}^\gamma(\cos \alpha) = 0 \quad N \text{ even}. \]

- Good approximation for four particles

<table>
<thead>
<tr>
<th>( m )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
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</thead>
<tbody>
<tr>
<td>( V_m )</td>
<td>( \frac{1}{24} )</td>
<td>( \frac{1}{5} )</td>
<td>( \frac{3}{8} )</td>
<td>( \frac{5}{8} )</td>
<td>( \frac{5}{6} )</td>
<td>( \frac{23}{24} )</td>
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<tr>
<td>( \alpha_m )</td>
<td>0.41113</td>
<td>0.84106</td>
<td>1.31811</td>
<td>1.82347</td>
<td>2.30052</td>
<td>2.73045</td>
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<tr>
<td>( \beta_m^{\text{cone}} )</td>
<td>2.67100</td>
<td>1.17208</td>
<td>0.64975</td>
<td>0.39047</td>
<td>0.24517</td>
<td>0.14988</td>
</tr>
<tr>
<td>( \beta_m )</td>
<td>3</td>
<td>1.39</td>
<td>0.839</td>
<td>0.455</td>
<td>0.275</td>
<td>0.160</td>
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</tbody>
</table>
Small number of particles

- By construction, cone approximation is exact for $N=3$
- Cone approximation produces close estimates for first-passage exponents when the number of particles is small
- Cone approximation gives a formal lower bound
Very large number of particles \( (N \to \infty) \)

- Gaussian equilibrium distribution implies

\[
V_m(N) \to \frac{1}{2} + \frac{1}{2} \text{erf}\left(\frac{z}{\sqrt{2}}\right) \quad \text{with} \quad z = \frac{m - \langle m \rangle}{\sigma}
\]

- Volume of cone is also given by error function

\[
V(\alpha, N) \to \frac{1}{2} + \frac{1}{2} \text{erf}\left(\frac{-y}{\sqrt{2}}\right) \quad \text{with} \quad y = (\cos \alpha)\sqrt{N}
\]

- First-passage exponent has the scaling form

\[
\beta_m(N) \to \beta(z) \quad \text{with} \quad z = \frac{m - \langle m \rangle}{\sigma}
\]

- Scaling function is root of equation involving parabolic cylinder function

\[
D_2\beta(-z) = 0
\]

Scaling exponents have scaling behavior!
Simulation results

Cone approximation is asymptotically exact!
Summary

• Inversion number as a measure for mixing
• Distribution of inversion number is Gaussian
• First-passage kinetics are rich
• Large spectrum of first-passage exponents
• Cone approximation gives good estimates for exponents
• Exponents follow a scaling behavior
• Cone approximation yields the exact scaling function
• Geometric proof for exactness
• Use inversion number to quantify mixing in 2 & 3 dimensions