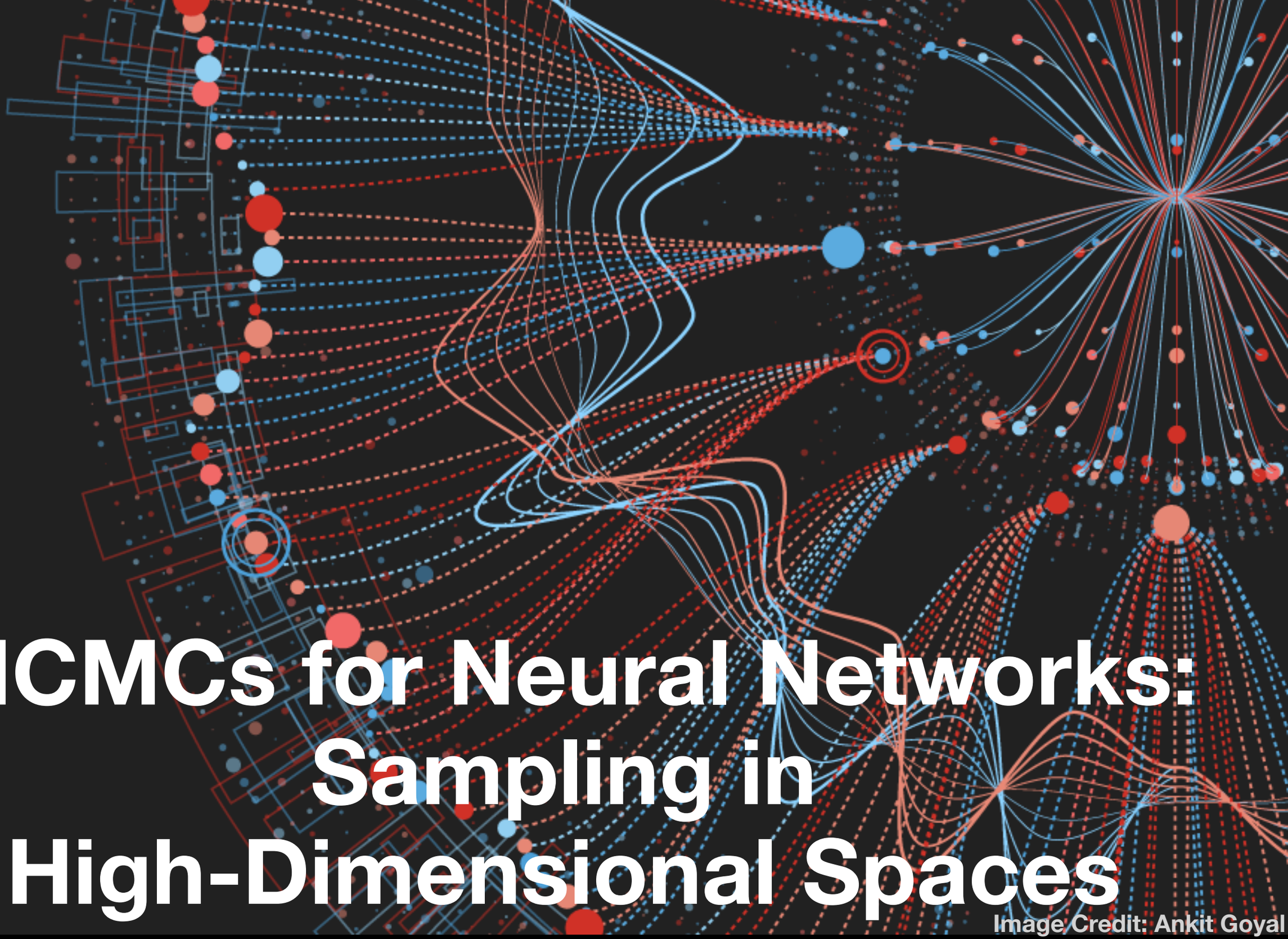


MCMCs for Neural Networks: Sampling in High-Dimensional Spaces

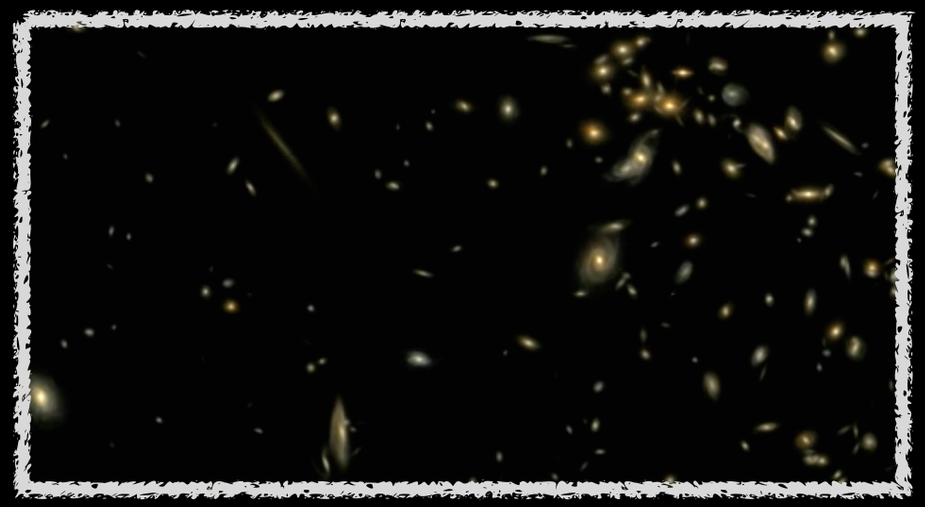
Image Credit: Ankit Goyal

Peter Behroozi (he/him)
U. Arizona + NAOJ

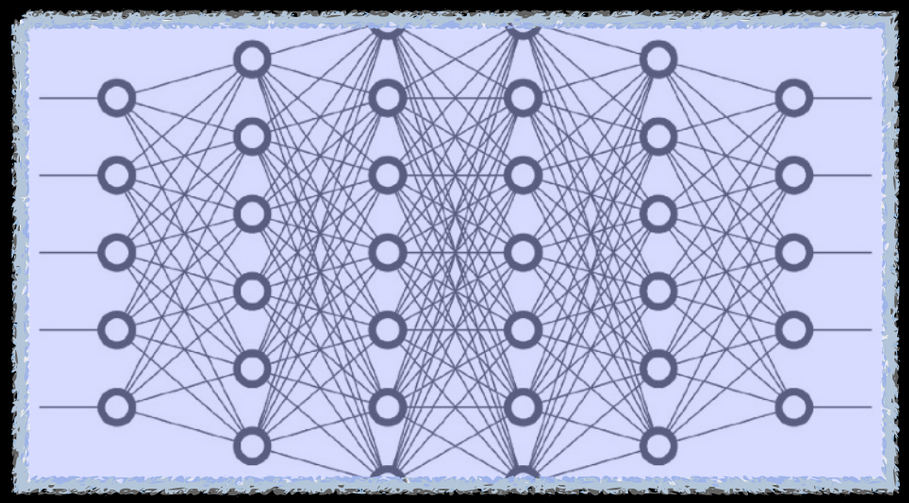
KITP-Galevo23

This talk will be very informal.

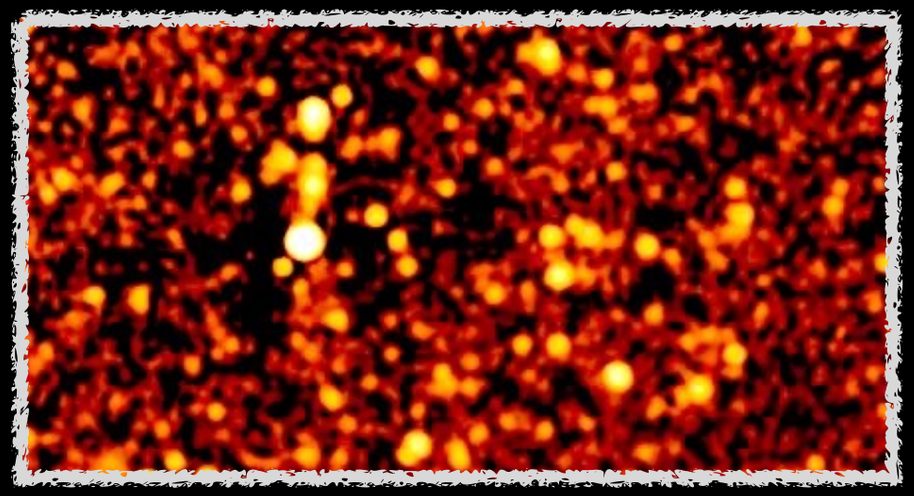
Motivation



Empirical Galaxy Modeling
50-100 dimensions



Deep Neural Networks
100-10^{14} dimensions



Confused Source Recovery
100 - 10^9 dimensions

Constrained Realizations
> 10^9 dimensions

Peter Behroozi

Image Credits: SDSS, Radu Raicea, Jim Condon, CLUES

MCMC Review

Observations

$$\mathcal{L}(x) = \exp(-\chi^2/2)$$

Parameter space → **MCMC**

Range of allowed parameters

MCMC Review

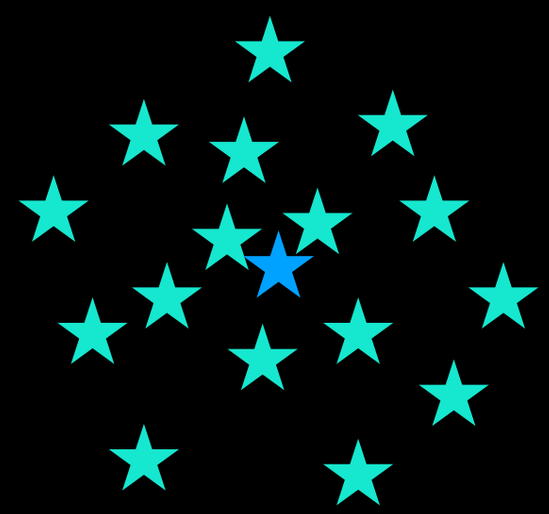
$$\pi(\mathbf{x} :\rightarrow \mathbf{y})$$

Transition Probability Density

MCMC Review

$$\pi(\mathbf{x} :\rightarrow \mathbf{y})$$

Transition Probability Density

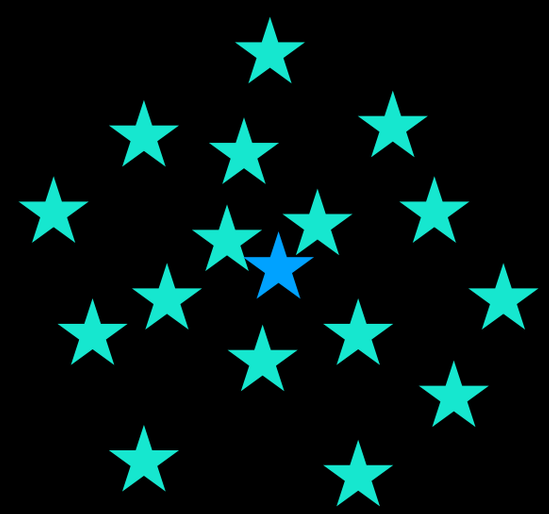


Gaussian Random Walk
(Metropolis-Hastings)

MCMC Review

$$\pi(\mathbf{x} :\rightarrow \mathbf{y})$$

Transition Probability Density



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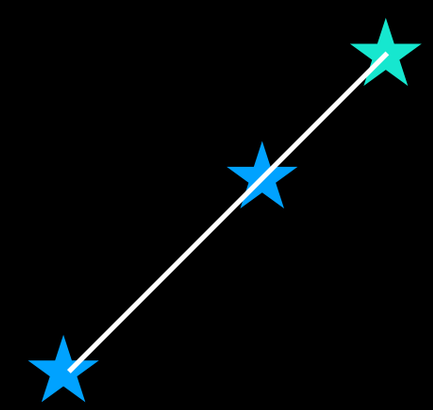
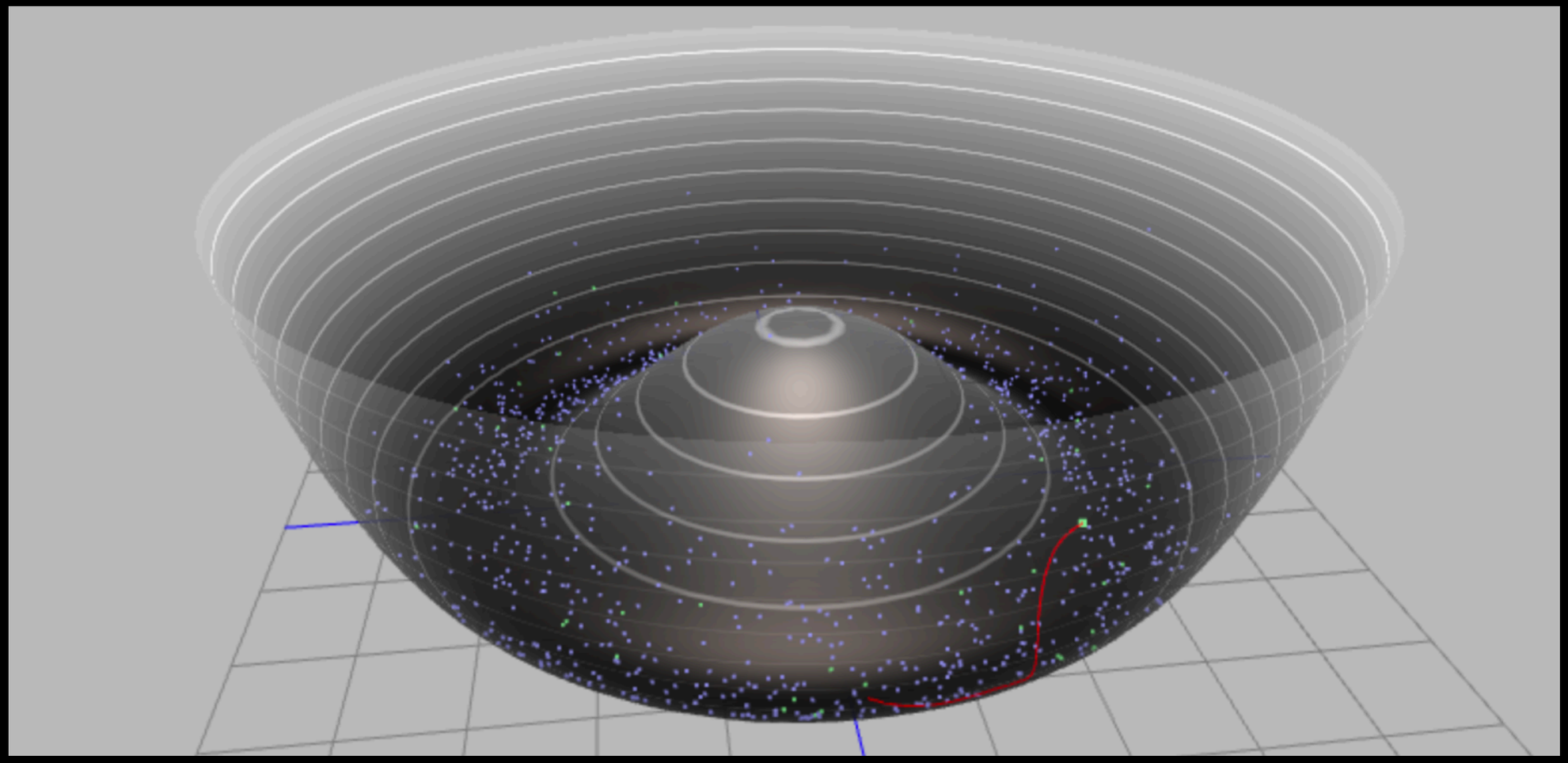


Stretch Step
(Goodman & Weare)

MCMC Review

$$\pi(\mathbf{x} :\rightarrow \mathbf{y})$$

Transition Probability Density



Hamiltonian Monte Carlo

https://arogozhnikov.github.io/2016/12/19/markov_chain_monte_carlo.html

High-D Spaces (D>10)

High-D Spaces (D>10)

$$P(\vec{x}) \propto \exp(-x^2)$$

Gaussian Distribution

High-D Spaces (D>10)

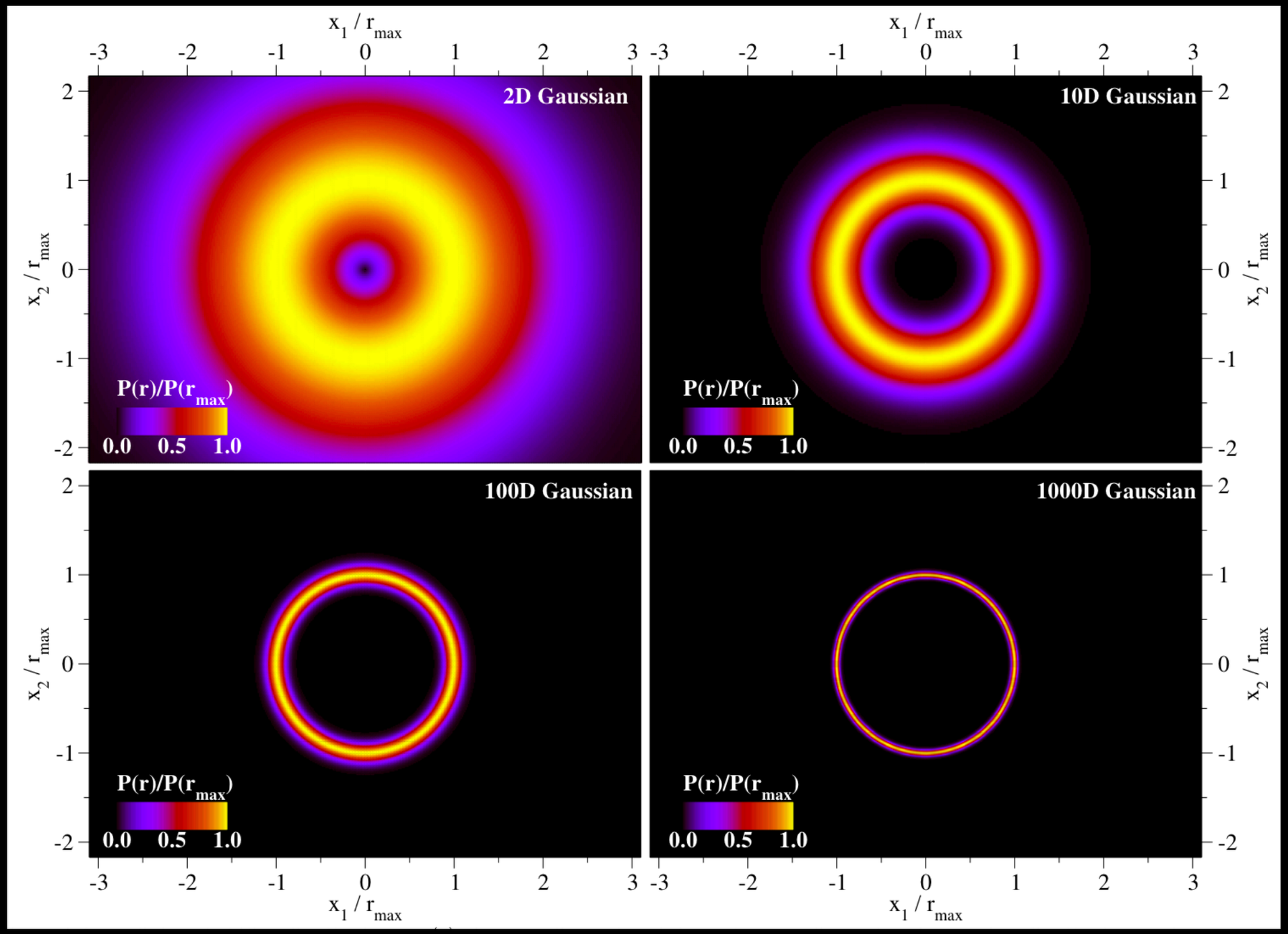
$$P(\vec{x}) \propto \exp(-x^2)$$

Gaussian Distribution

$$P(r) \propto r^{D-1} \exp(-r^2)$$

Distribution of Radii

High-D Spaces (D>10)



High-D Spaces (D>10)

Coffee

Lemon

Pizza

Credits: Julius Schorzman; https://food.ndtv.com/ingredient/lemon-701101; Valerio Capello

High-D Spaces (D>10)

Coffee

$\cdot$

Pizza

$=$

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$=$

$$|\text{Coffee}||\text{Pizza}|\cos\theta$$

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High-D Spaces (D>10)

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Pizza

$=$

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High-D Spaces (D>10)

Coffee

$\cdot$

Pizza

$=$

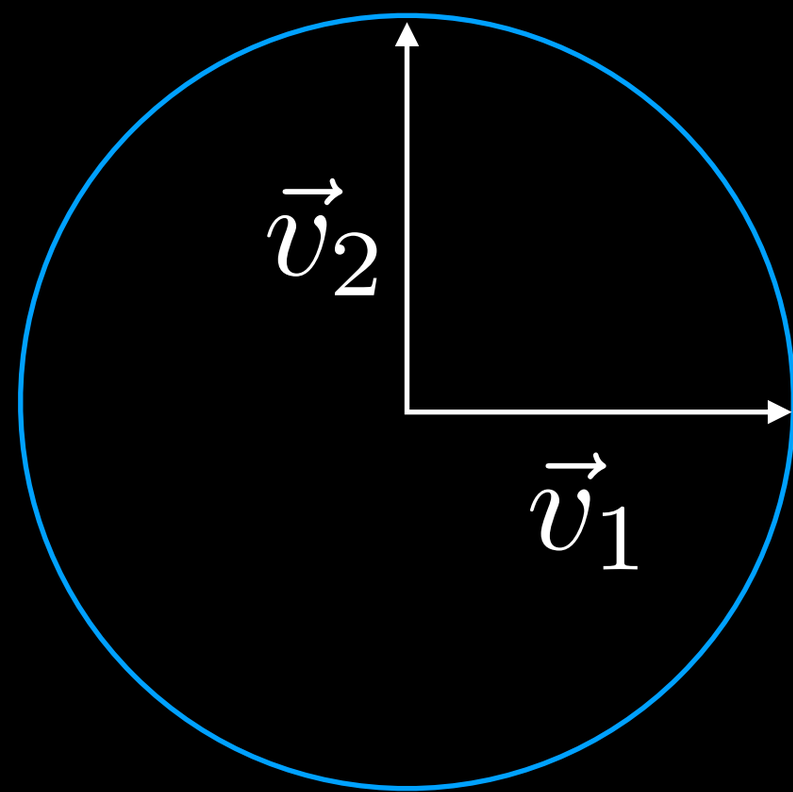
$$|\text{Coffee}||\text{Pizza}|\cos\theta \sim 0$$

$$\langle(\hat{v}_1 \cdot \hat{v}_2)^2\rangle = \frac{1}{D}$$

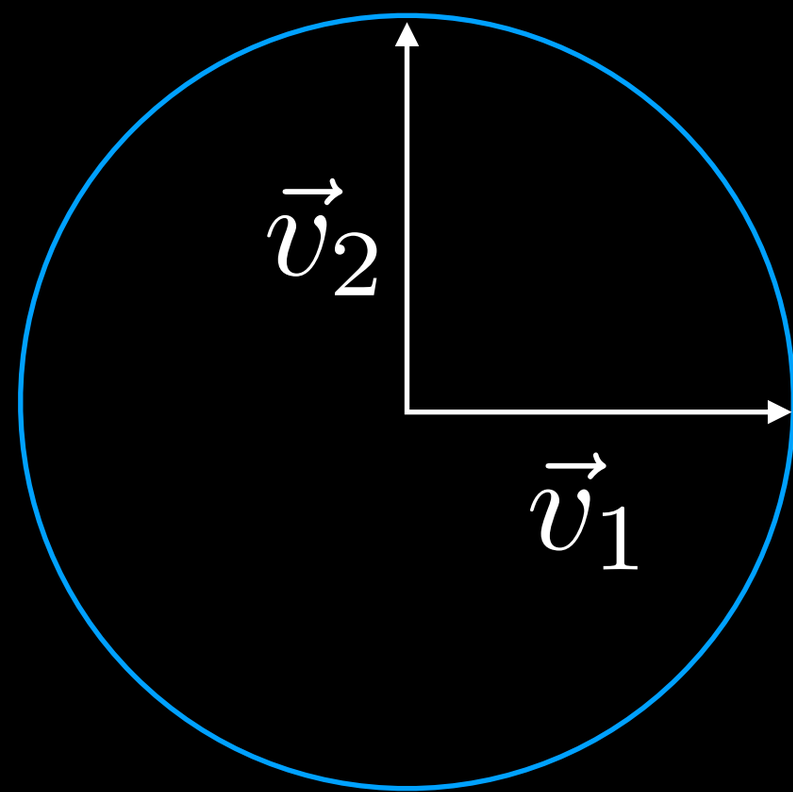
Random vectors in high dimensional spaces are orthogonal!

Credits: Julius Schorzman; https://food.ndtv.com/ingredient/lemon-701101; Valerio Capello

High-D Spaces



Why is it so hard?



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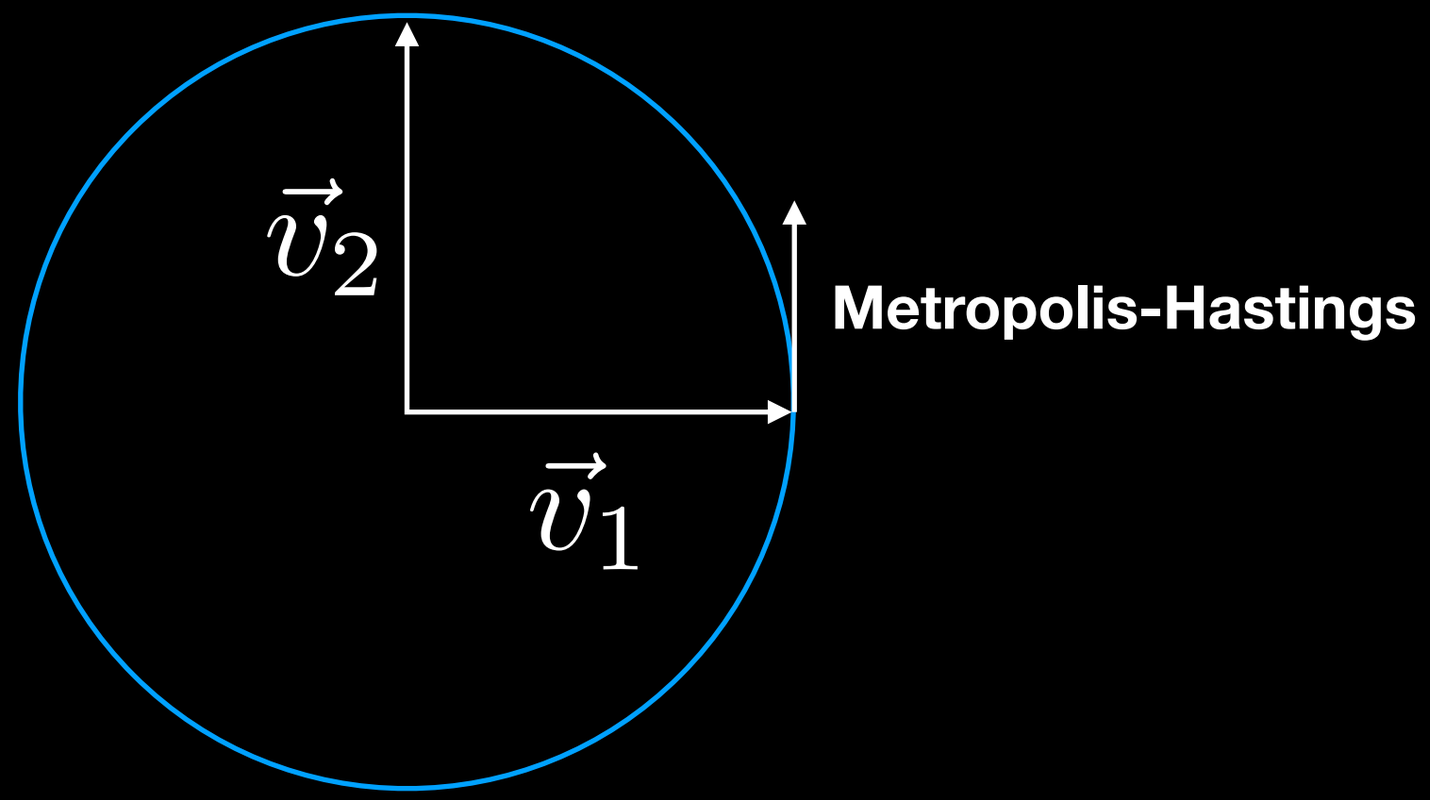

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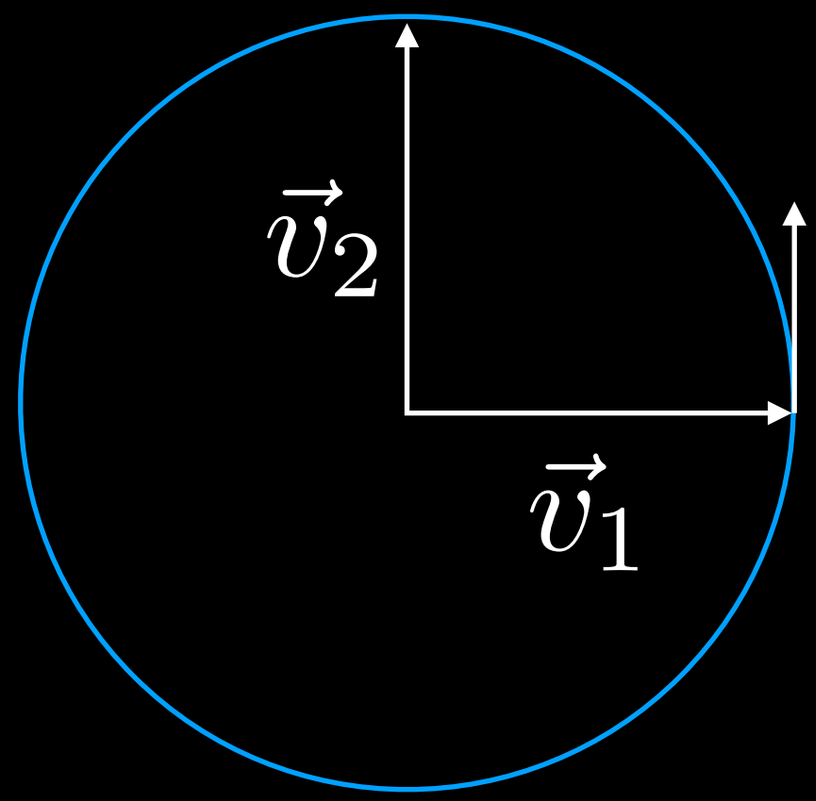
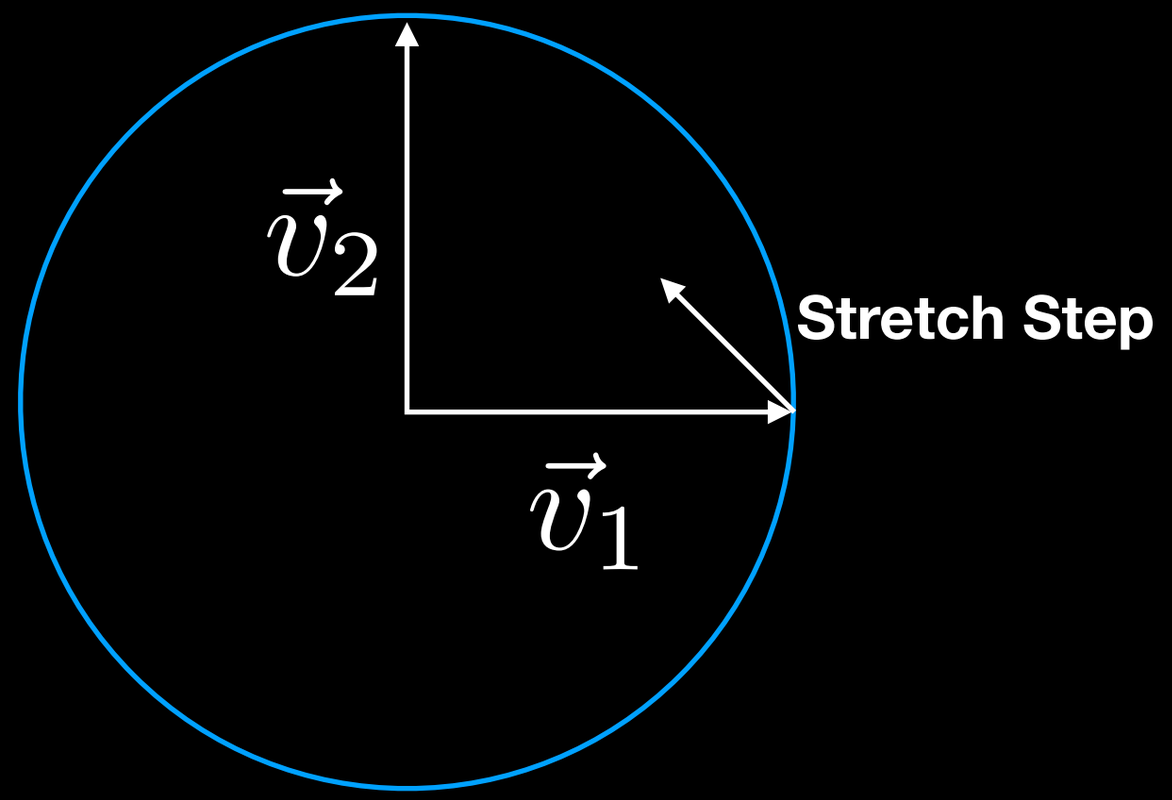


Metropolis-Hastings

$\mathcal{O}(D)$

Why is it so hard?



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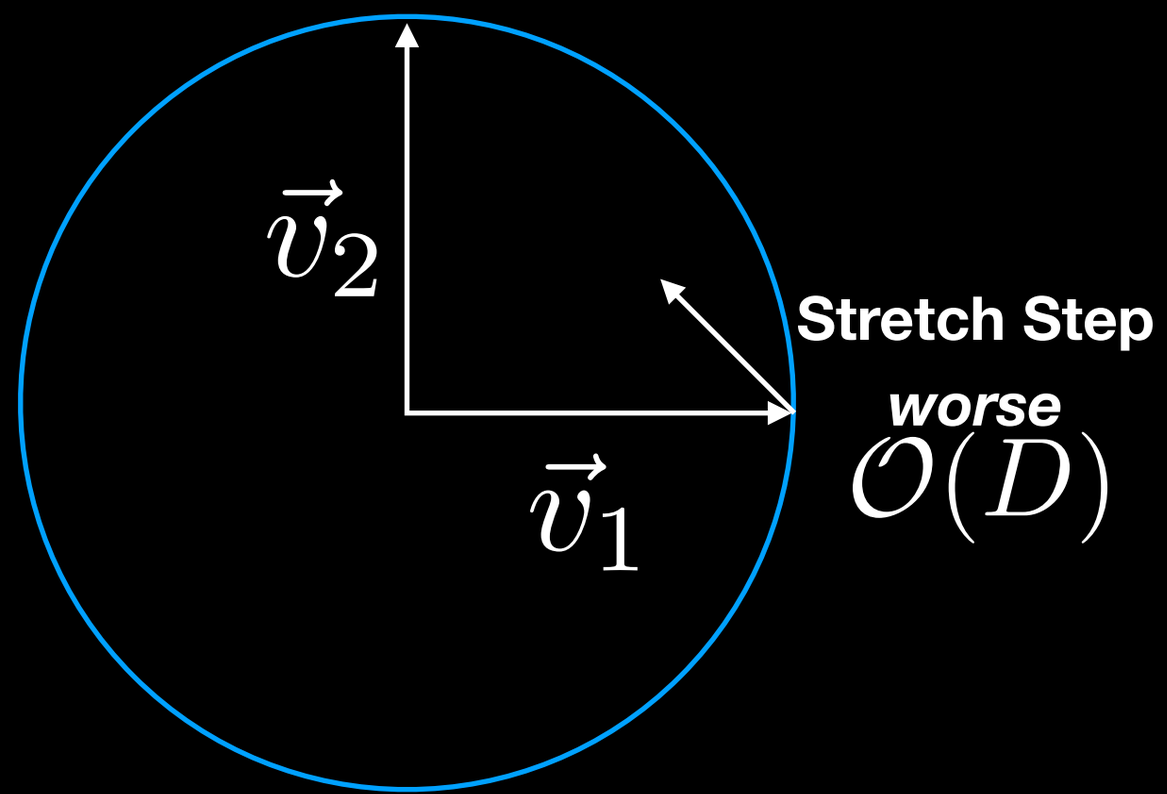

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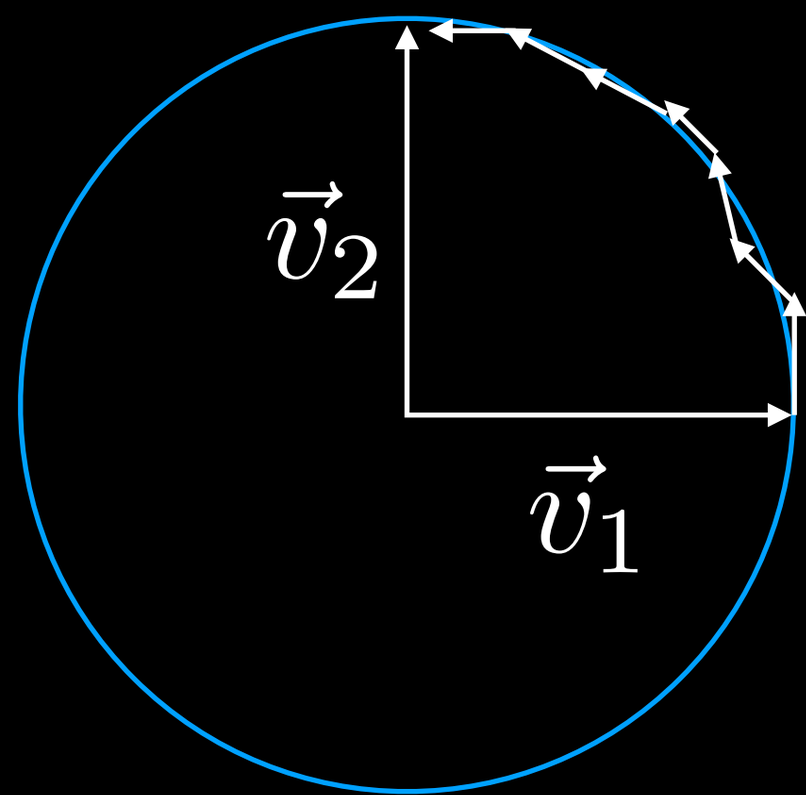


Hamiltonian MC

Metropolis-Hastings

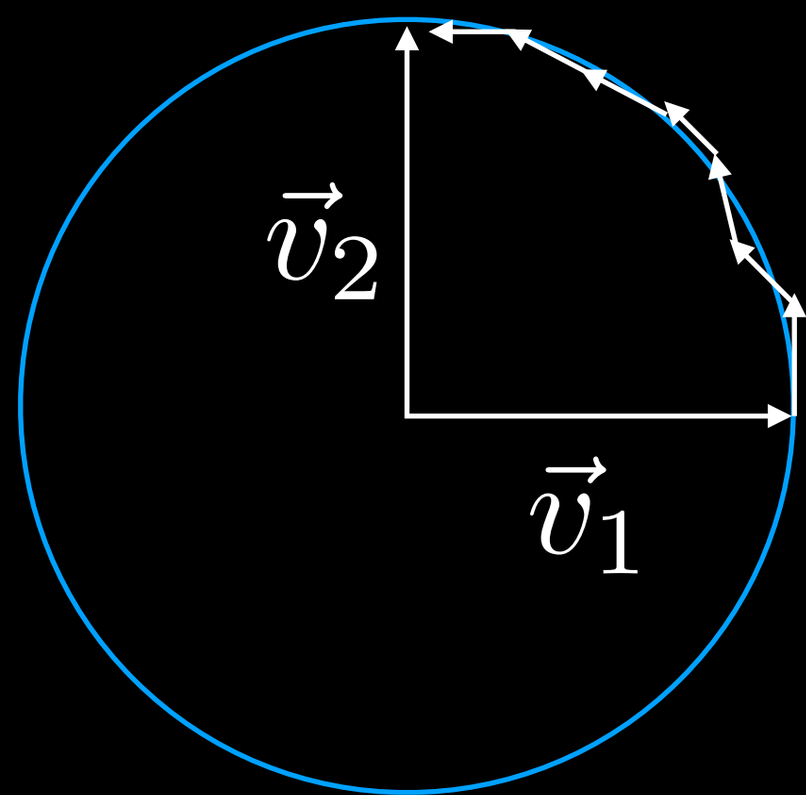
$$\mathcal{O}(D)$$

Stretch Step

worse

$$\mathcal{O}(D)$$

Why is it so hard?



Hamiltonian MC

$$\mathcal{O}(D^{1/4}) \cdot T(\vec{\nabla})$$

Metropolis-Hastings

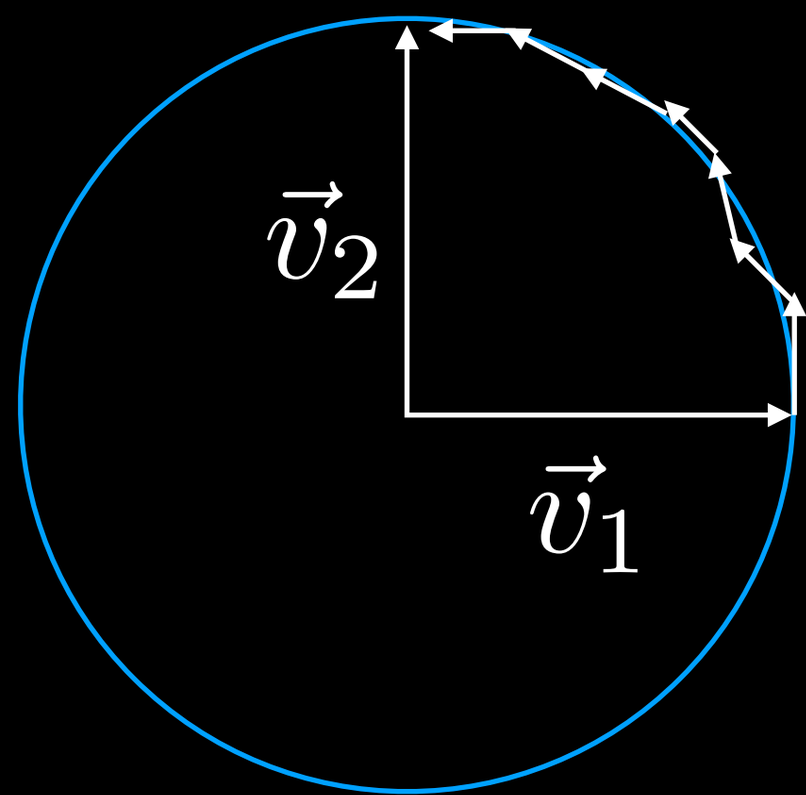
$$\mathcal{O}(D)$$

Stretch Step

worse

$$\mathcal{O}(D)$$

Why is it so hard?



Metropolis-Hastings

$$\mathcal{O}(D)$$

Stretch Step

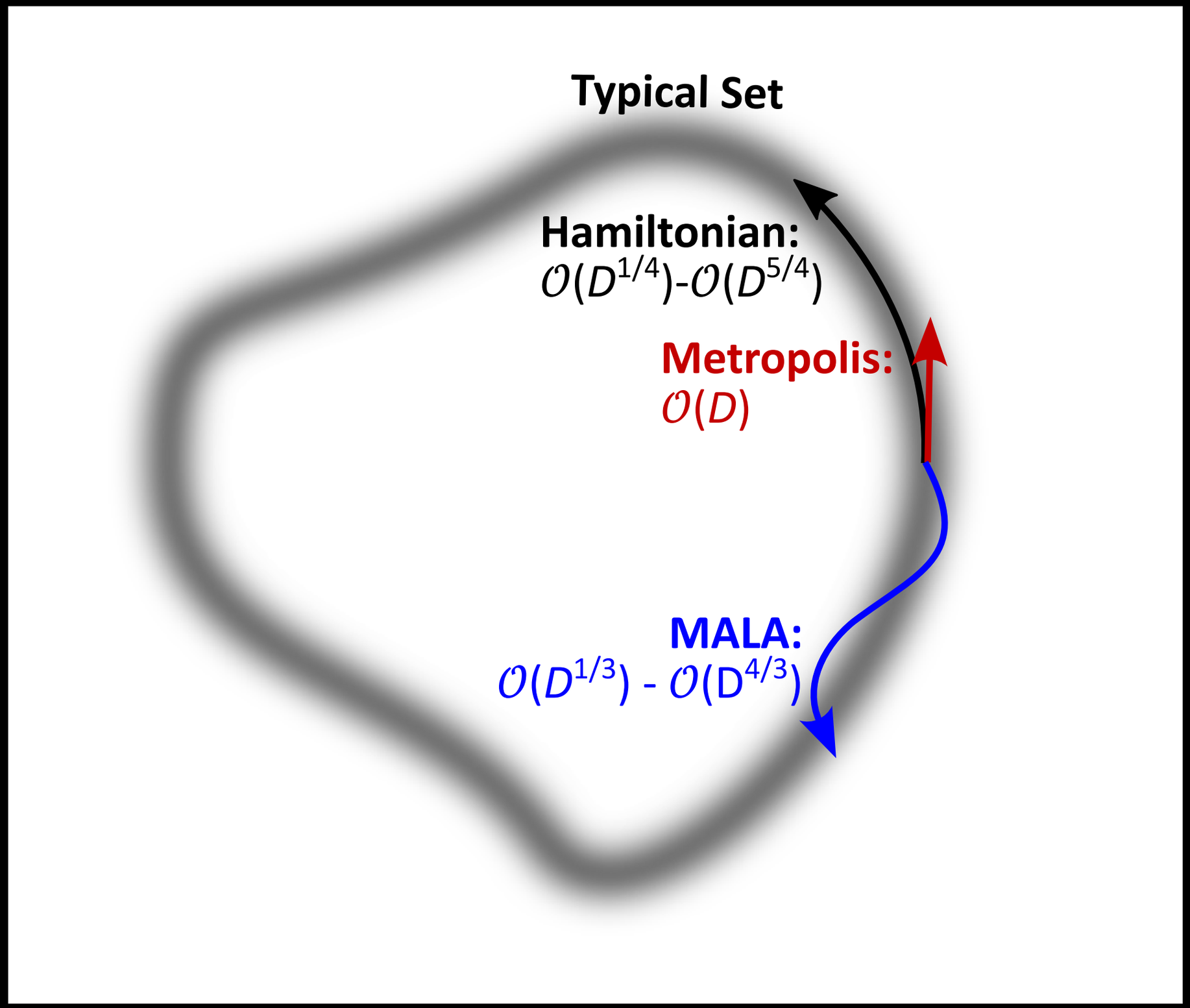
worse

$$\mathcal{O}(D)$$

Hamiltonian MC

$$\mathcal{O}(D^{1/4}) - \mathcal{O}(D^{5/4})$$

Why is it so hard?



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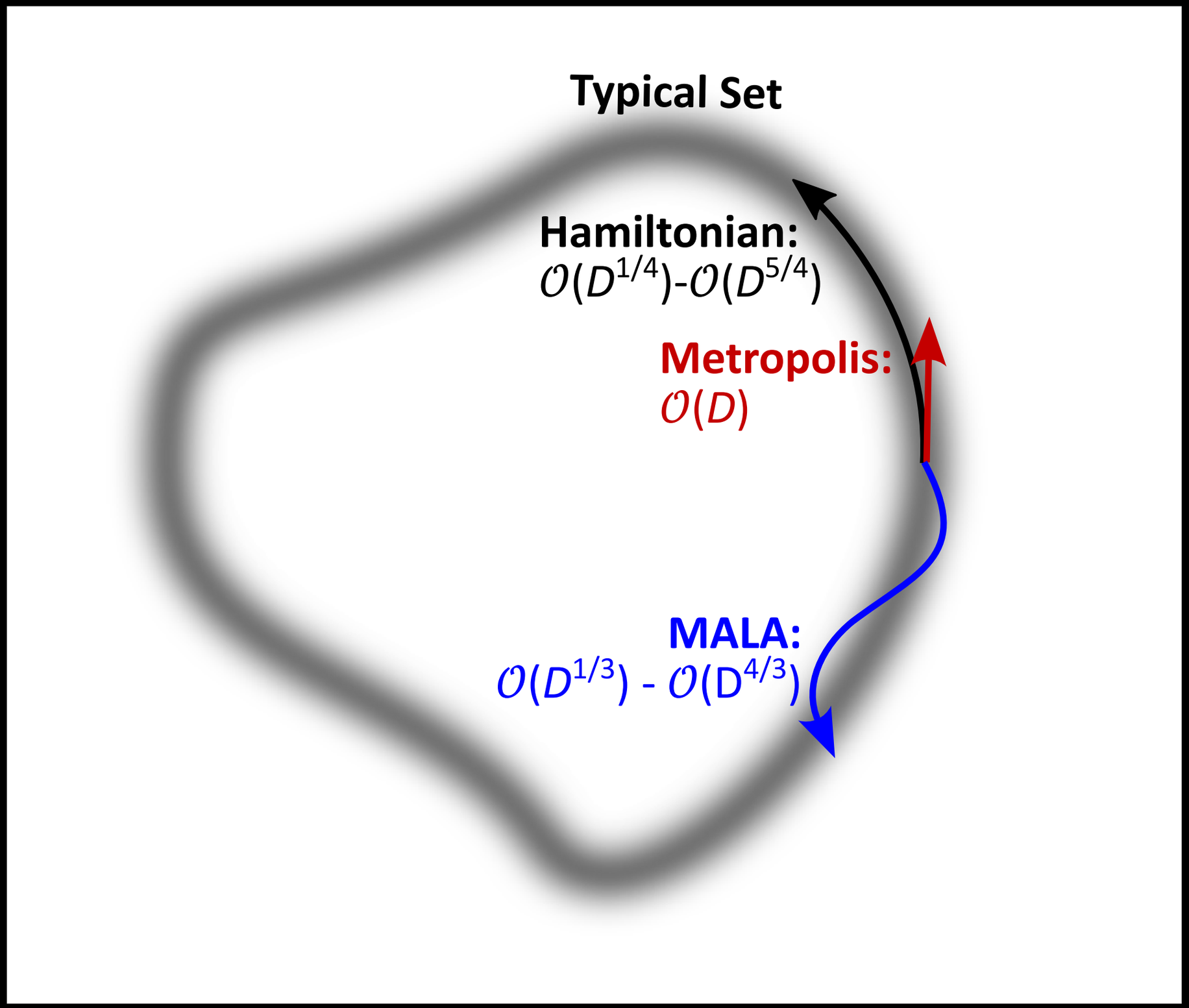

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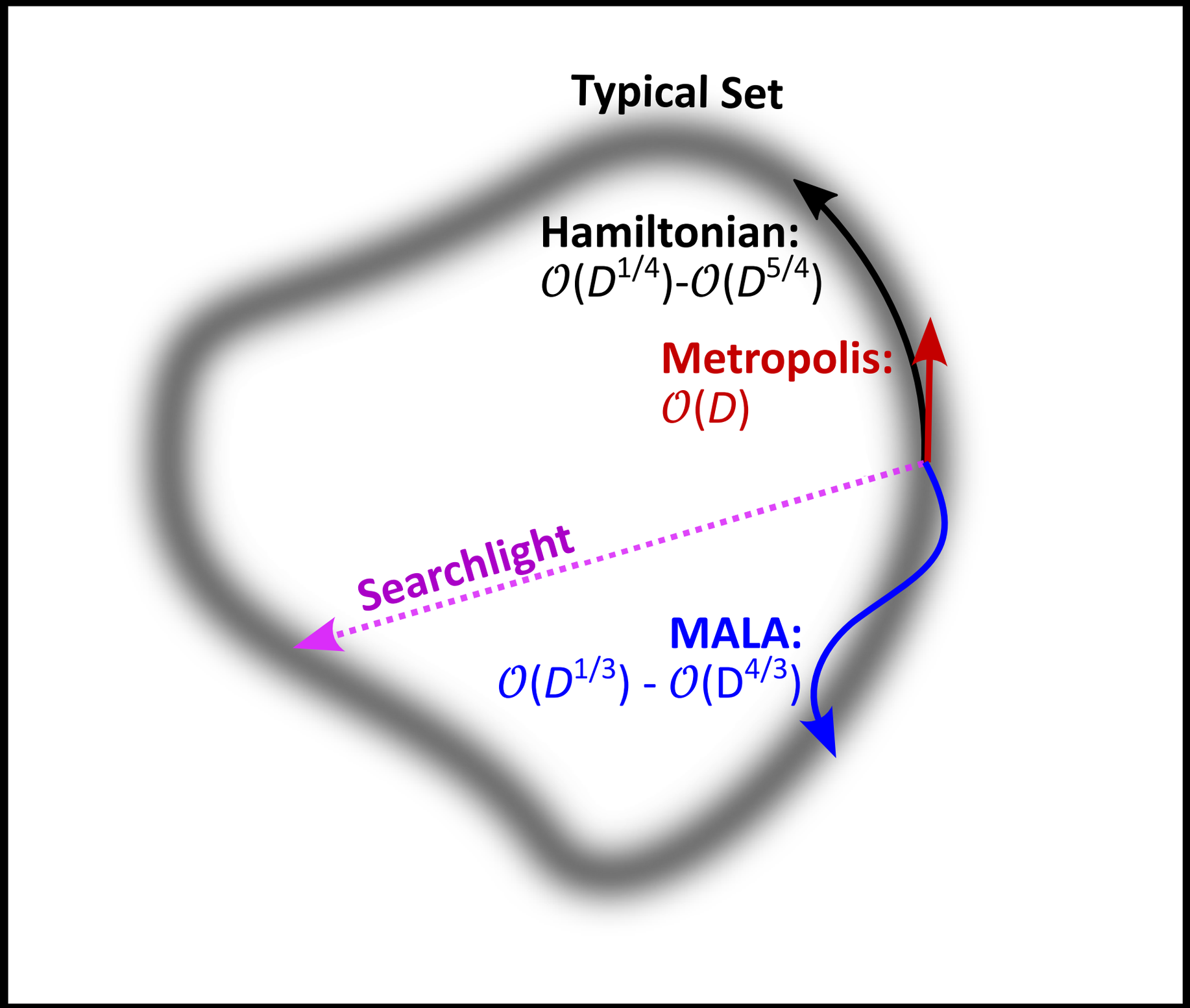

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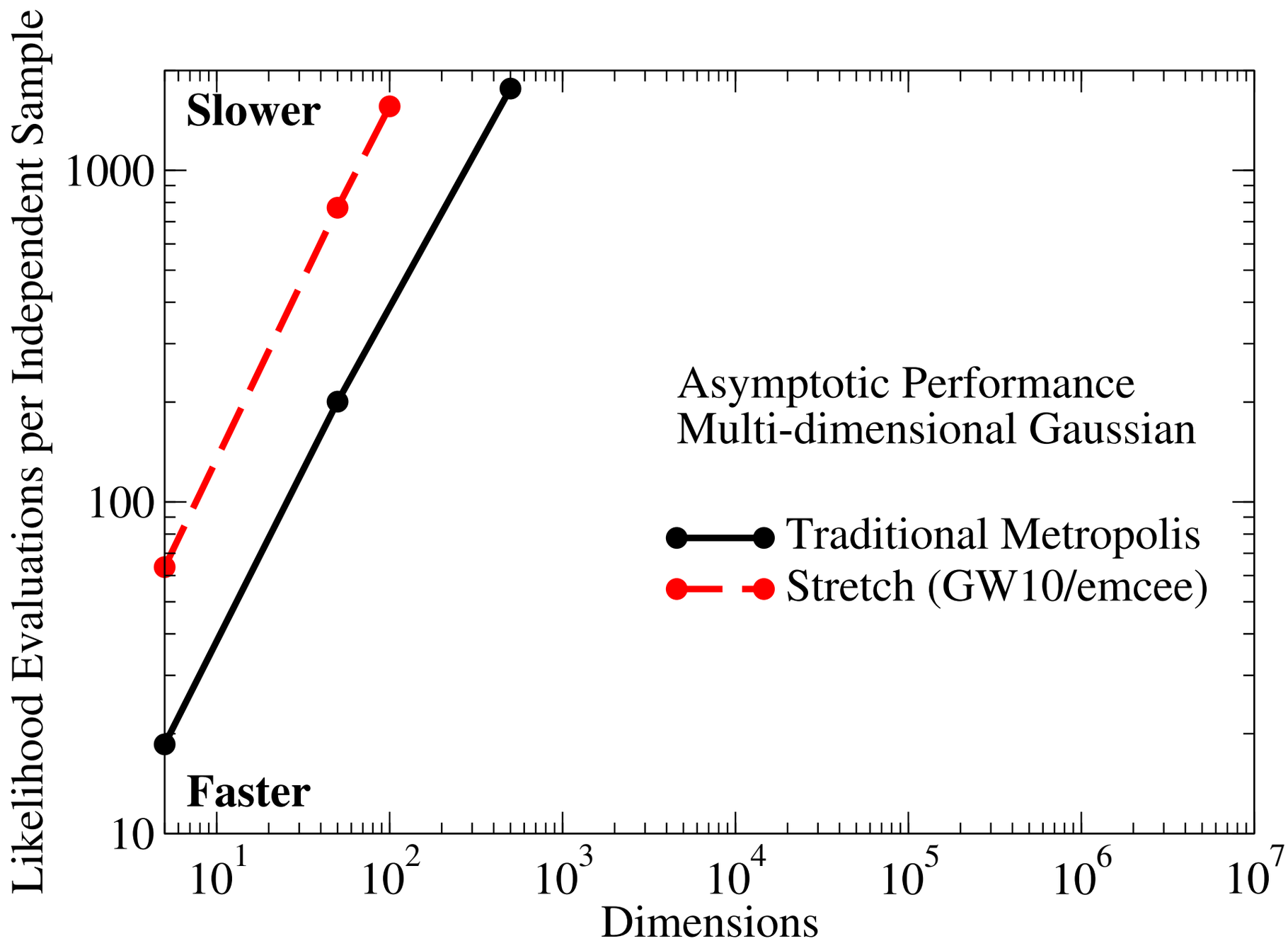

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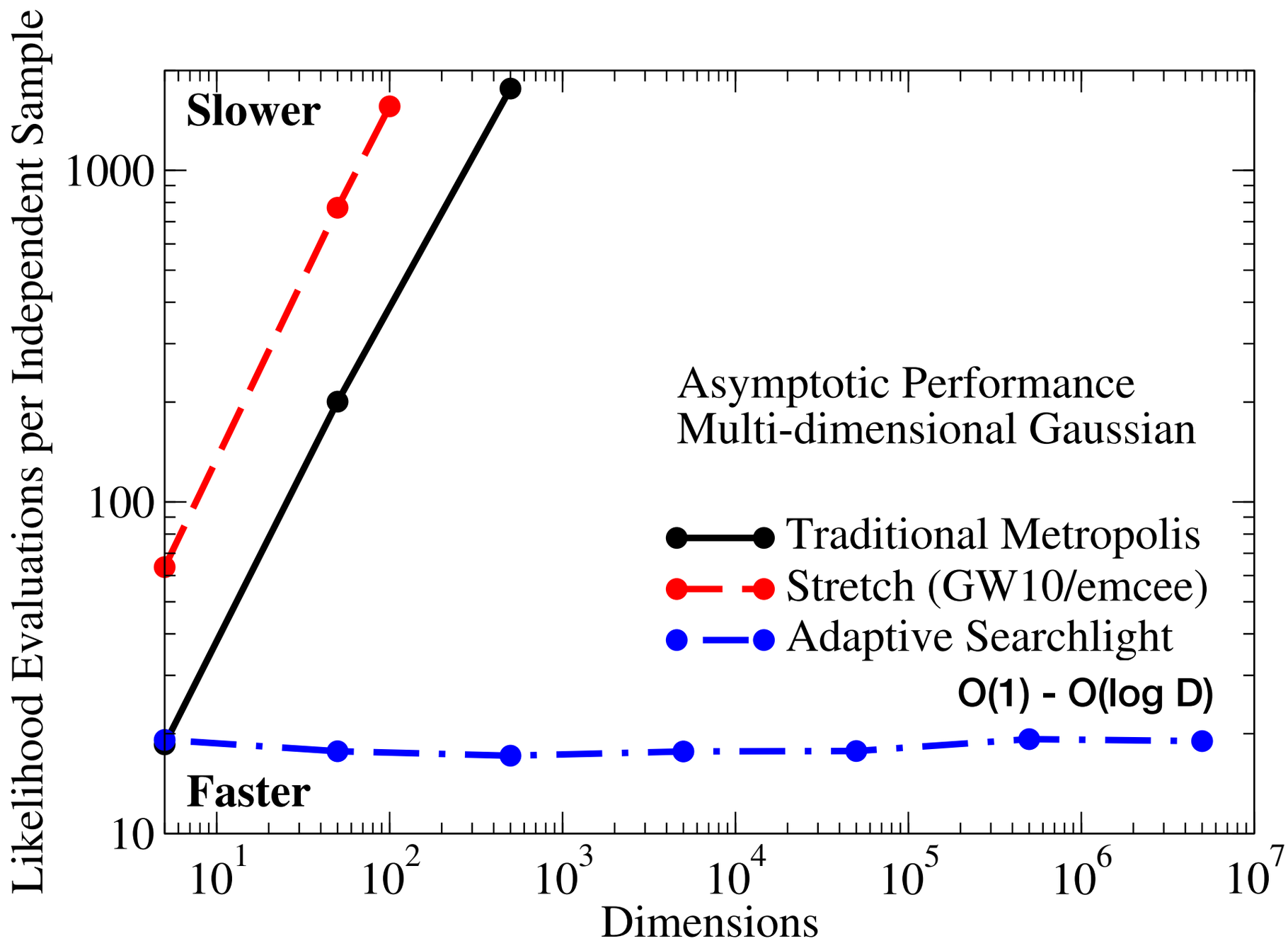
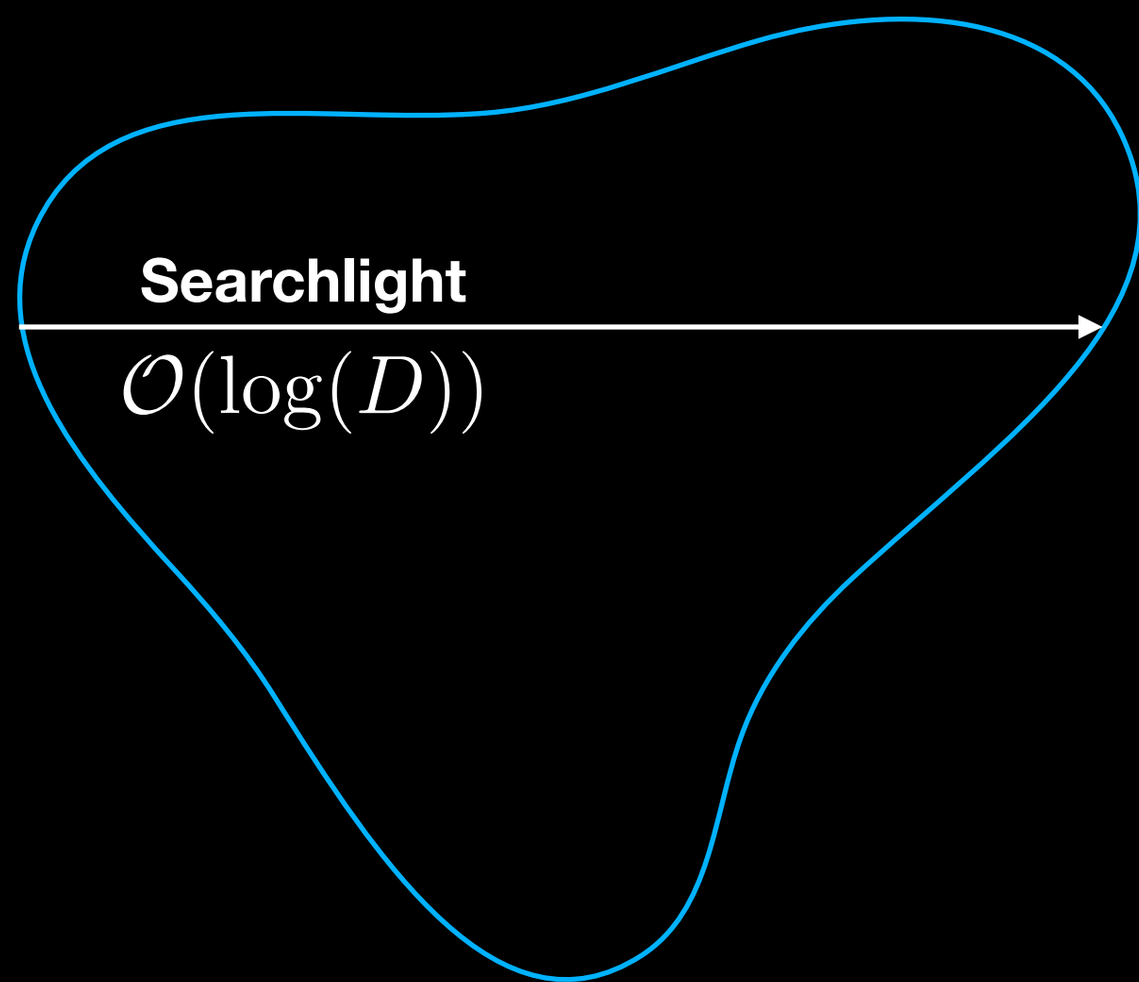


Should it be so hard?

Why not combine MCMCs with search algorithms?



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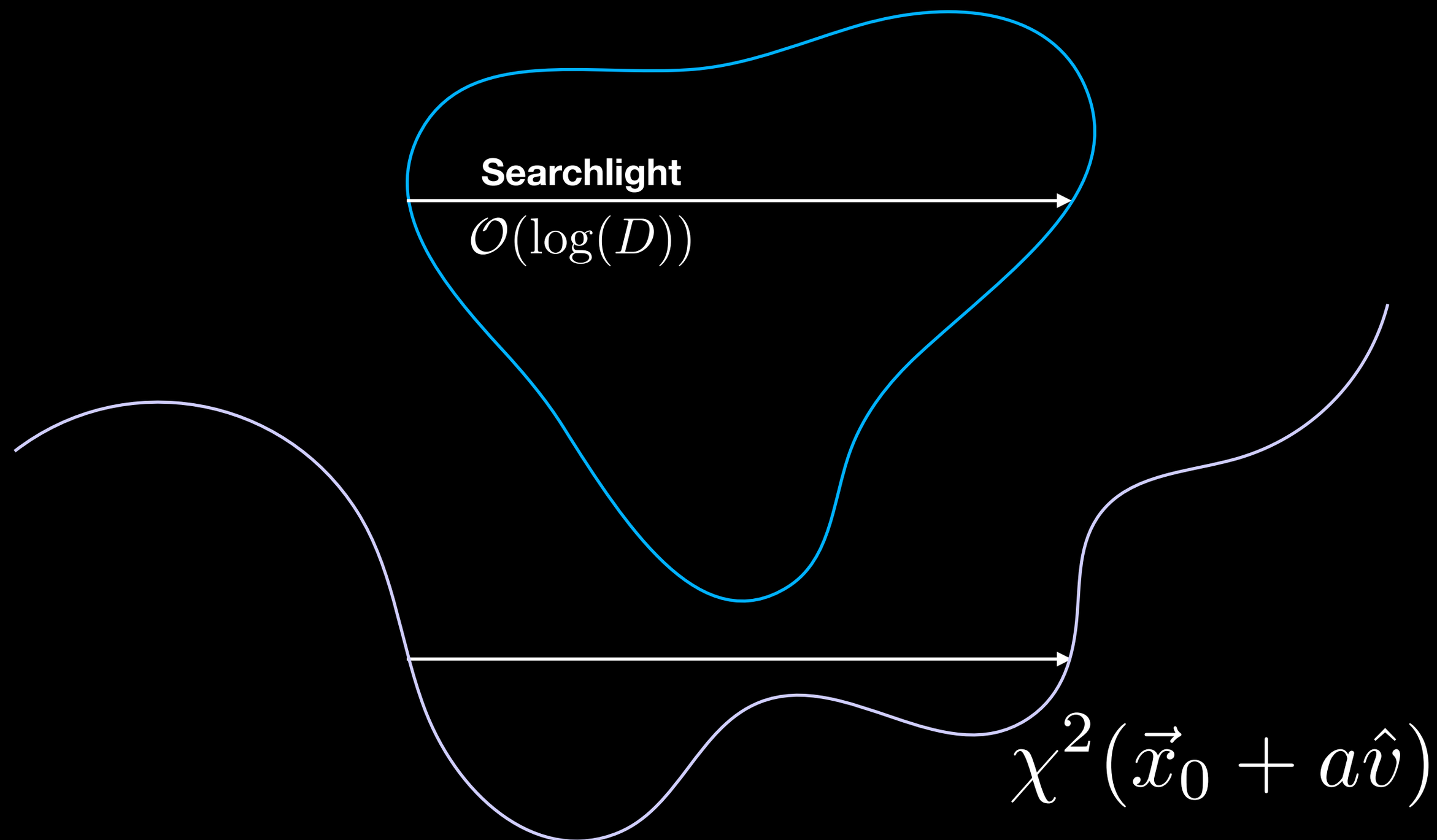

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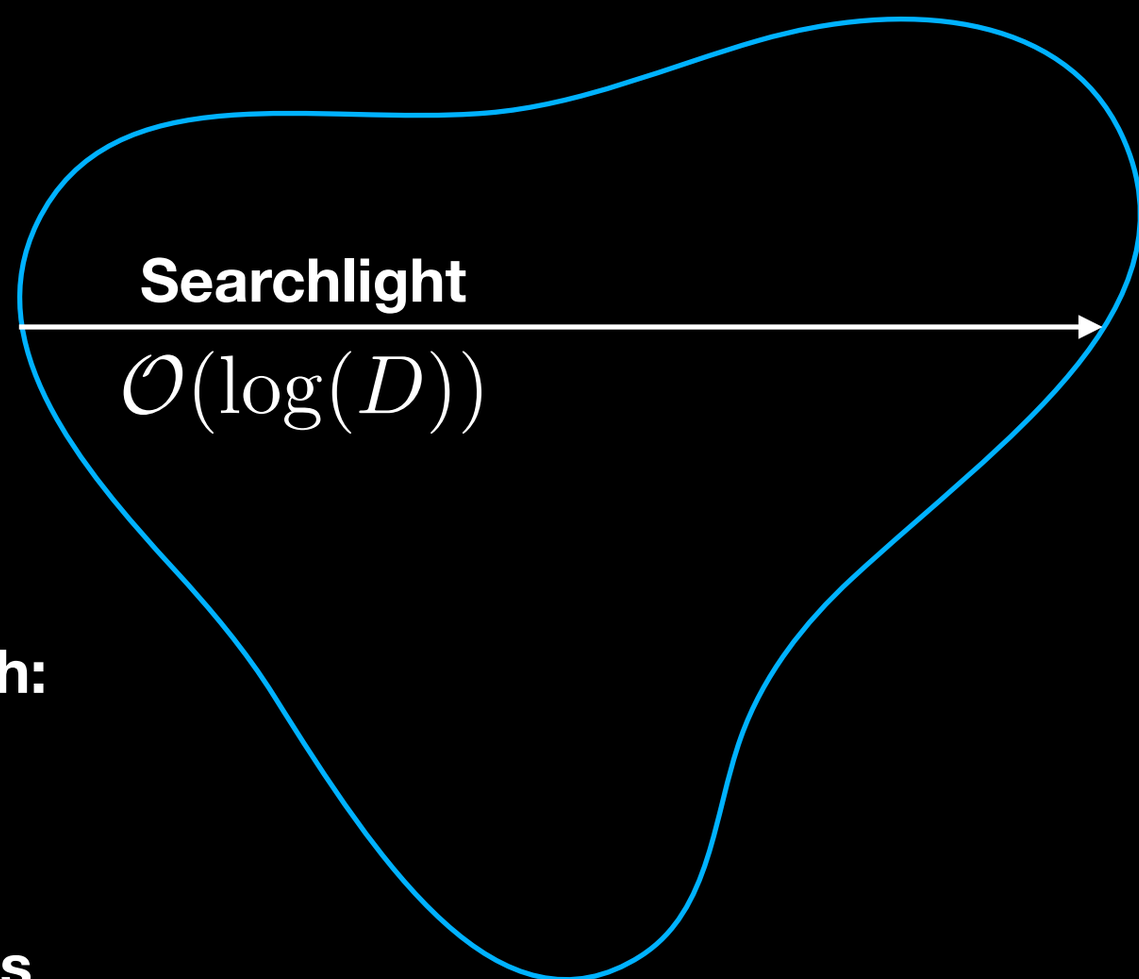


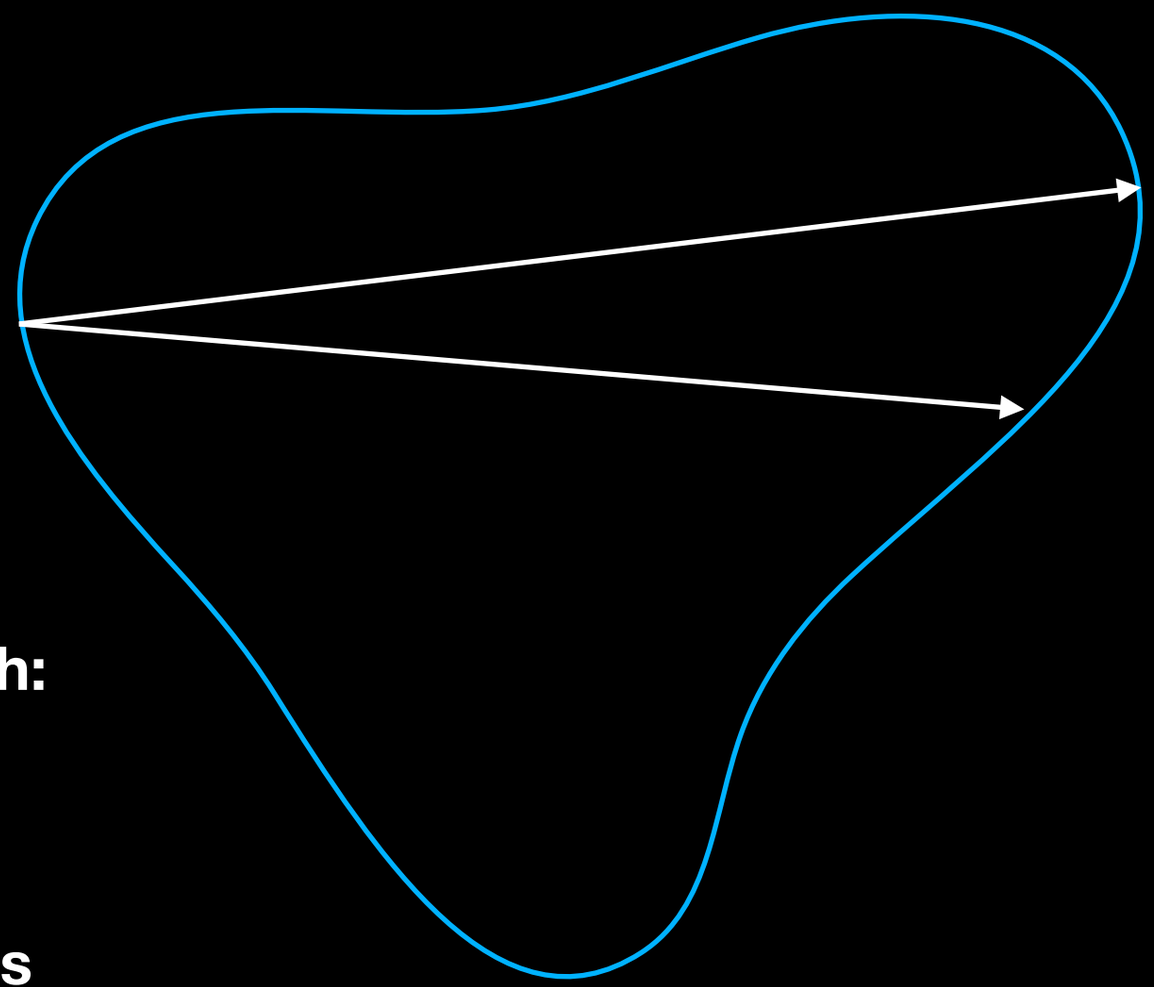
Metropolis / Stretch:
Diffusion

Hamiltonian:
Gravitational Orbits

Searchlight:
Optical Paths

Should it be so hard?

Searchlight: blackbody radiation from isolikelihood surfaces.



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$$L(r) \propto r^{1-D}$$

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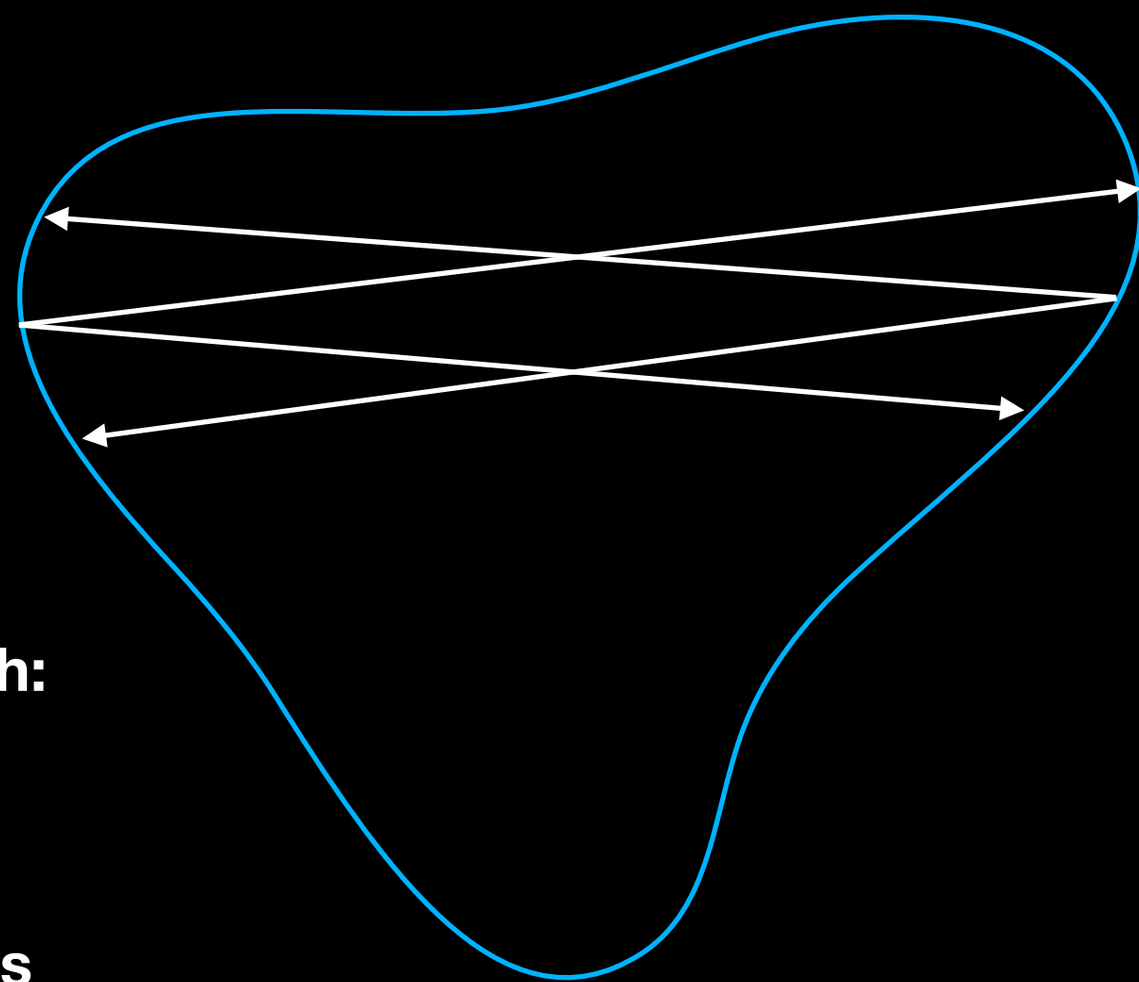

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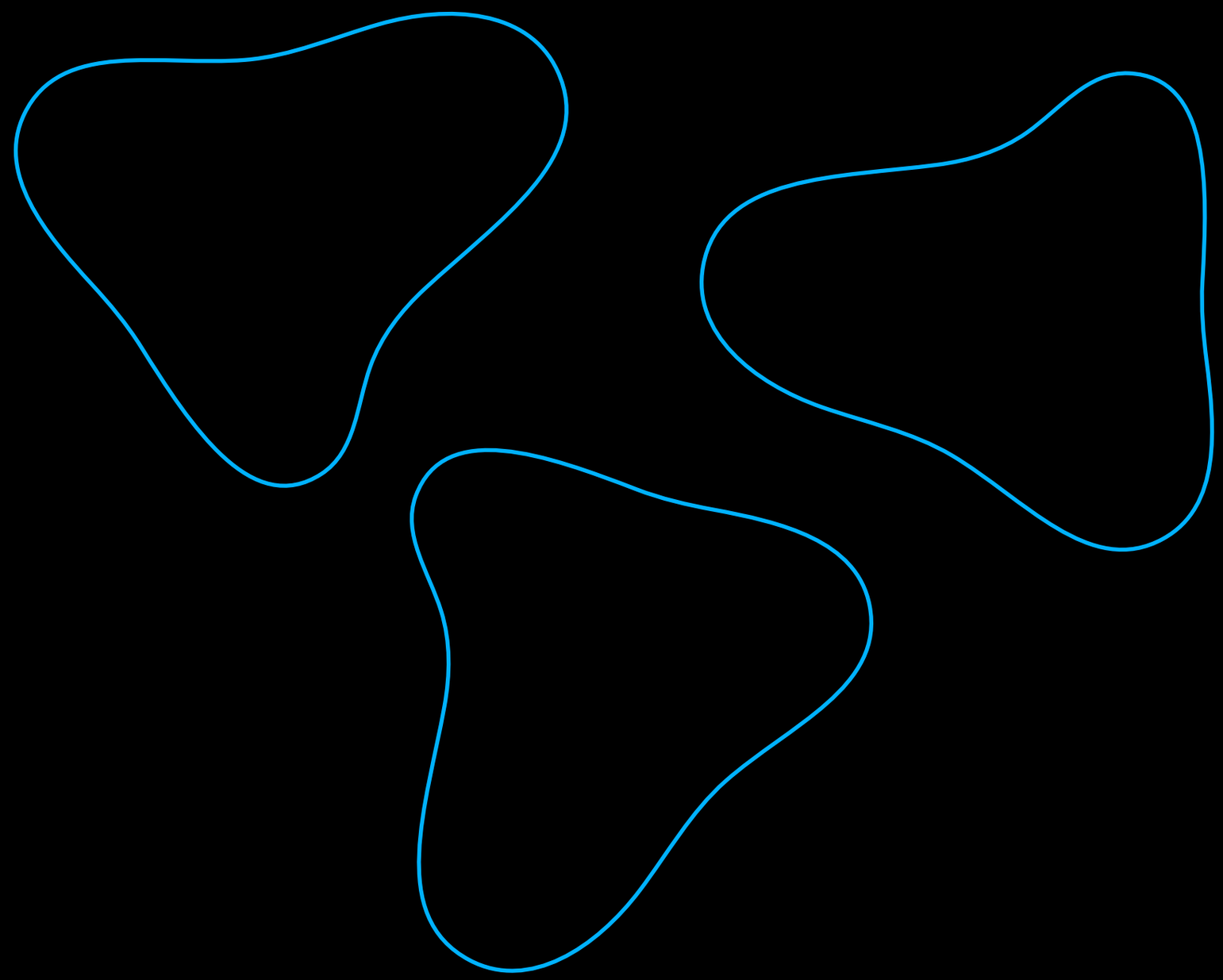

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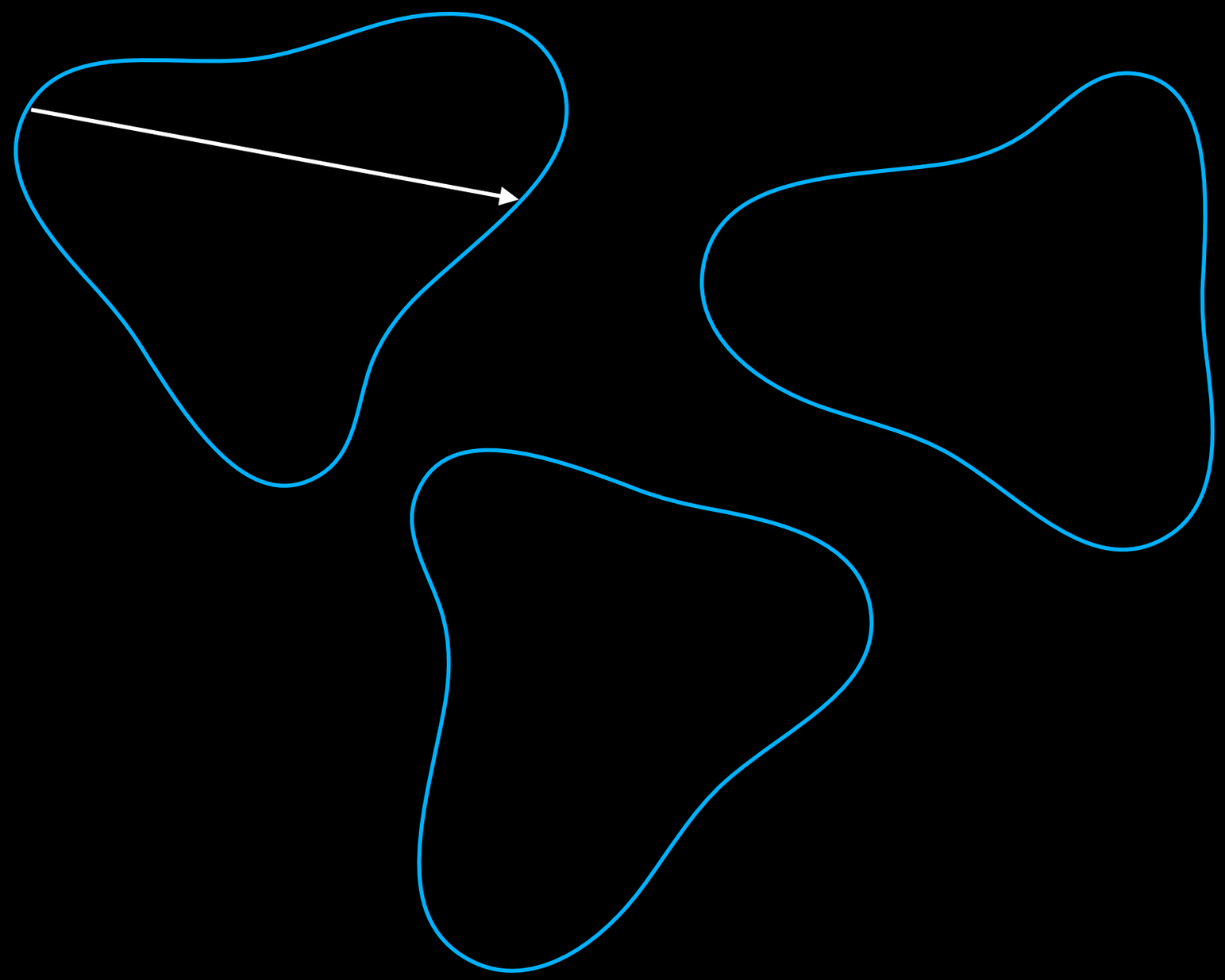

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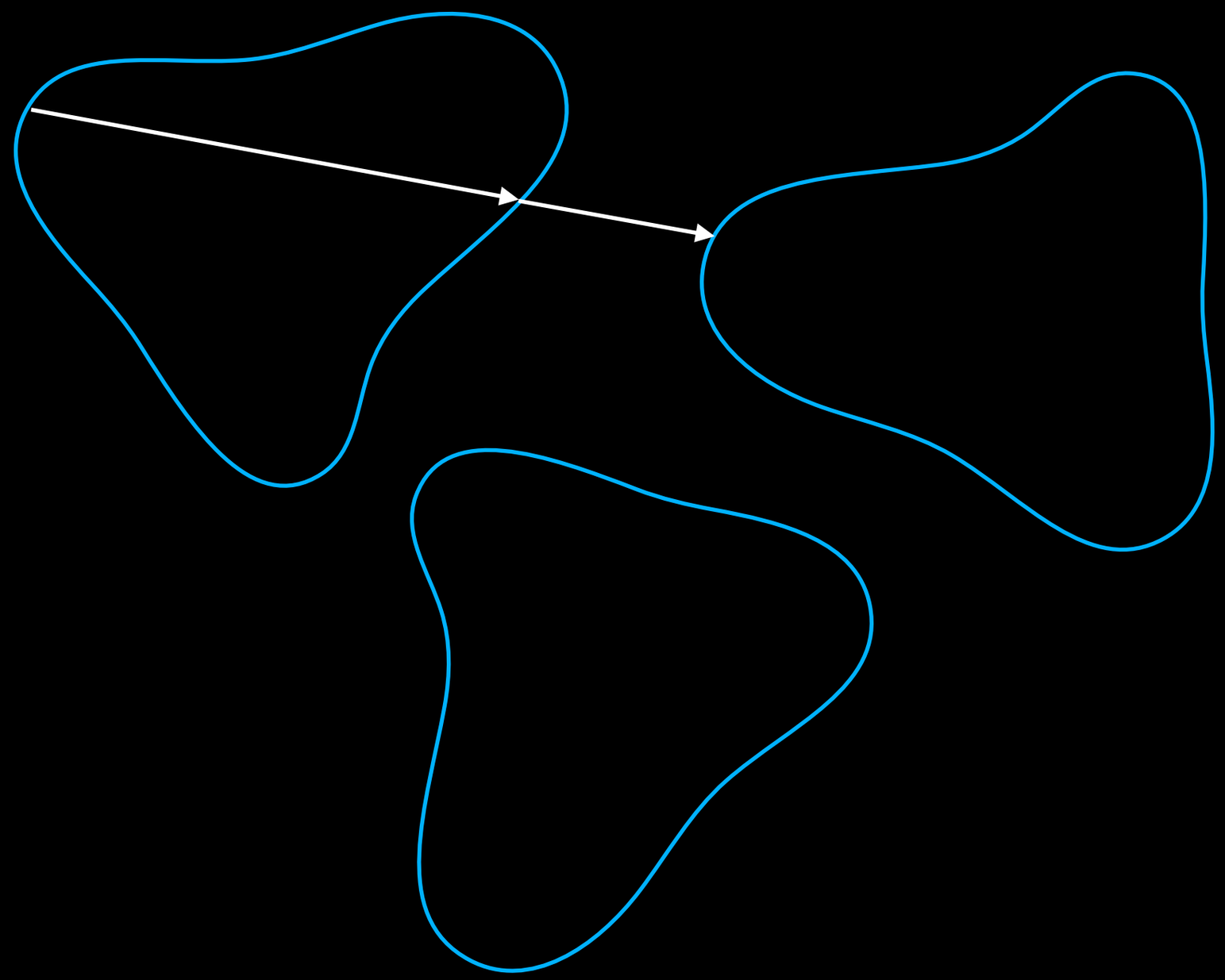

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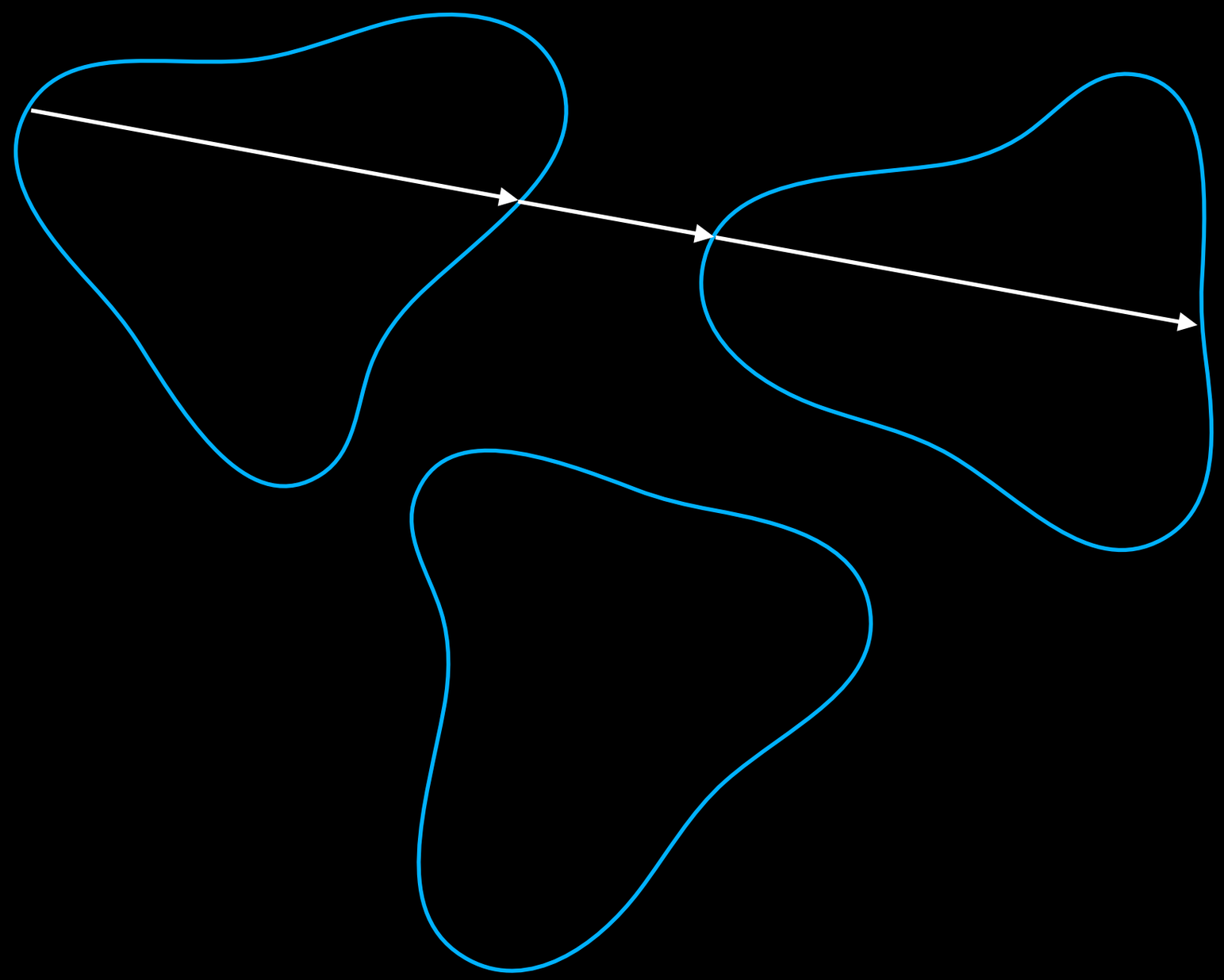

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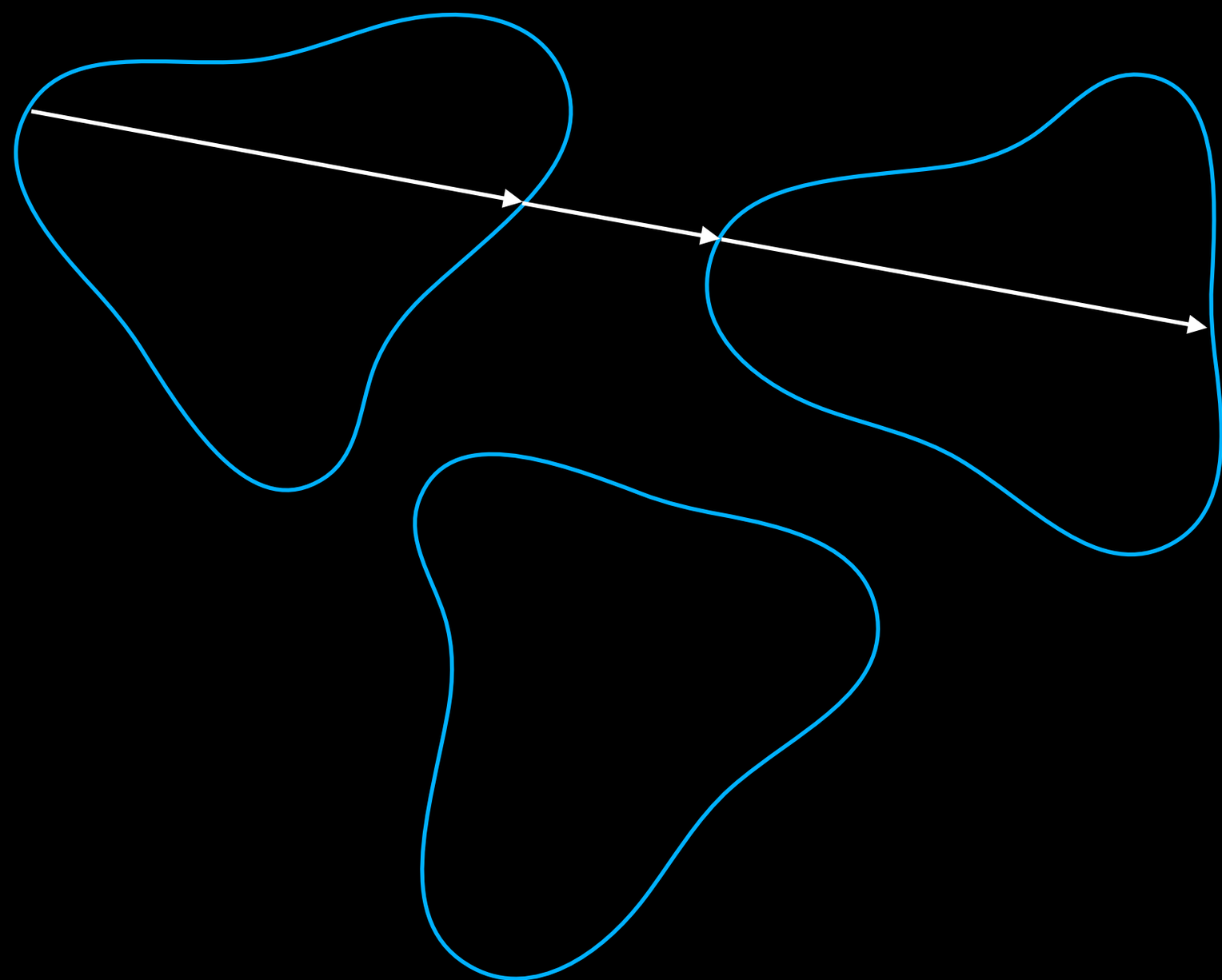
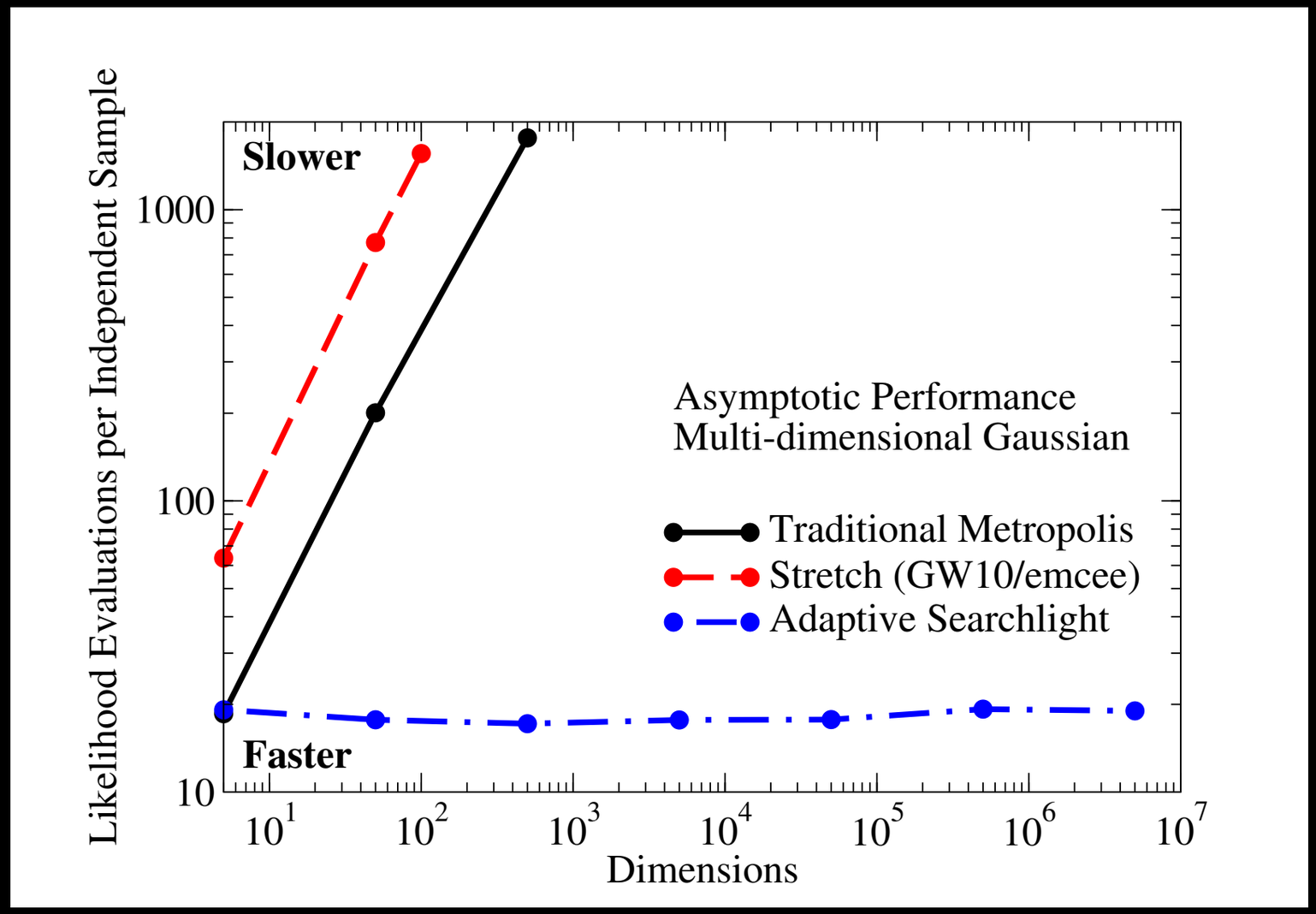


Naturally handles disjoint isoprobability surfaces(!)

Summary



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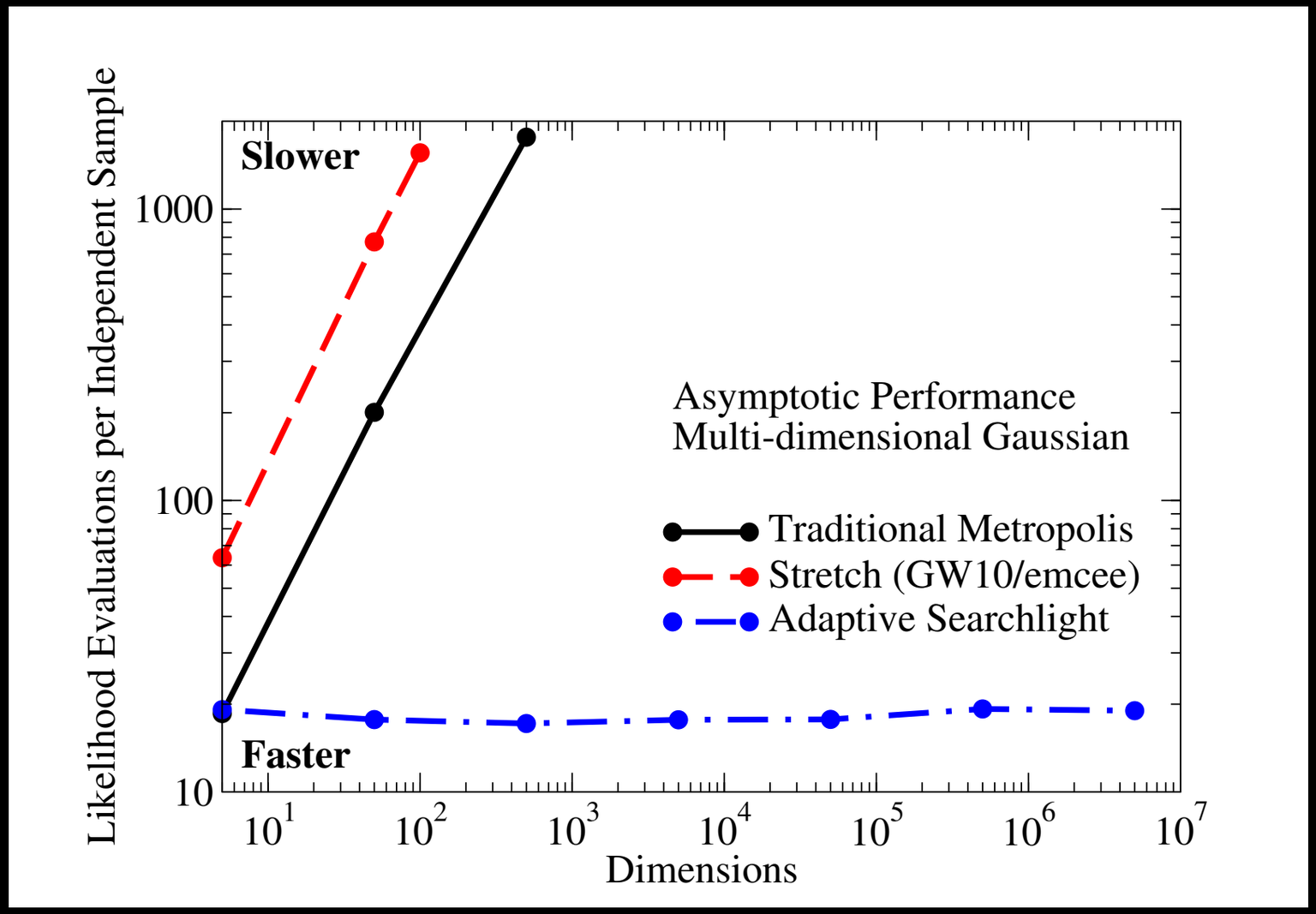
Connects MCMCs to Hamiltonian optics.

Naturally handles disjoint isoprobability surfaces(!)

O(1) - O(Log D) scaling with dimensionality

Summary



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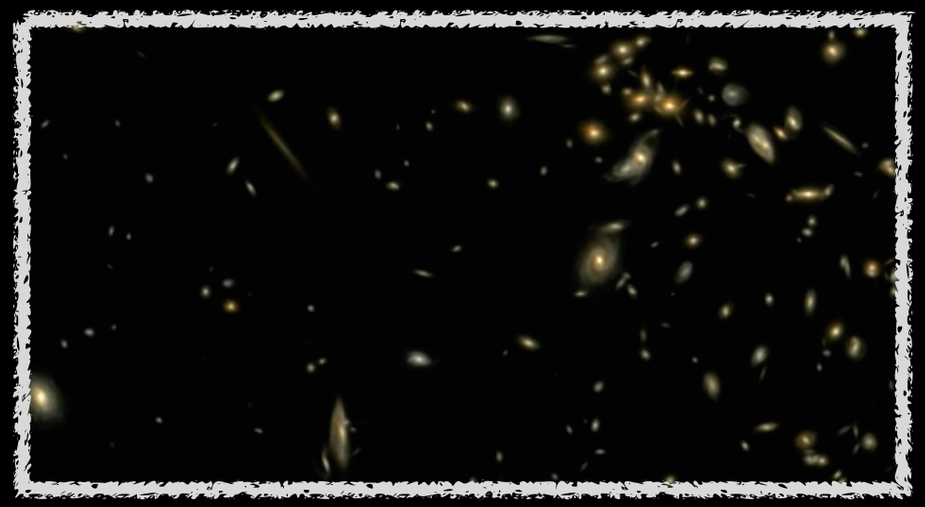
Connects MCMCs to Hamiltonian optics.

Naturally handles disjoint isoprobability surfaces(!)

O(1) - O(Log D) scaling with dimensionality

Combining with normalizing flows would yield even better performance(!)

Motivation



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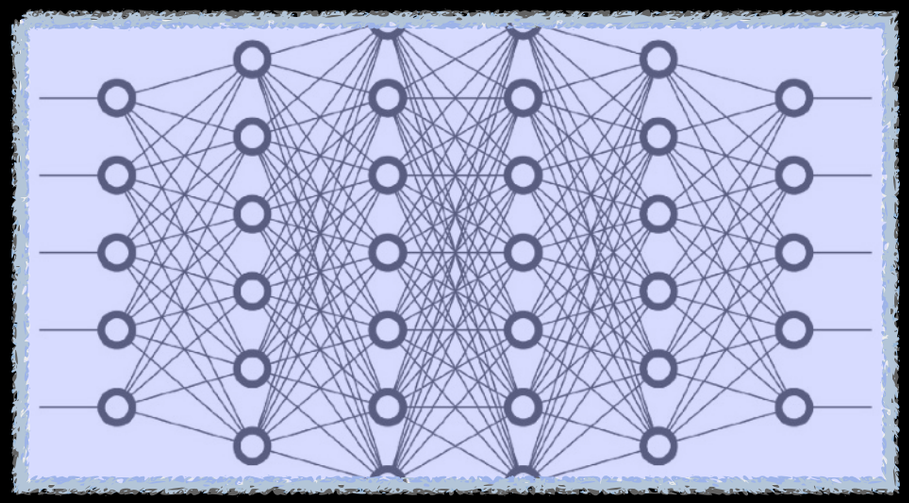

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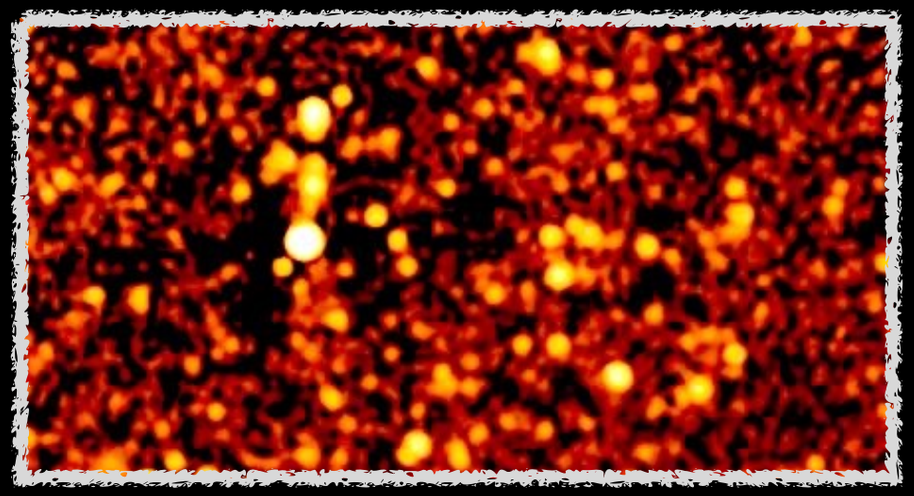

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Peter Behroozi

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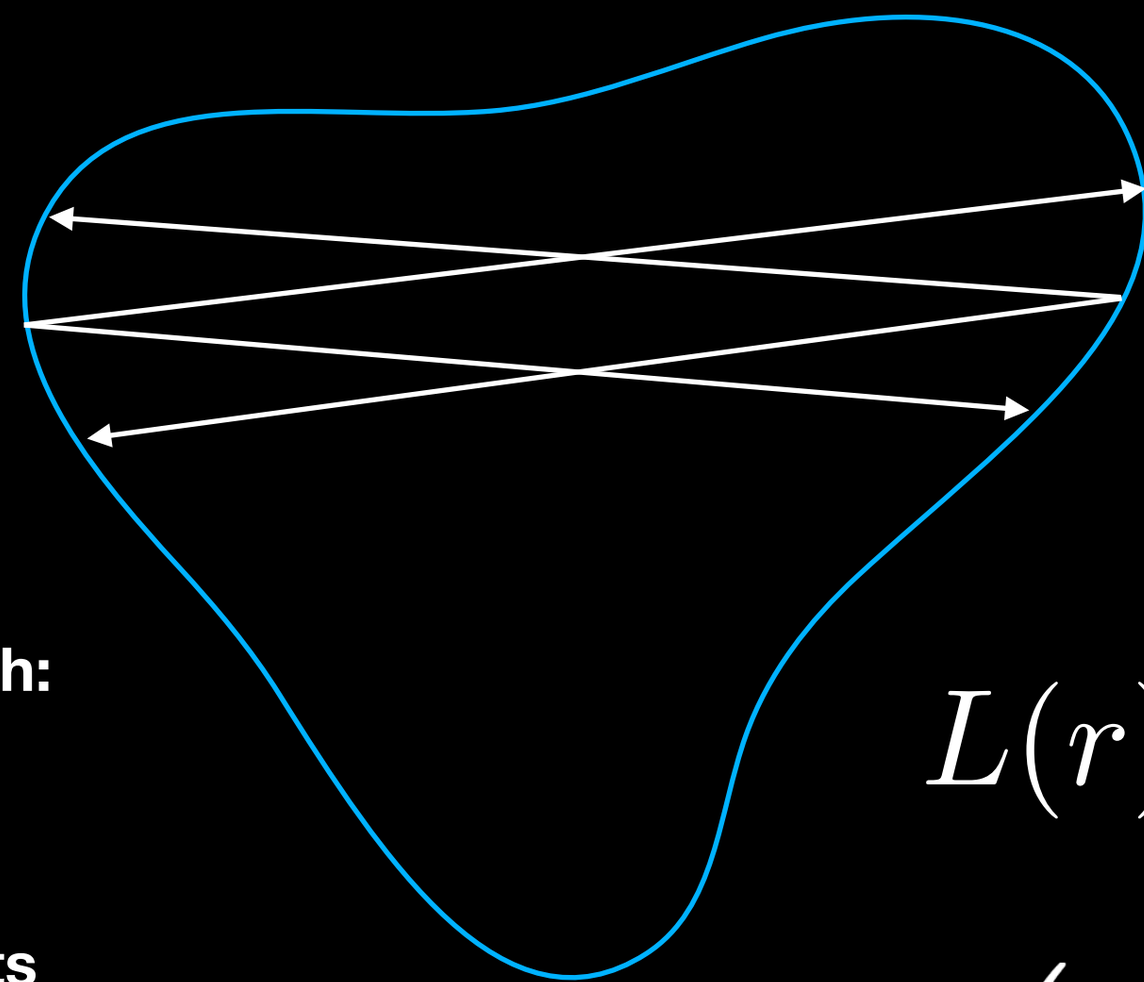

Metropolis / Stretch: Diffusion

Hamiltonian: Gravitational Orbits

$$L(r) \propto r^{1-D}$$

Searchlight: Optical Paths

$$P(x \to y) = \min\left(1, \frac{\hat{v} \cdot \vec{\nabla}\mathcal{L}(x)}{\hat{v} \cdot \vec{\nabla}\mathcal{L}(y)}\right)$$