First Passage in High Dimensions

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E. Ben-Naim and P.L. Krapivsky, J. Phys. A **43**, 495007 & 495008 (2010)

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

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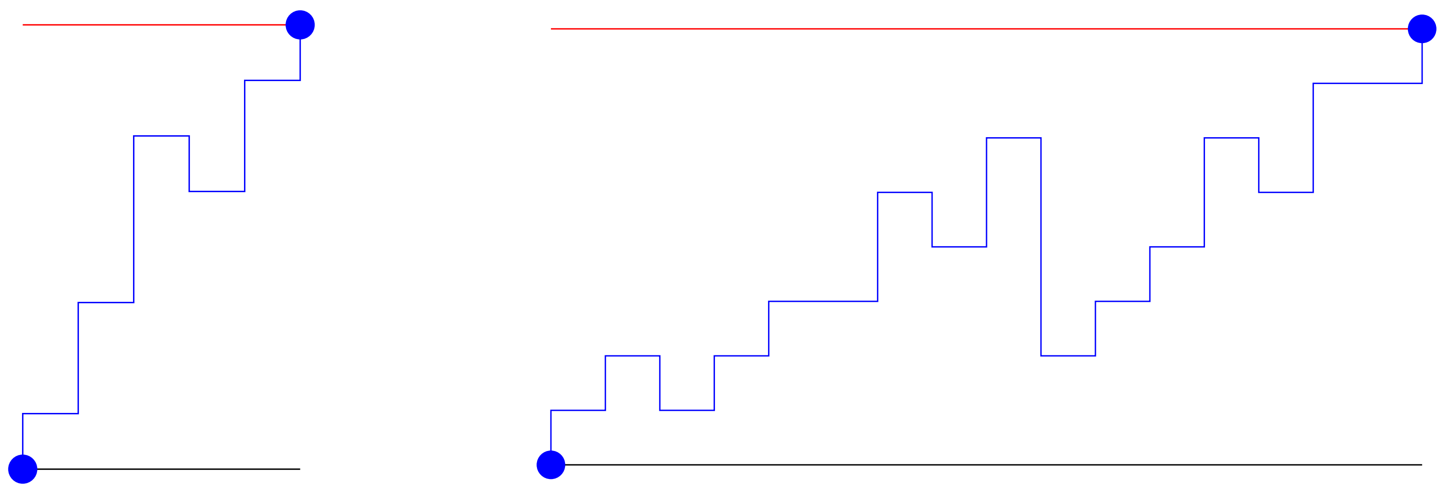
Outline

1. First Passage 101
2. The capture problem = ordering of multiple random walks
3. First passage in a spherical cone
4. The cone approximation

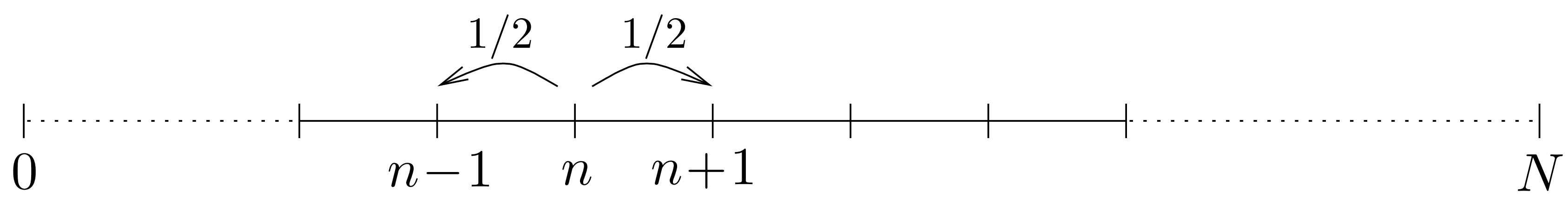
First-Passage Processes



- 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.

S. Redner, A Guide to First-Passage Processes, 2001

Gambler Ruin Problem



- You versus casino. Fair coin. Your wealth = n, Casino = N-n
- Game ends with ruin. What is your winning probability E_n ?
- Winning probability satisfies discrete Laplace equation

$$E_n = \frac{E_{n-1} + E_{n+1}}{2}$$

$$\nabla^2 E = 0$$

- Boundary conditions are <u>crucial</u>

$$E_0 = 0 \qquad \text{and} \qquad E_N = 1$$

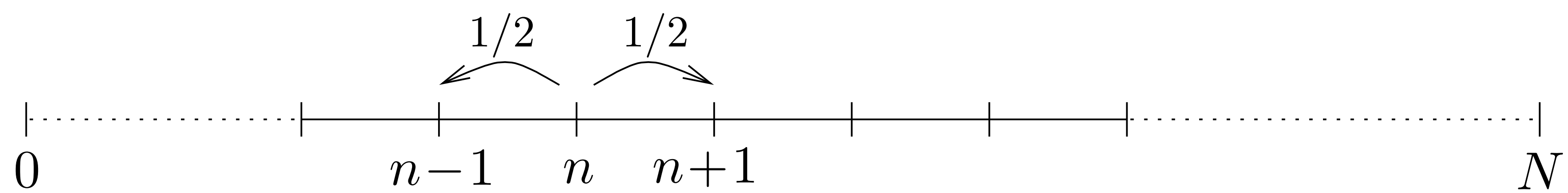
- Winning probability is proportional to your wealth

$$E_n = \frac{n}{N}$$

Feller 1968

First-passage probability satisfies a simple equation

First-Passage Time



- Average duration of game is T_n
- Duration satisfies discrete Poisson equation

$$T_n = \frac{T_{n-1}}{2} + \frac{T_{n+1}}{2} + 1 \qquad D\nabla^2 T = -1$$

- Boundary conditions: $T_0 = T_N = 0$
- Duration is quadratic

$$T_n = n(N-n)$$

- Small wealth = short game, big wealth = long game

$$T_n \sim \begin{cases} N & n = \mathcal{O}(1) \\ N^2 & n = \mathcal{O}(N) \end{cases} \qquad \begin{aligned} D\nabla^2(T_+E_+) &= -E_+ \\ D\nabla^2(T_-E_-) &= -E_- \end{aligned}$$

First-passage time satisfies a simple equation

Brute Force Approach

- Start with time-dependent diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = D\nabla^2 P(x,t)$$

- Impose absorbing boundary conditions & initial conditions

$$P(x,t)\big|_{x=0} = P(x,t)\big|_{x=N} = 0 \quad \text{and} \quad P(x,t=0) = \delta(x-n)$$

- Obtain full time-dependent solution

$$P(x,t) = \frac{2}{N}\sum_{l\geq 1} \sin\frac{l\pi x}{N}\sin\frac{l\pi n}{N} e^{-(l\pi)^2 Dt/N^2}$$

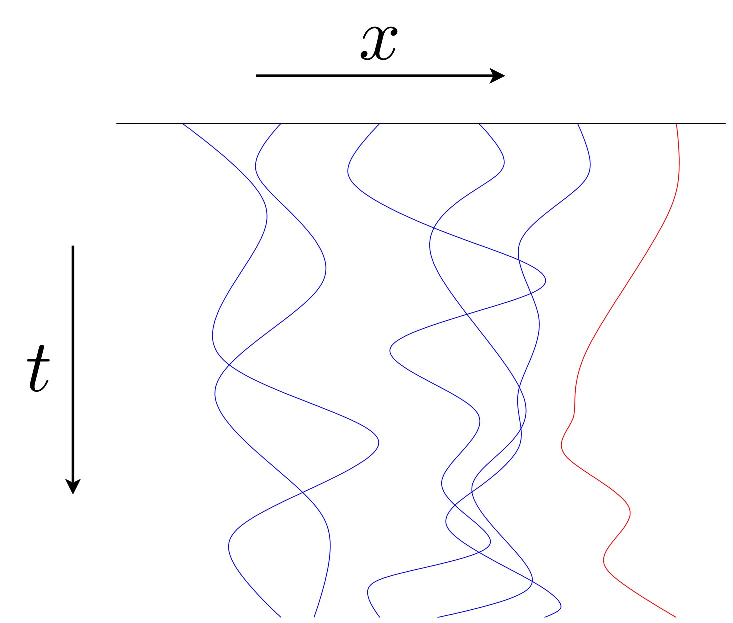
- Integrate flux to calculate winning probability and duration

$$E_n = -\int_0^\infty dt\, D\frac{\partial P(x,t)}{\partial x}\Big|_{x=N} \quad \Longrightarrow \quad E_n = \frac{n}{N}$$

Lesson: focus on quantity of interest

The capture problem

- System: N independent diffusing particles in one dimension
- What is the probability that original leader maintains the lead?
- N Diffusing 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 "lamb" survives "lions" until t
- Independent of initial conditions, power-law asymptotic behavior

$$S(t) \sim t^{-\beta} \qquad \text{as} \qquad t \to \infty$$

- Monte Carlo: nontrivial exponents that depend on N

Bramson 91
Redner 96
benAvraham 02
Grassberger 03

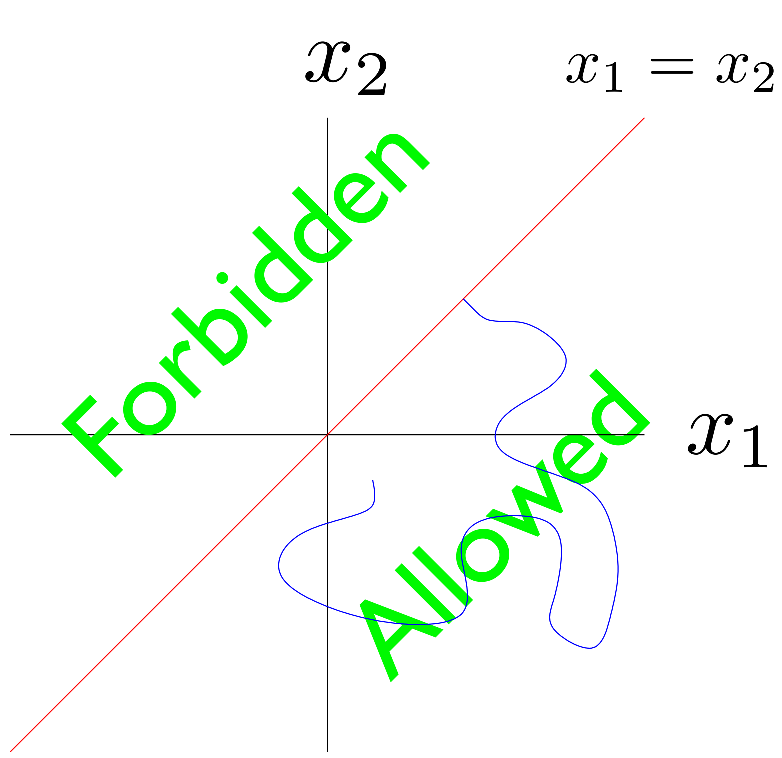
N	2	3	4	5	6	10
$\beta(N)$	$1/2$	$3/4$	0.913	1.032	1.11	1.37

No theoretical computation of exponents

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

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

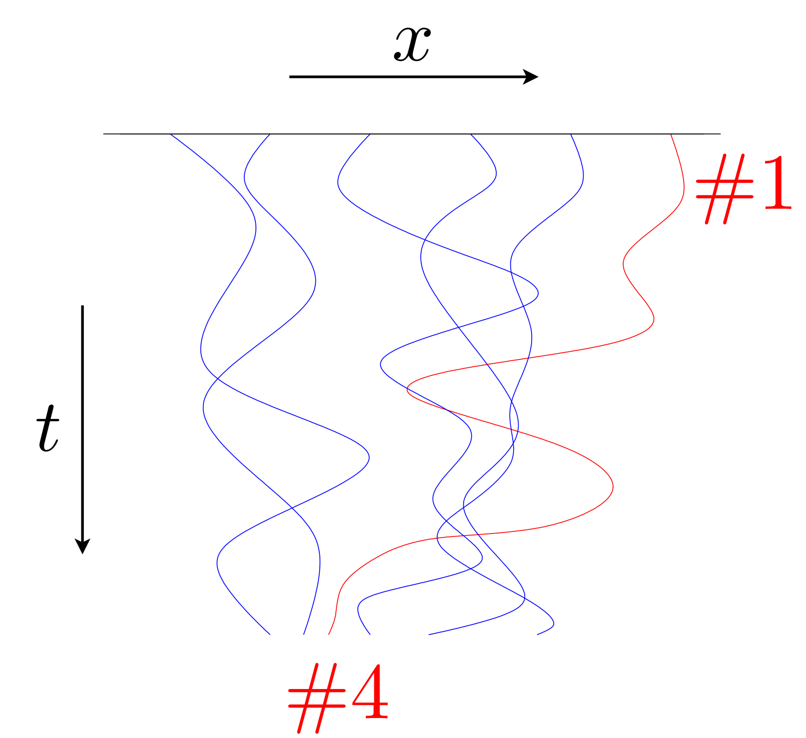


- In general, map N one-dimensional walk onto one walk in N dimension with complex boundary conditions

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 maintains the lead
- $S_{N-1}(t)$ is the probability that leader never becomes laggard
- Power-law asymptotic behavior is generic

$$S_m(t) \sim t^{-\beta_m(N)}$$



- Spectrum of first-passage exponents

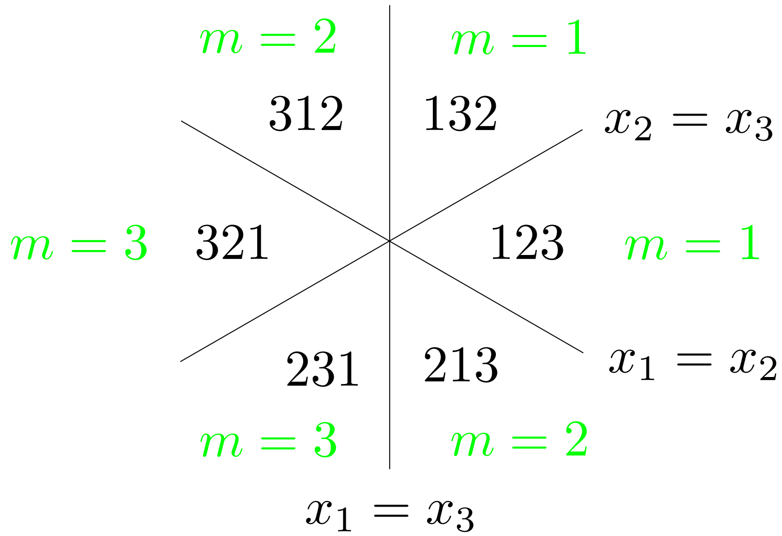
$$\beta_1(N) > \beta_2(N) > \cdots > \beta_{N-1}(N)$$

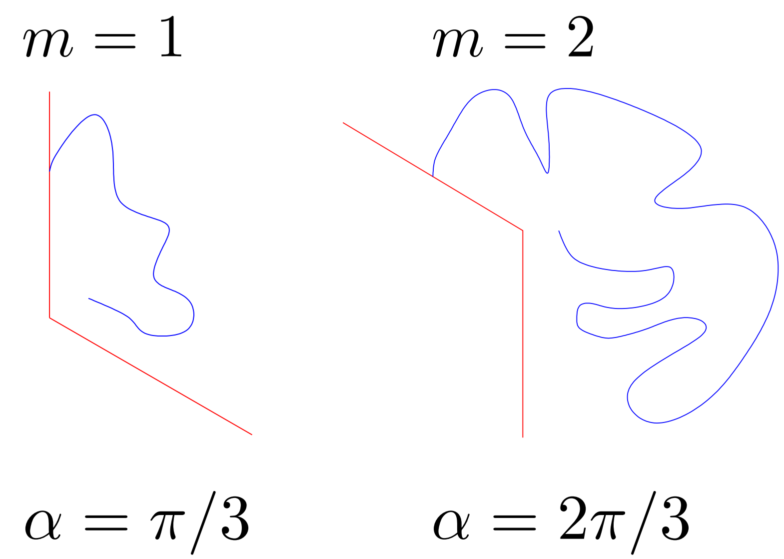
Can't solve the problem? Make it bigger!

Lindenberg 01

Three Particles

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





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

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

Spitzer 58
Fisher 84

- 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

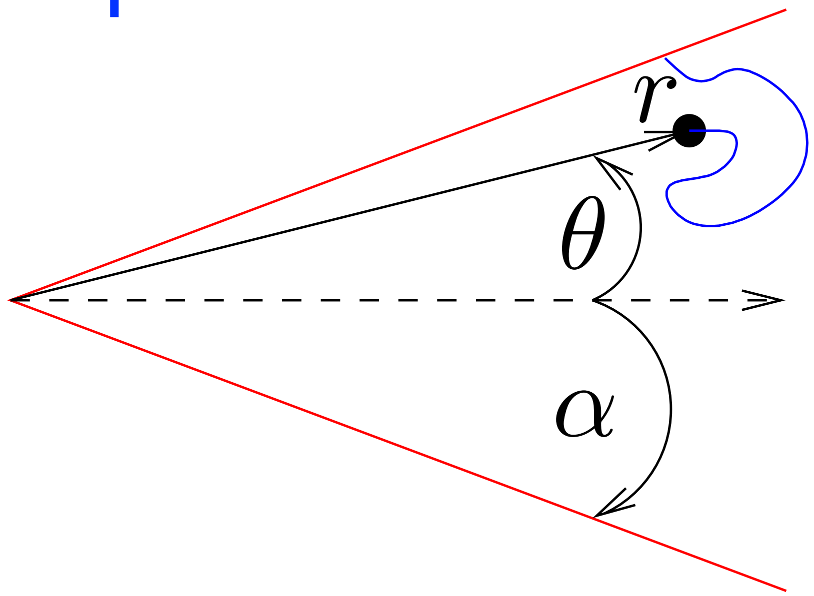
$$S_m\sim t^{-\beta_m}\qquad \text{with}\qquad \beta_1>\beta_2>\cdots>\beta_{N-1}$$

Large spectrum of first-passage exponents

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

$$S(r,\theta,t) \simeq \Phi(r,\theta)\, t^{-\beta}$$

- Amplitude obeys Laplace's equation

$$\nabla^2 \Phi(r,\theta) = 0$$

- Use dimensional analysis

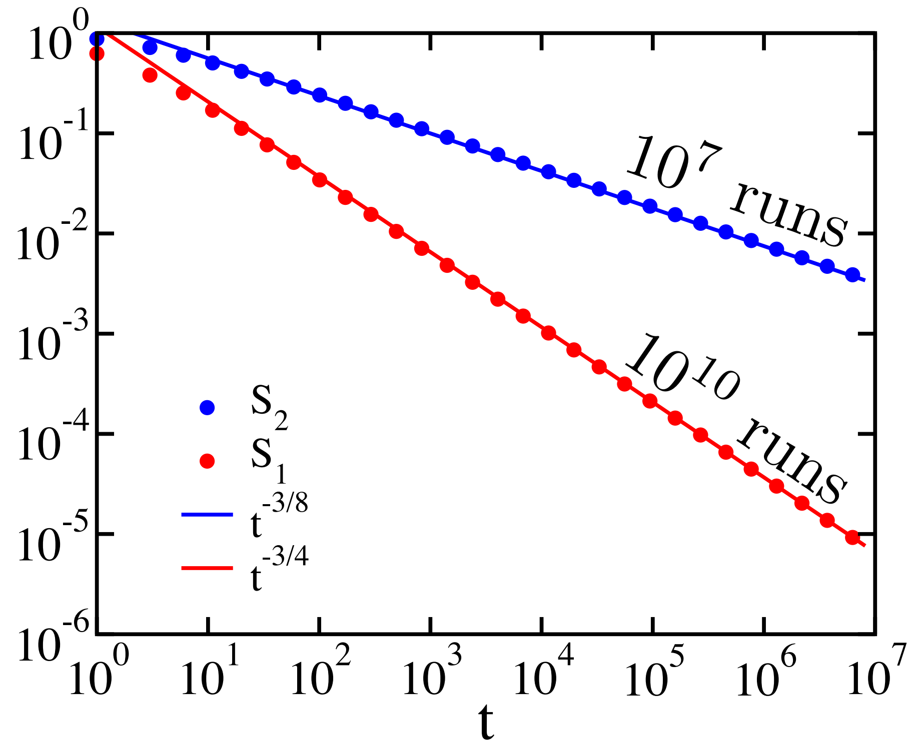
$$\Phi(r,\theta) \sim (r^2/D)^\beta \psi(\theta) \quad \Longrightarrow \quad \psi_{\theta\theta} + (2\beta)^2\psi = 0$$

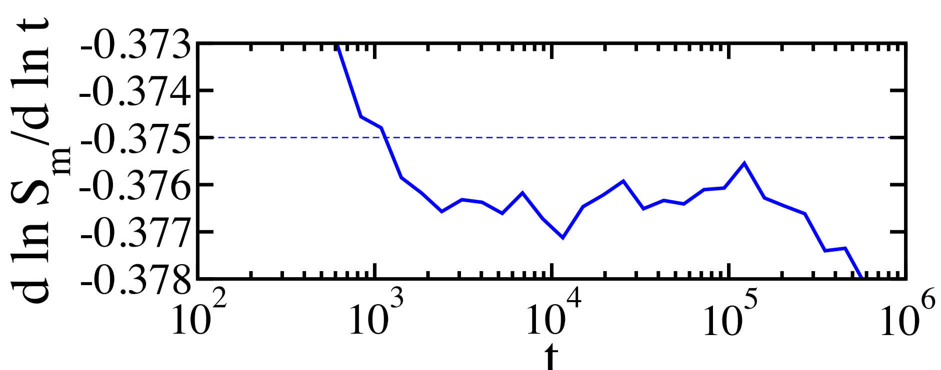
- Enforce boundary condition $S|_{\theta=\alpha} = \Phi|_{\theta=\alpha} = \psi|_{\theta=\alpha}$
- Lowest eigenvalue is the relevant one

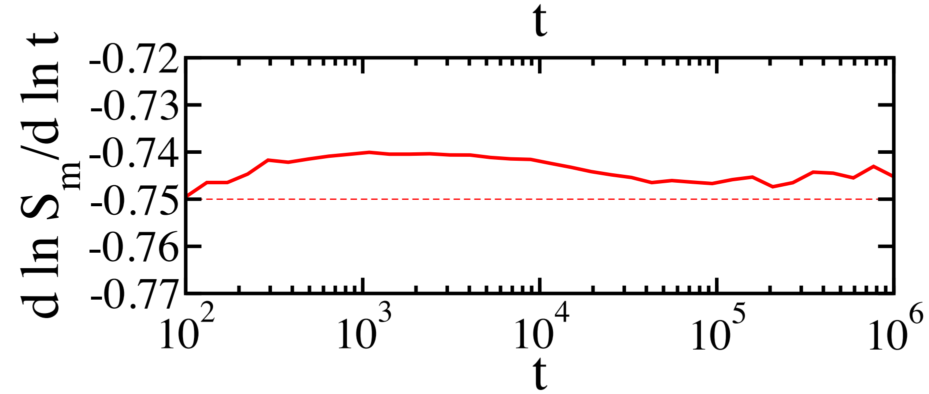
$$\psi_2(\theta) = \cos(2\beta\theta) \quad \Longrightarrow \quad \beta = \frac{\pi}{4\alpha}$$

Monte Carlo Simulations

3 particles

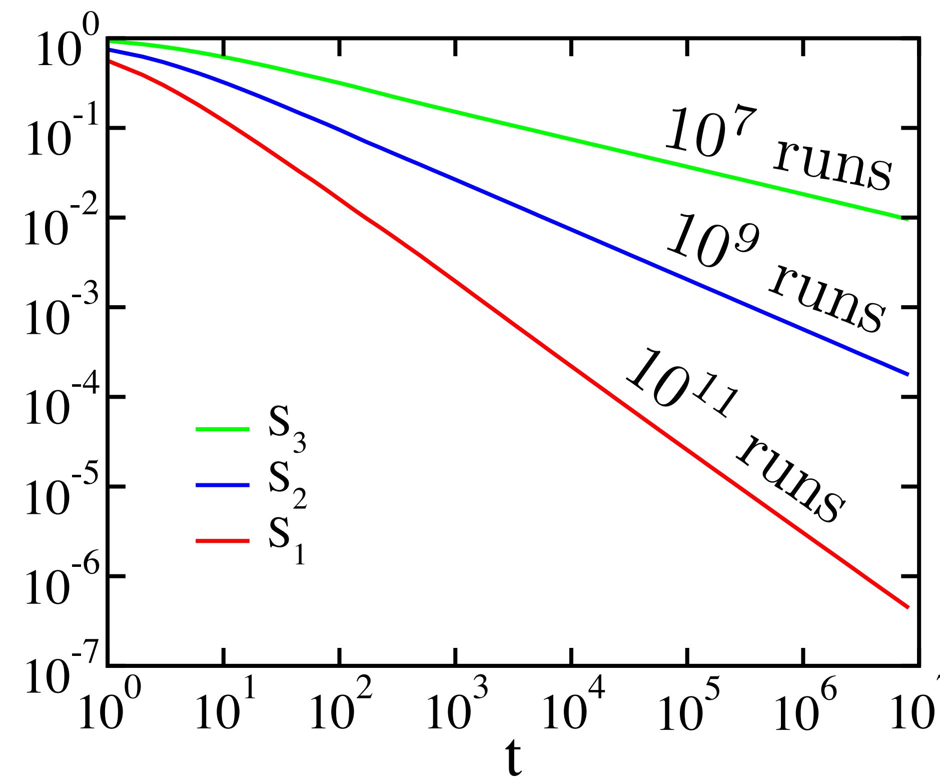






confirm wedge theory results

4 particles



$$\beta_1 = 0.913$$

$$\beta_2 = 0.556$$

$$\beta_3 = 0.306$$

as expected, there are 3 nontrivial exponents

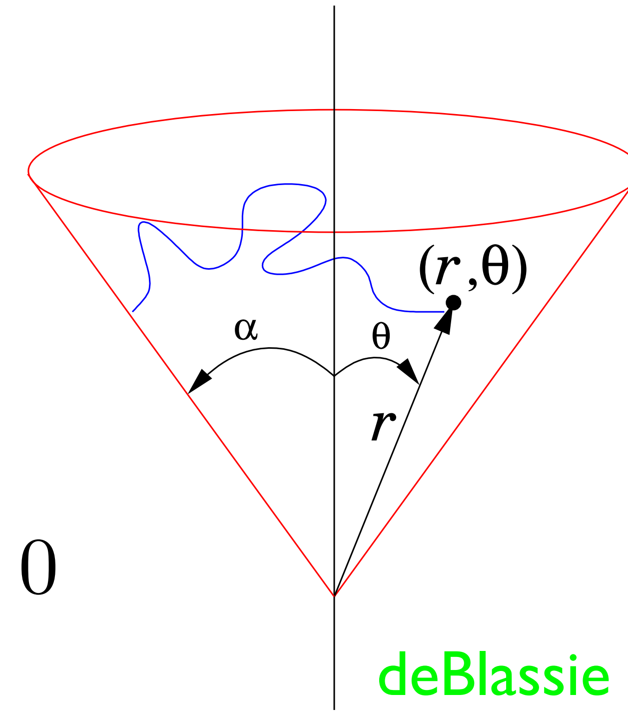
Kinetics of First Passage in a Cone

- Repeat wedge calculation step by step

$$S(r,\theta,t) \sim \psi(\theta)(Dt/r^2)^{-\beta}$$

- Angular function obeys Poisson-like equation

$$\frac{1}{(\sin\theta)^{d-2}}\frac{d}{d\theta}\left[(\sin\theta)^{d-2}\frac{d\psi}{d\theta}\right] + 2\beta(2\beta+d-2)\psi = 0$$



deBlassie 88

- Solution in terms of associated Legendre functions

$$\psi_d(\theta) = \begin{cases} (\sin\theta)^{-\delta} P^{\delta}_{2\beta+\delta}(\cos\theta) & d \text{ odd}, \\ (\sin\theta)^{-\delta} Q^{\delta}_{2\beta+\delta}(\cos\theta) & d \text{ even} \end{cases} \qquad \delta = \frac{d-3}{2}$$

- Enforce boundary condition, choose lowest eigenvalue

$$P^{\delta}_{2\beta+\delta}(\cos\alpha) = 0 \qquad d \text{ odd},$$
$$Q^{\delta}_{2\beta+\delta}(\cos\alpha) = 0 \qquad d \text{ even}.$$

Exponent is nontrivial root of Legendre function

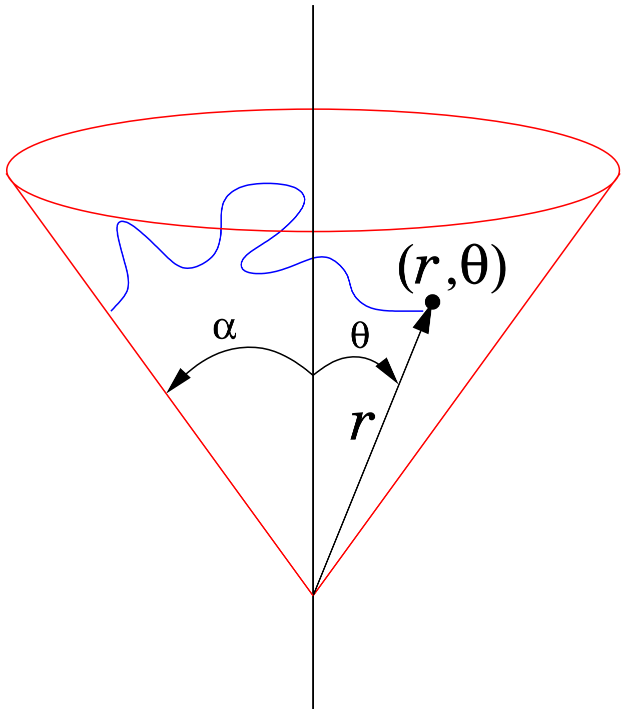
Additional Results

- 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

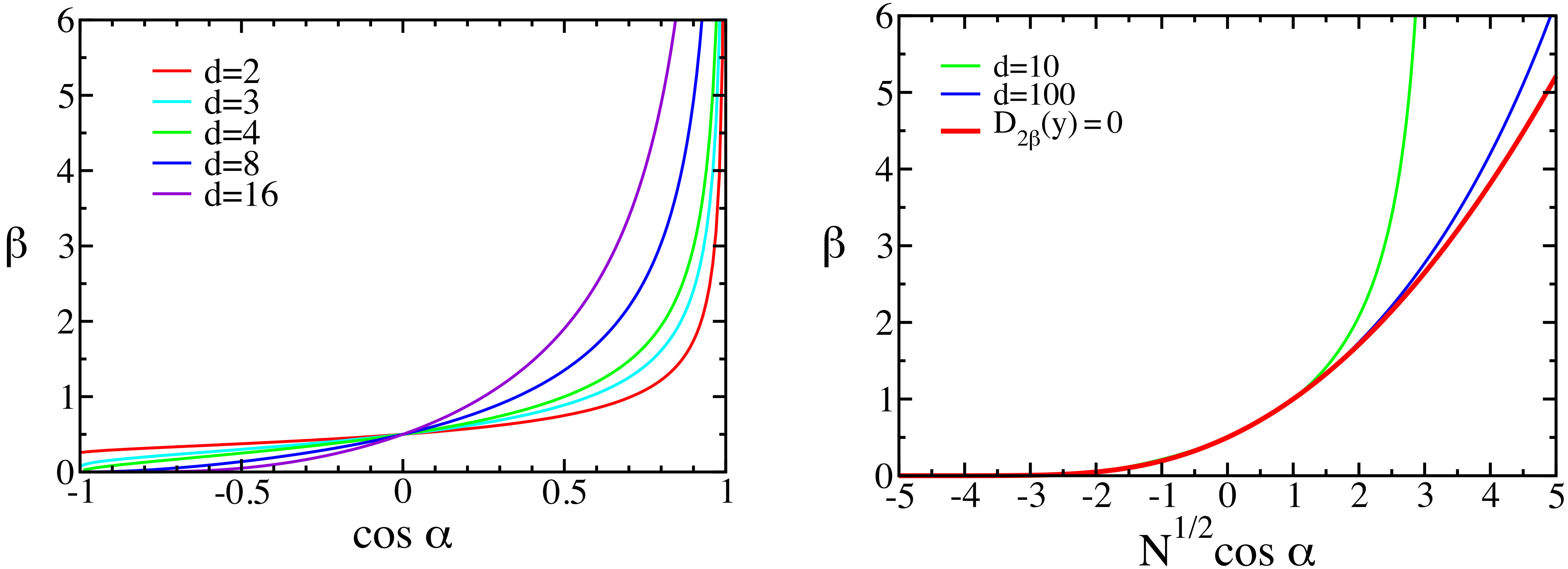
$$D\nabla^2 T(r,\theta) = -1$$

- First-passage time (when finite)

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

$$\alpha < \cos^{-1}(1/\sqrt{d})$$

High Dimensions



- Exponent varies sharply for opening angles near $\pi/2$
- Universal behavior in high dimensions

$$\beta_d(\alpha) \to \beta(\sqrt{N}\cos\alpha)$$

- Scaling function is smallest root of parabolic cylinder function

$$D_{2\beta}(y) = 0$$

Exponent is function of one scaling variable, not two

Asymptotic Analysis

- Limiting behavior of scaling function

$$\beta(y) \simeq \begin{cases} \sqrt{y^2/8\pi}\,\exp\left(-y^2/2\right) & y \to -\infty, \\ y^2/8 & y \to \infty. \end{cases}$$

- Thin cones: exponent diverges

$$\beta_d(\alpha) \simeq B_d \alpha^{-1} \quad \text{with} \quad J_\delta(2B_d) = 0$$

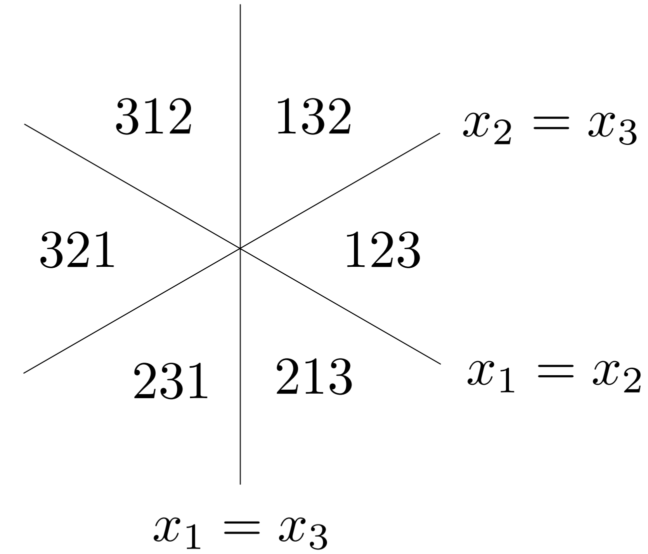
- Wide cones: exponent vanishes when $d \geq 3$

$$\beta_d(\alpha) \simeq A_d\,(\pi - \alpha)^{d-3} \quad \text{with} \quad A_d = \frac{1}{2} B\left(\frac{1}{2}, \frac{d-3}{2}\right)$$

- A needle is reached with certainty only when $d < 3$
- Large dimensions

$$\beta_d(\alpha) \simeq \begin{cases} \frac{d}{4}\left(\frac{1}{\sin\alpha} - 1\right) & \alpha < \pi/2, \\ C(\sin\alpha)^d & \alpha > \pi/2. \end{cases}$$

Diffusion in High Dimensions

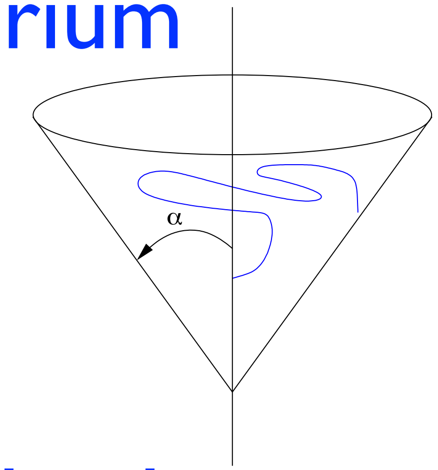


- In general, map N one-dimensional walk onto one walk in N dimension with complex boundary conditions
- There are $\binom{N}{2} = \frac{N(N-1)}{2}$ planes of the type $x_i = x_j$
- These planes divide space into $N!$ "chambers"
- Particle order is unique to each chamber
- The absorbing boundary encloses 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

$$Q^{\gamma}_{2\beta+\gamma}(\cos\alpha) = 0 \qquad N \text{ odd},$$
$$P^{\gamma}_{2\beta+\gamma}(\cos\alpha) = 0 \qquad N \text{ even}.$$

$$\gamma = \frac{N-4}{2}$$

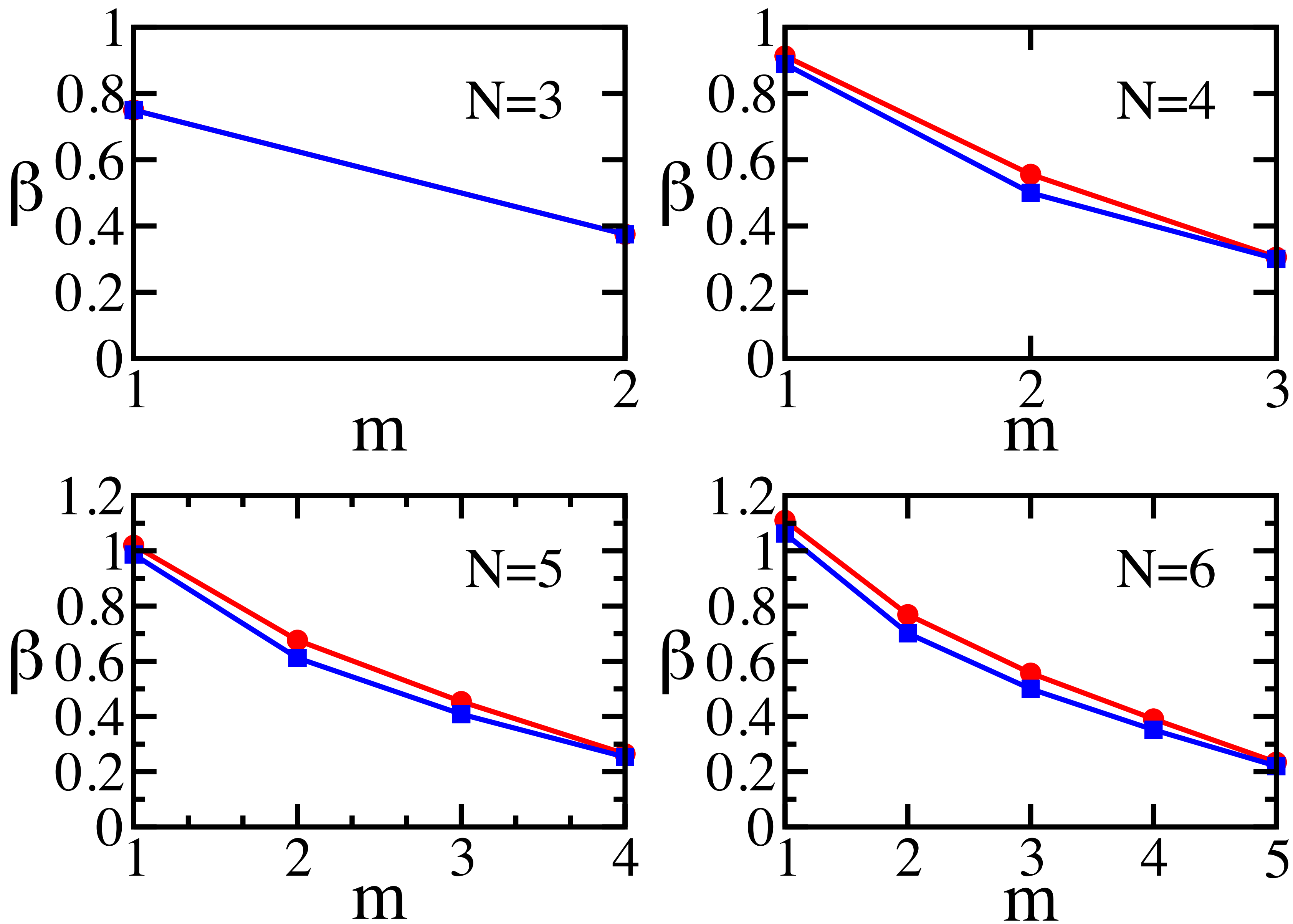
- Good approximation for four particles

m	1	2	3
V_m	$1/4$	$1/2$	$3/4$
β_m^{cone}	0.888644	$1/2$	0.300754
β_m	0.913	0.556	0.306

Small Number of Particles

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

Rayleigh 1877
Faber-Krahn theorem



Excellent, consistent approximation!

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

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

- First-passage exponent has the scaling form

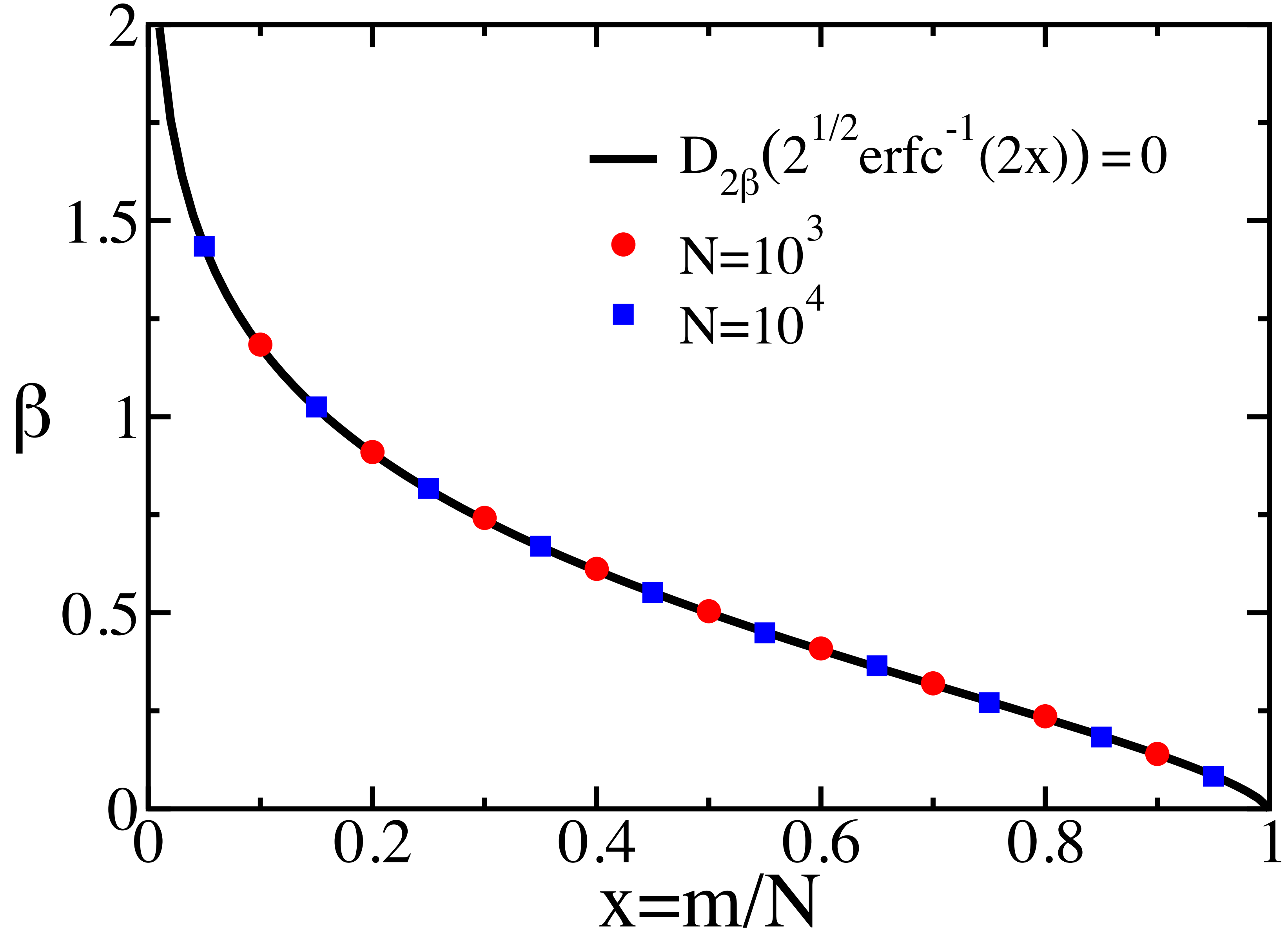
$$\beta_m(N) \to \beta(x) \quad \text{with} \quad x = m/N$$

- 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

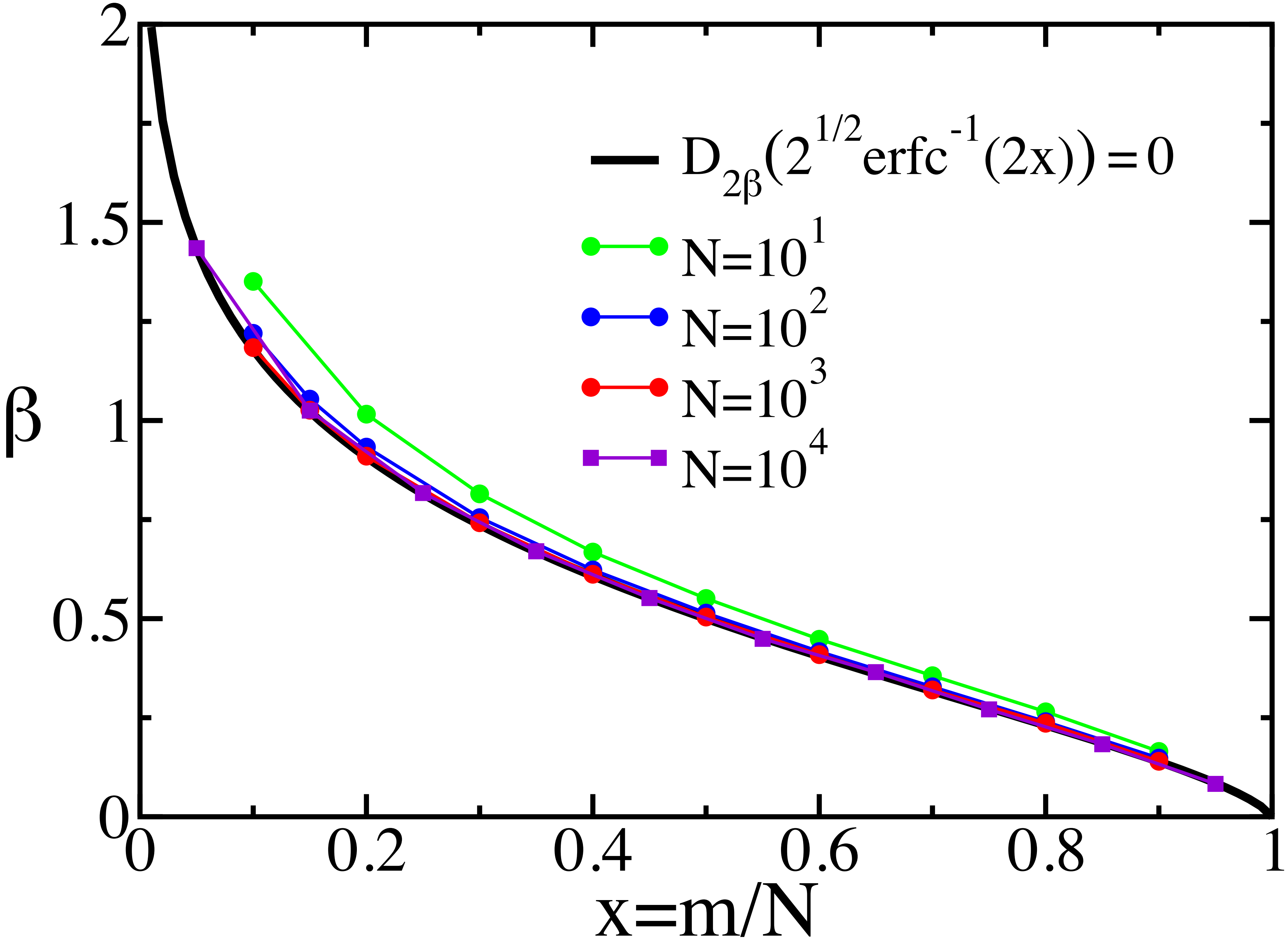


Numerical simulation of diffusion in 10,000 dimensions!

Only 10 measurements confirm scaling function!

Cone approximation is asymptotically exact!

Approach to Scaling



Scaling function converges quickly

Is spherical cone a limiting shape?

Small Number of Particles

N	β_1^{cone}	β_1
3	$3/4$	$3/4$
4	0.888644	0.91
5	0.986694	1.02
6	1.062297	1.11
7	1.123652	1.19
8	1.175189	1.27
9	1.219569	1.33
10	1.258510	1.37

N	$\beta_{N-1}^{\text{cone}}$	β_{N-1}
2	$1/2$	$1/2$
3	$3/8$	$3/8$
4	0.300754	0.306
5	0.253371	0.265
6	0.220490	0.234
7	0.196216	0.212
8	0.177469	0.190
9	0.162496	0.178
10	0.150221	0.165

Decent approximation for the exponents even for small number of particles

Extreme Exponents

- Extremal behavior of first-passage exponents

$$\beta(x) \simeq \begin{cases} \frac{1}{4} \ln \frac{1}{2x} & x \to 0 \\ (1-x) \ln \frac{1}{2(1-x)} & x \to 1 \end{cases}$$

- Probability leader never loses the lead (capture problem)

$$\beta_1 \simeq \frac{1}{4} \ln N$$

- Probability leader never becomes last (laggard problem)

$$\beta_{N-1} \simeq \frac{1}{N} \ln N$$

- Both agree with previous heuristic arguments

Krapivsky 02

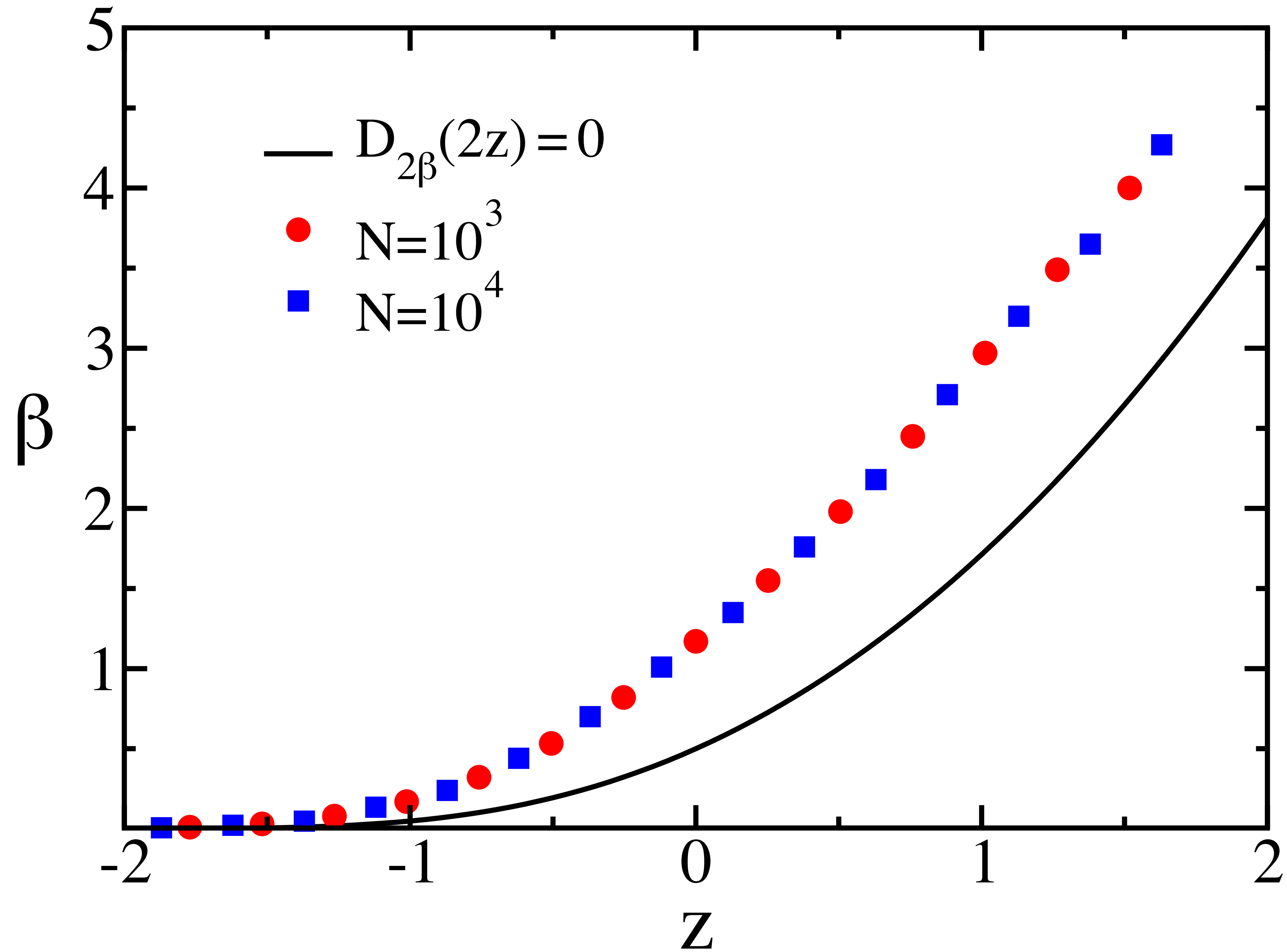
Extremal exponents can not be measured directly
Indirect measurement via exact scaling function

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 approach is not always asymptotically exact
- Geometric proof for exactness
- Limiting shapes in general



Counter example: cone is not limiting shape