Scaling Laws for First-Passage Exponents

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

STATPHYS25, Seoul, Korea, July 22, 2013
Process by which a fluctuating quantity reaches a threshold for the first time.

**First-passage probability:** for the random variable to reach the threshold as a function of time.

**Total probability:** that threshold is ever reached. May or may not equal 1.

**First-passage time:** the mean duration of the first-passage process. Can be finite or infinite.

Typically defined by a single threshold

Ordering of Brownian particles

- System: $N$ independent Brownian particles in one dimension
- What is the probability that original leader maintains the lead?
- $N$ Brownian particles
  \[ \frac{\partial \varphi_i(x, t)}{\partial t} = D \nabla^2 \varphi_i(x, t) \]
- Initial conditions
  \[ x_N(0) < x_{N-1}(0) < \cdots < x_2(0) < x_1(0) \]
- Survival probability $S(t)$ = probability leader remains first until $t$
- Independent of initial conditions, power-law asymptotic behavior
  \[ S(t) \sim t^{-\beta} \quad \text{as} \quad t \to \infty \]
- Monte Carlo: nontrivial exponents that depend on $N$

<table>
<thead>
<tr>
<th>$N$</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta(N)$</td>
<td>1/2</td>
<td>3/4</td>
<td>0.913</td>
<td>1.032</td>
<td>1.11</td>
<td>1.37</td>
</tr>
</tbody>
</table>

No analytic expressions for exponents

References:
Bramson 91
Redner 96
benAvraham 02
Grassberger 03
Order statistics

- Generalize the capture problem: \( S_m(t) \) is the probability that the leader does not fall below rank \( m \) until time \( t \)
- \( S_1(t) \) is the probability that leader remains first
- \( S_{N-1}(t) \) is the probability that leader never becomes last
- Power-law asymptotic behavior is generic
  \[ S_m(t) \sim t^{-\beta_m(N)} \]
- Spectrum of first-passage exponents
  \[ \beta_1(N) > \beta_2(N) > \cdots > \beta_{N-1}(N) \]

Can’t solve the problem? Make it bigger!
Two particles

- We need the probability that two particles do not meet
- Map two one-dimensional walks onto one two-dimensional walk
- Space is divided into allowed and forbidden regions
- Boundary separating the two regions is absorbing
- Coordinate $x_1 - x_2$ performs one-dimensional random walk
- Survival probability decays as power-law
  \[ S_1(t) \sim t^{-1/2} \]
- In general, map $N$ one-dimensional walk onto one walk in $N$ dimension with complex boundary conditions
Three particles

- Diffusion in three dimensions; now, allowed regions are wedges

\[
\begin{array}{c|c}
  m = 2 & m = 1 \\
  312 & 132 \quad x_2 = x_3 \\
  m = 3 & 321 \\
  231 & 213 \quad x_1 = x_2 \\
  m = 3 & m = 2 \\
  x_1 = x_3 \\
\end{array}
\]

- Survival probability in wedge with opening angle \(0 < \alpha < \pi\)

\[
S(t) \sim t^{-\pi/(4\alpha)}
\]

- Survival probabilities decay as power-law with time

\[
S_1 \sim t^{-3/4} \quad \text{and} \quad S_2 \sim t^{-3/8}
\]

- Indeed, a family of nontrivial first-passage exponents

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

Large spectrum of first-passage exponents

Spitzer 58
Fisher 84
First passage in a wedge

- Survival probability obeys the diffusion equation
  \[ \frac{\partial S(r, \theta, t)}{\partial t} = D \nabla^2 S(r, \theta, t) \]

- Focus on long-time limit
  \[ S(r, \theta, t) \sim \Phi(r, \theta) t^{-\beta} \]

- Amplitude obeys Laplace’s equation
  \[ \nabla^2 \Phi(r, \theta) = 0 \]

- Use dimensional analysis
  \[ \Phi(r, \theta) \sim \left( \frac{r^2}{D} \right)^\beta \psi(\theta) \implies \psi_{\theta\theta} + (2\beta)^2 \psi = 0 \]

- Enforce boundary condition
  \[ S|_{\theta=\alpha} = \Phi|_{\theta=\alpha} = \psi|_{\theta=\alpha} \]

- Lowest eigenvalue is the relevant one
  \[ \psi_2(\theta) = \cos(2\beta \theta) \implies \beta = \frac{\pi}{4\alpha} \]
Monte Carlo simulations

3 particles

4 particles

$\beta_1 = 0.913$

$\beta_2 = 0.556$

$\beta_3 = 0.306$

as expected, there are 3 nontrivial exponents

confirm wedge theory results
Simulations: small number of particles strongly hints at asymptotic scaling behavior!

\[ \beta_m(N) \to F(m/N) \quad \text{when} \quad N \to \infty \]

Scaling law for first-passage exponents
Kinetics of first passage in a cone

- Repeat wedge calculation step by step
  \[ S(r, \theta, t) \sim \psi(\theta)(Dt/r^2)^{-\beta} \]

- Angular function obeys Poisson-like equation
  \[
  \frac{1}{(\sin \theta)^{d-2}} \frac{d}{d\theta} \left[ (\sin \theta)^{d-2} \frac{d\psi}{d\theta} \right] + 2\beta(2\beta + d - 2)\psi = 0
  \]

- Solution in terms of associated Legendre functions
  \[
  \psi_d(\theta) = \begin{cases} 
  (\sin \theta)^{-\delta} P_{2\beta+\delta}^{\delta}(\cos \theta) & d \text{ odd}, \\
  (\sin \theta)^{-\delta} Q_{2\beta+\delta}^{\delta}(\cos \theta) & d \text{ even}
  \end{cases}
  \]
  \[ \delta = \frac{d - 3}{2} \]

- Enforce boundary condition, choose **lowest** eigenvalue
  \[
  P_{2\beta+\delta}^{\delta}(\cos \alpha) = 0 \quad d \text{ odd,}
  \]
  \[
  Q_{2\beta+\delta}^{\delta}(\cos \alpha) = 0 \quad d \text{ even.}
  \]

Exponent is root of Legendre function
Additional results

- Explicit results in 2d and 4d

\[ \beta_2(\alpha) = \frac{\pi}{4\alpha} \quad \text{and} \quad \beta_4(\alpha) = \frac{\pi - \alpha}{2\alpha} \]

- Root of ordinary Legendre function in 3d

\[ P_{2\beta}(\cos \alpha) = 0 \]

- Flat cone is equivalent to one-dimension

\[ \beta_d(\alpha = \pi/2) = 1/2 \]

- First-passage time obeys Poisson’s equation

\[ D \nabla^2 T(r, \theta) = -1 \]

- First-passage time (when finite)

\[ T(r, \theta) = \frac{r^2}{2D} \frac{\cos^2 \theta - \cos^2 \alpha}{d \cos^2 \alpha - 1} \]

\[ \alpha < \cos^{-1}(1/\sqrt{d}) \]
Asymptotic analysis

- Limiting behavior of scaling function
  \[ \beta(y) \sim \begin{cases} \sqrt{\frac{y^2}{8\pi}} \exp\left(-\frac{y^2}{2}\right) & y \to -\infty, \\ \frac{y^2}{8} & y \to \infty. \end{cases} \]

- Thin cones: exponent diverges
  \[ \beta_d(\alpha) \sim B_d \alpha^{-1} \quad \text{with} \quad J_\delta(2B_d) = 0 \]

- Wide cones: exponent vanishes when \( d \geq 3 \)
  \[ \beta_d(\alpha) \sim A_d (\pi - \alpha)^{d-3} \quad \text{with} \quad A_d = \frac{1}{2} B \left(\frac{1}{2}, \frac{d-3}{2}\right) \]

- A needle is reached with certainty only when \( d < 3 \)

- Large dimensions
  \[ \beta_d(\alpha) \sim \begin{cases} \frac{d}{4} \left(\frac{1}{\sin \alpha} - 1\right) & \alpha < \frac{\pi}{2}, \\ C(\sin \alpha)^d & \alpha > \frac{\pi}{2}. \end{cases} \]
High dimensions

- Exponent varies sharply for opening angles near $\pi/2$
- Universal behavior in high dimensions
  \[ \beta_d(\alpha) \rightarrow \beta(\sqrt{N}\cos \alpha) \]
- Scaling function is smallest root of parabolic cylinder function
  \[ D_{2\beta}(y) = 0 \]

Exponent is function of one scaling variable, not two
In general, map $N$ one-dimensional walk onto one walk in $N$ dimension with complex boundary conditions.

There are \( \binom{N}{2} = \frac{N(N-1)}{2} \) planes of the type $x_i = x_j$.

These planes divide space into $N!$ “chambers.”

Particle order is unique to each chamber.

The absorbing boundary encloses multiple chambers.

We do not know the shape of the allowed region.

However, we do know the volume of the allowed region.

Equilibrium distribution of particle order

\[
V_m = \frac{m}{N}
\]
Cone approximation

- Fractional volume of allowed region given by equilibrium distribution of particle order
  \[ V_m(N) = \frac{m}{N} \]

- Replace allowed region with cone of same fractional volume
  \[ V(\alpha) = \frac{\int_{0}^{\alpha} d\theta (\sin \theta)^{N-3}}{\int_{0}^{\pi} d\theta (\sin \theta)^{N-3}} \]
  \[ d\Omega \propto \sin^{d-2} \theta \, d\theta \]
  \[ d = N - 1 \]

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

- Good approximation for four particles

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<tr>
<th></th>
<th>1</th>
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<th>3</th>
</tr>
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<tbody>
<tr>
<td>( m )</td>
<td>1/4</td>
<td>1/2</td>
<td>3/4</td>
</tr>
<tr>
<td>( V_m )</td>
<td>1/4</td>
<td>1/2</td>
<td>3/4</td>
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<tr>
<td>( \beta_{\text{cone}}^m )</td>
<td>0.888644</td>
<td>1/2</td>
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Small number of particles

• By construction, cone approximation is exact for $N=3$
• Cone approximation gives a formal lower bound

![Graphs showing the approximation for different values of $N$](image)

Excellent, consistent approximation!

Rayleigh 1877
Faber-Krahn theorem
Very large number of particles \((N \to \infty)\)

- Equilibrium distribution is simple
  \[
  V_m = \frac{m}{N}
  \]

- 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
  \[
  \beta_m(N) \to \beta(x) \quad \text{with} \quad x = m/N
  \]

- Scaling function is root of equation involving parabolic cylinder function
  \[
  D_{2\beta} \left( \sqrt{2} \text{erfc}^{-1}(2x) \right) = 0
  \]

Scaling law for scaling exponents!
Simulation results

\[ D_{2\beta}(2^{1/2} \text{erfc}^{-1}(2x)) = 0 \]

Numerical simulation of diffusion in 10,000 dimensions!
Cone approximation is asymptotically exact!
Extreme exponents

- Extremal behavior of first-passage exponents

\[ \beta(x) \approx \begin{cases} 
\frac{1}{4} \ln \frac{1}{2x} & x \to 0 \\
(1 - x) \ln \frac{1}{2(1-x)} & x \to 1 
\end{cases} \]

- Probability leader never loses the lead (capture problem)

\[ \beta_1 \approx \frac{1}{4} \ln N \]

- Probability leader never becomes last (laggard problem)

\[ \beta_{N-1} \approx \frac{1}{N} \ln N \]

- Both agree with previous heuristic arguments

Krapivsky 02

Extremal exponents can not be measured directly
Indirect measurement via exact scaling function
**Small number of particles**

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<tr>
<th>$N$</th>
<th>$\beta_{1}^{\text{cone}}$</th>
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Decent approximation for the exponents even for small number of particles
Summary

• First-passage kinetics are rich
• Family of first-passage exponents
• Cone approximation gives good estimates for exponents
• Exponents follow a scaling behavior in high dimensions
• Cone approximation yields the exact scaling function
• Combine equilibrium distribution and geometry to obtain exact or approximate nonequilibrium behavior, namely, first-passage kinetics
Outlook

• Heterogeneous Diffusion
• Accelerated Monte Carlo methods
• Scaling occurs in general
• Cone approximation: sometimes exact,
• is not always asymptotically exact
• Geometric proof for exactness
• Limiting shapes in general
Cone approximation is asymptotically exact!
Number of particles avoiding the origin

Counter example: cone is not limiting shape