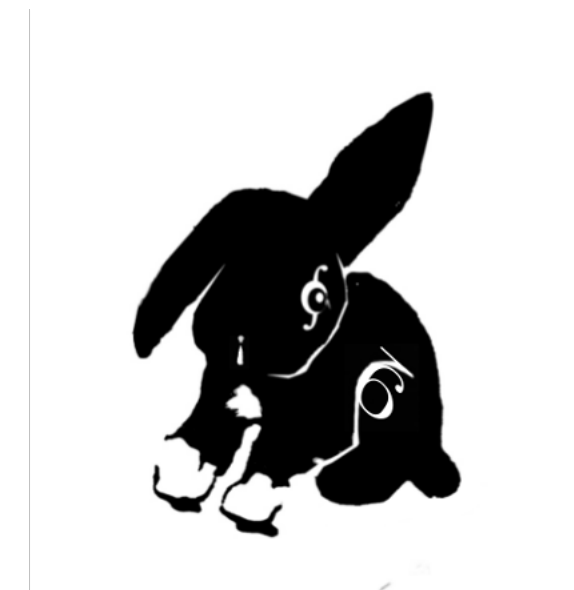


# Quantum-inspired techniques for learning the geometry of data

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Instituto de Telecomunicações,  
Instituto Superior Técnico, Lisboa



Physics of Information and Quantum Technologies Group

Mohan Sarovar

Sandia National Labs, Livermore, CA



QuantHEP 2023, Istituto Nazionale di Fisica Nucleare

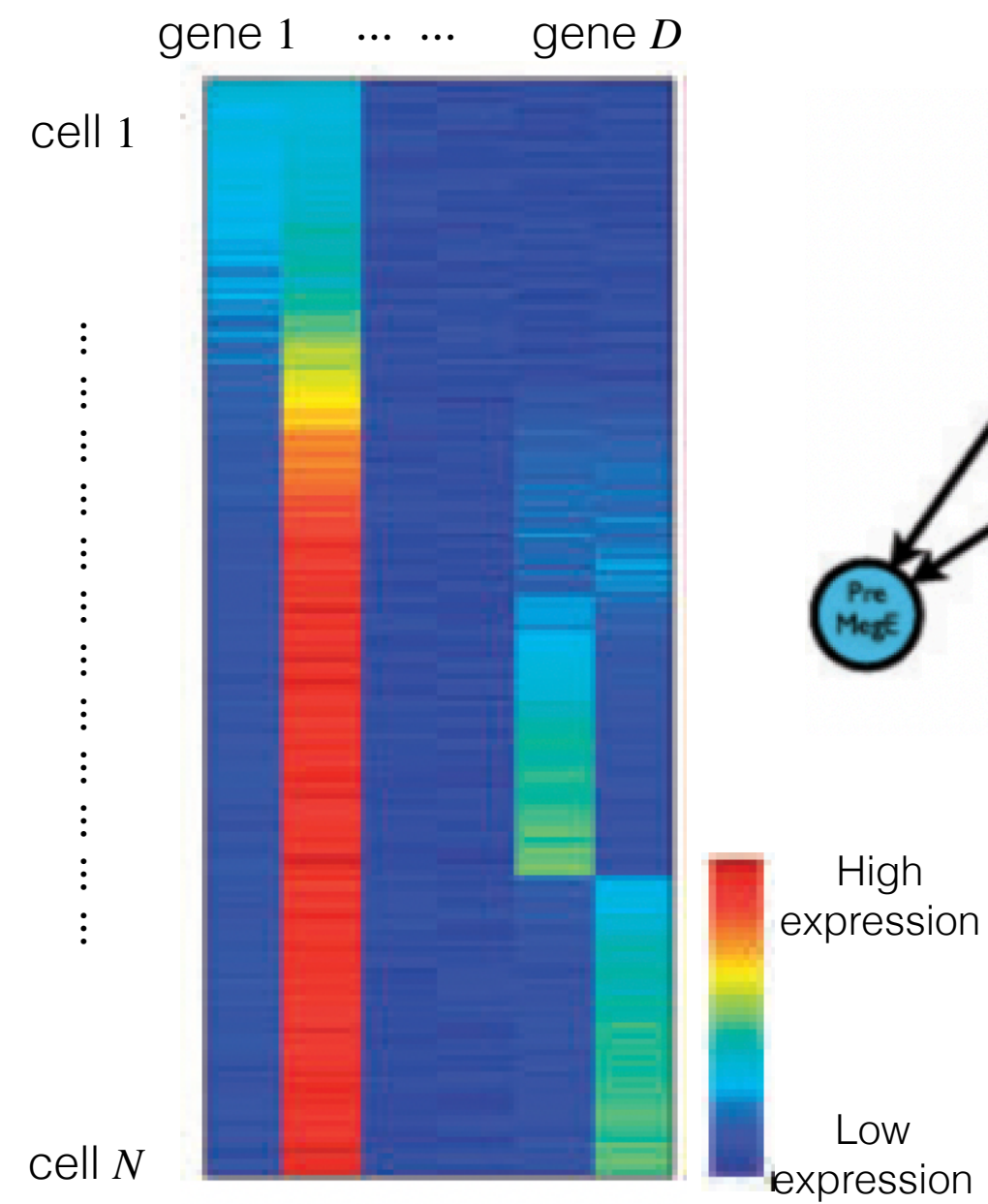
September 26, 2023

- **Data analysis tasks are *often* geometric analysis of data**
- **Geometry of HEP data analysis**
- **Quantum dynamics underlying the geometry of data**
  - **Example applications**
- **Future directions for HEP applications**

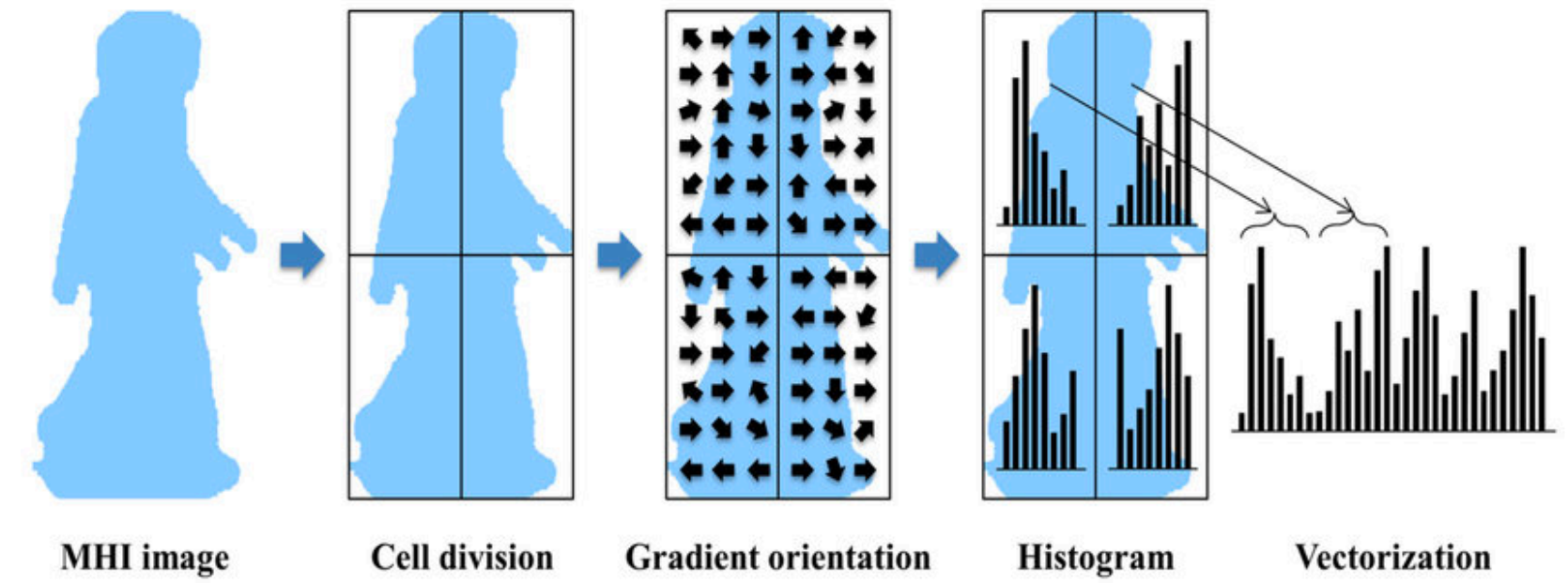
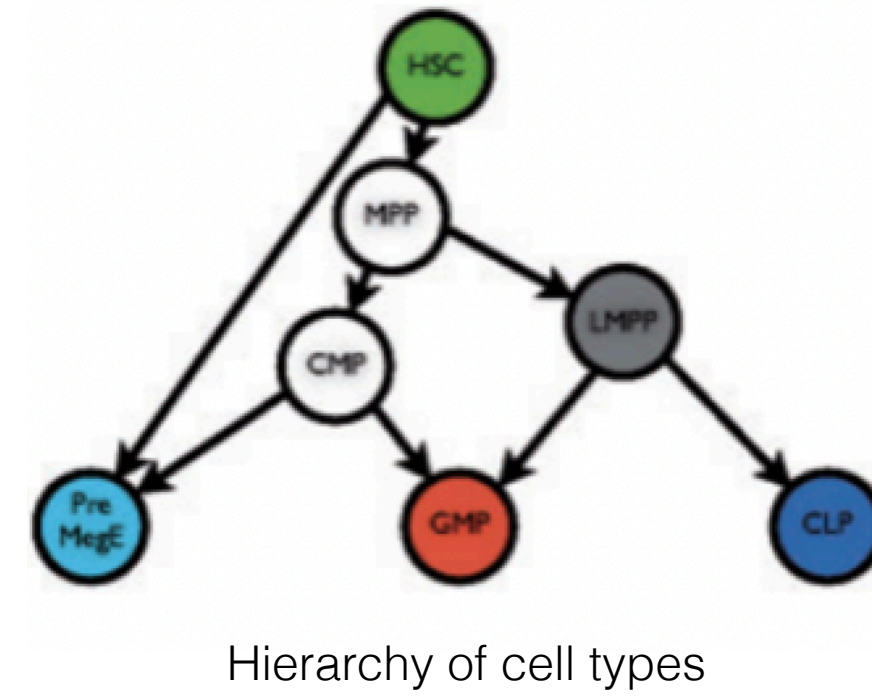
***Data is often an organized point cloud***

# What is "data"?

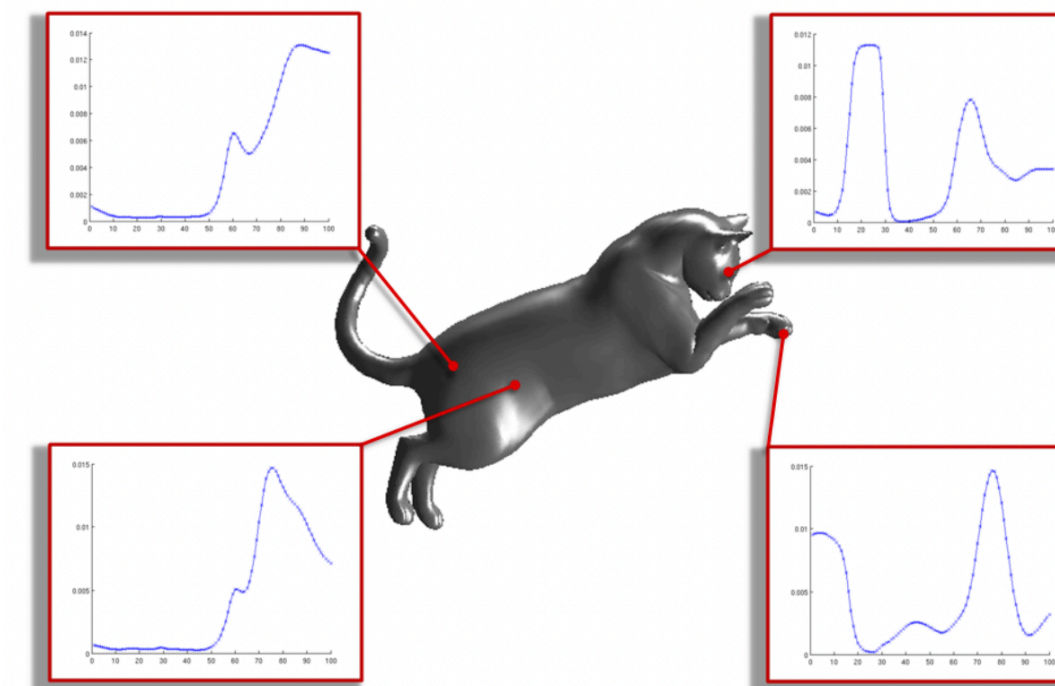
$N$  vectors in  $\mathbb{R}^D$



Hagverdi et al., *Bioinformatics* (2015)



Eum et al., *Sensors* (2015)



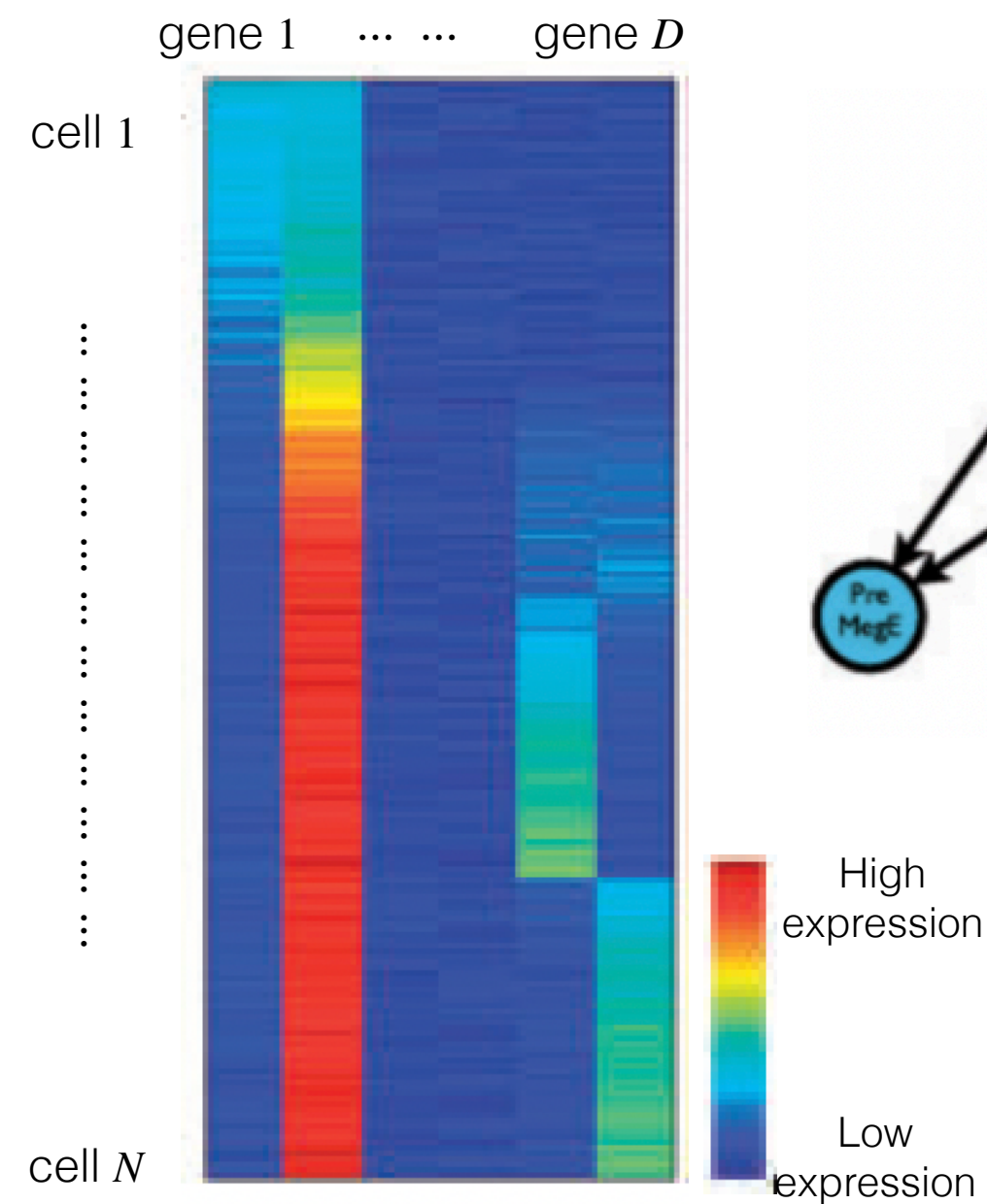
Aubry et al., *ICCV workshop, IEEE* (2011)

**Measurements**, including statistics of natural processes, constitute **data**

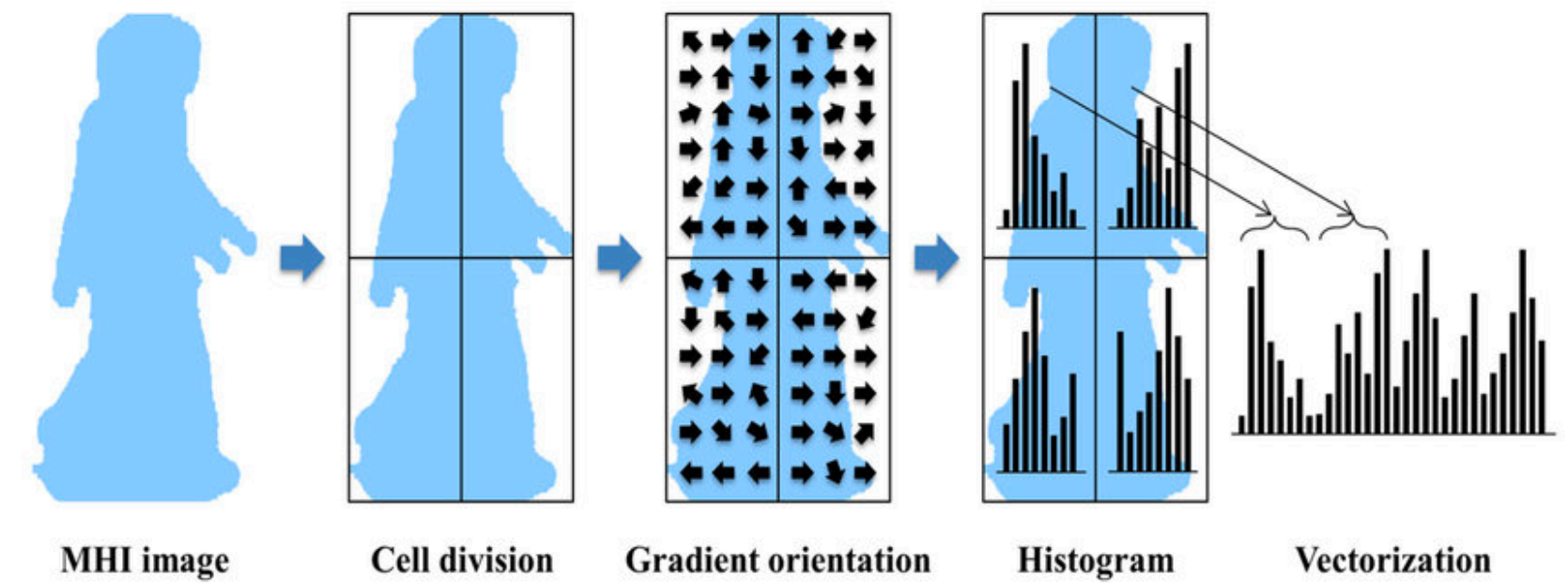
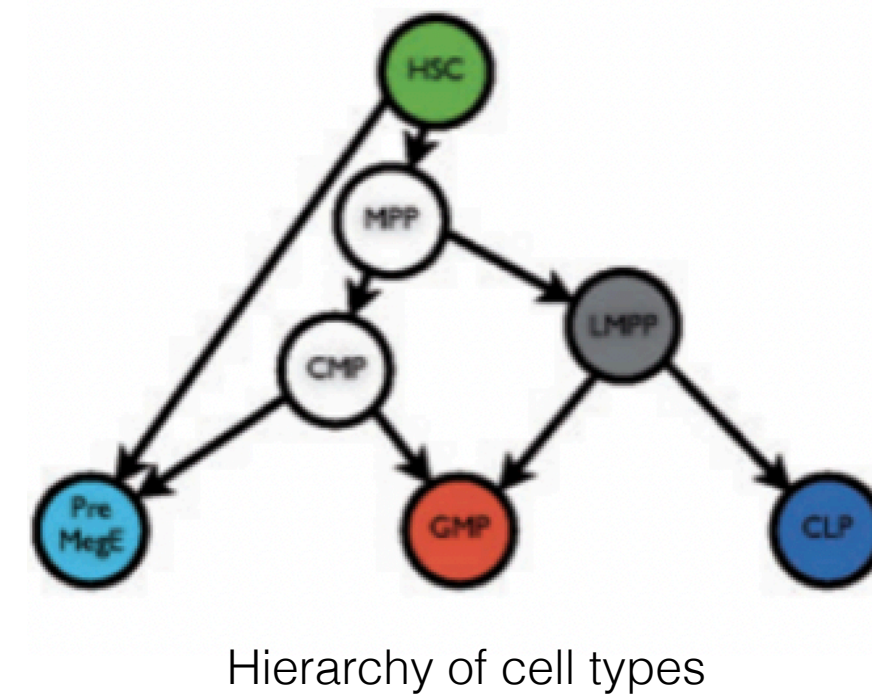


# What is “data”?

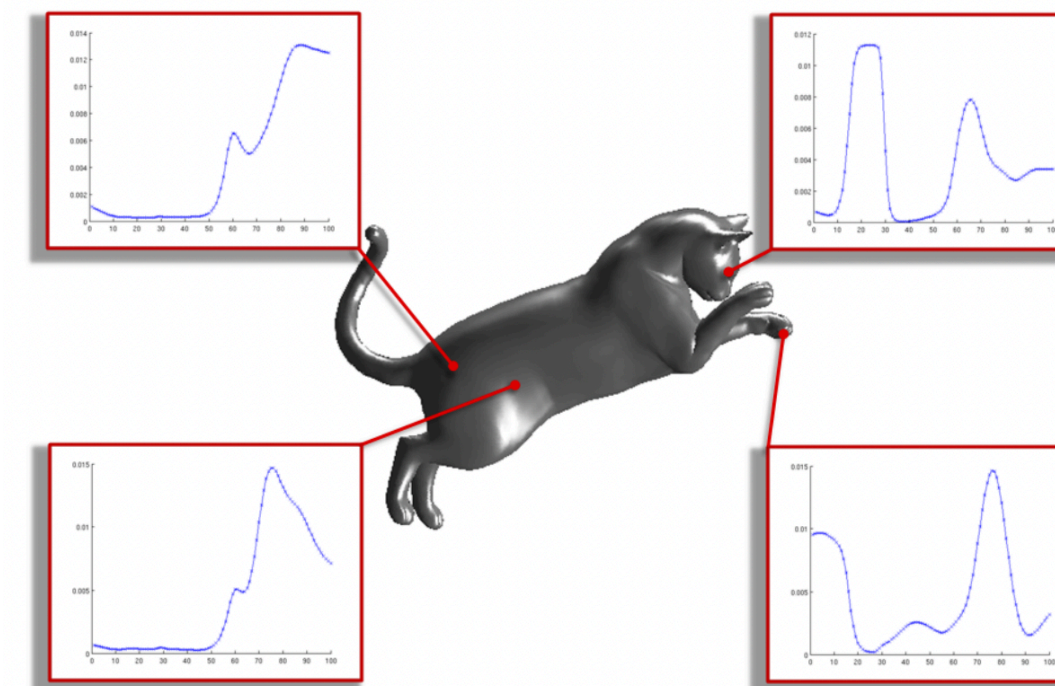
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Haghighi et al., *Bioinformatics* (2015)



Eum et al., *Sensors* (2015)



Aubry et al., *ICCV workshop, IEEE* (2011)

**Measurements**, including statistics of natural processes, constitute **data**

- measuring/sampling  $D$  variables in an experiment
- recording the output of  $D$  sensors

}

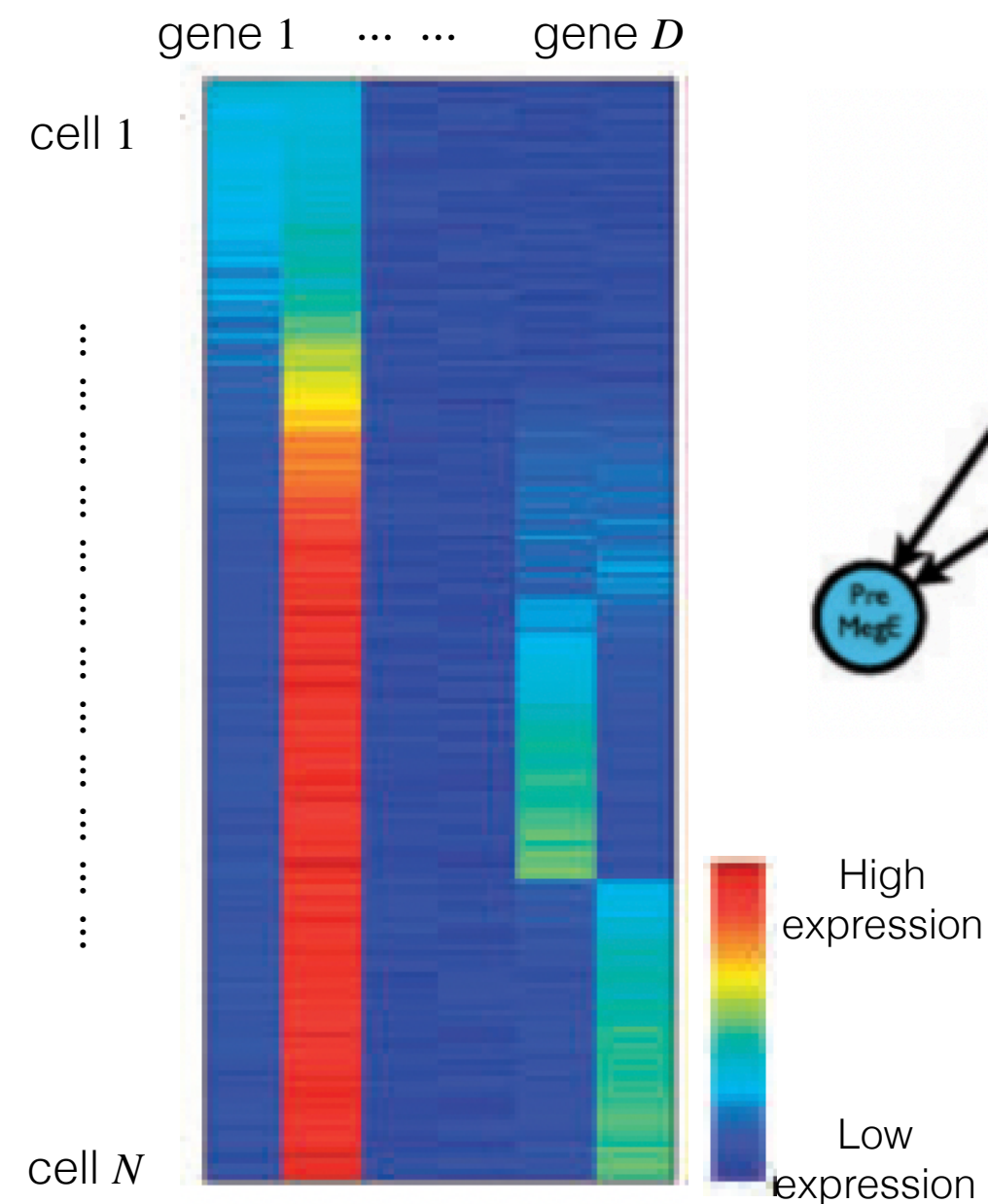
$$v := (\text{meas.}_1, \dots, \text{meas.}_D) \in \mathbb{R}^D$$

“feature vector”

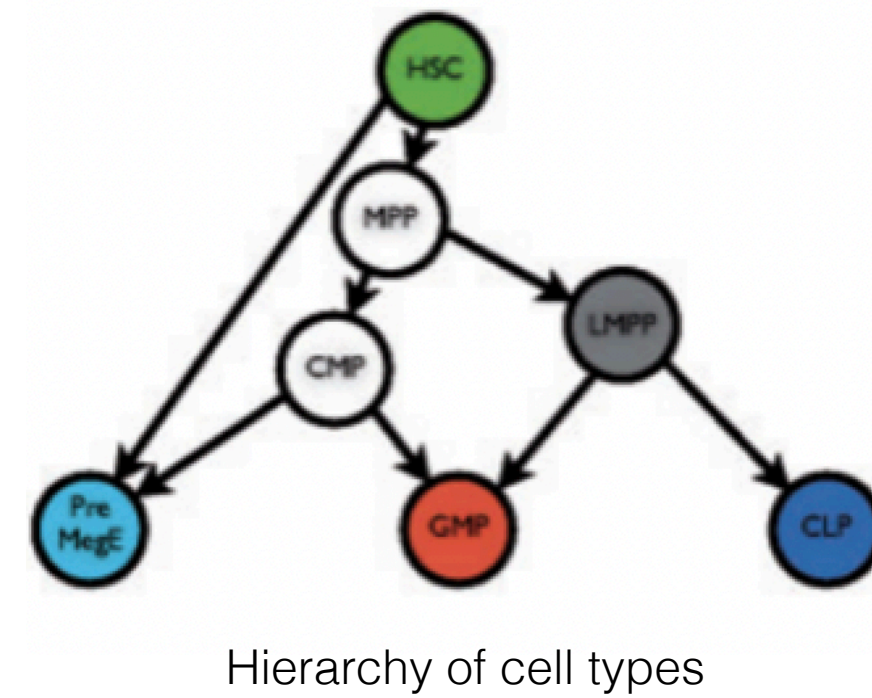


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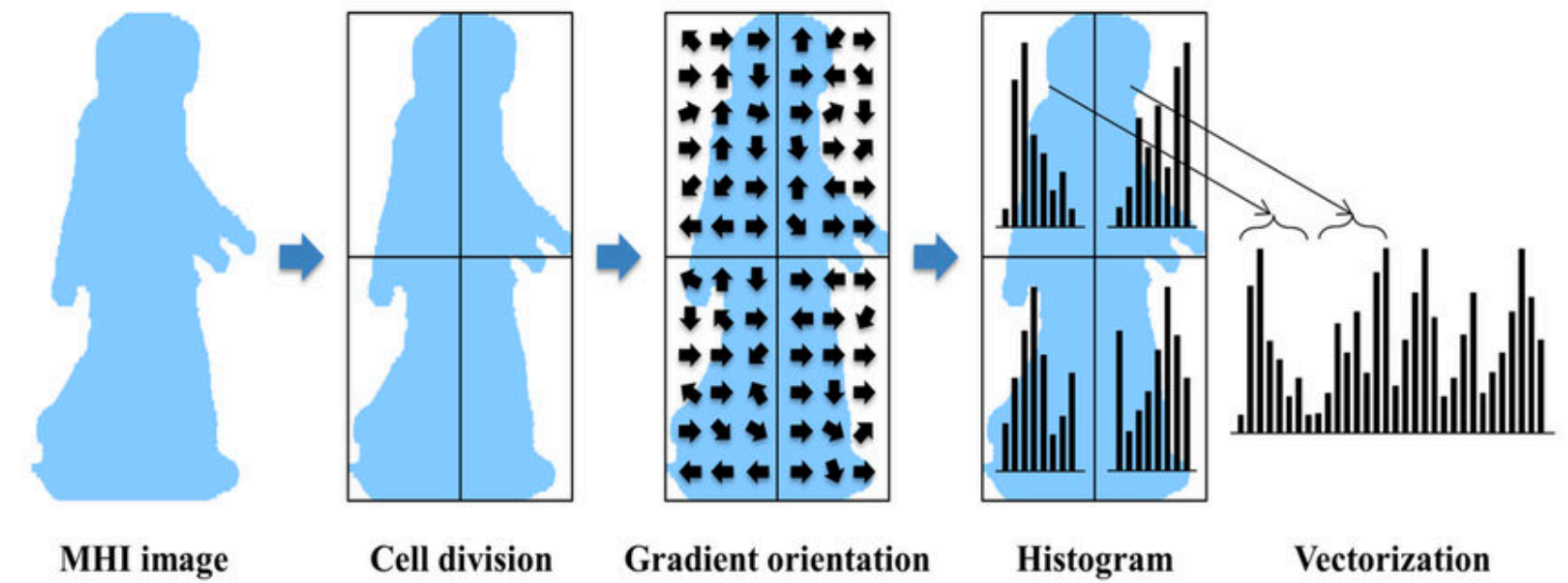
$N$  vectors on low-dim. submanifold



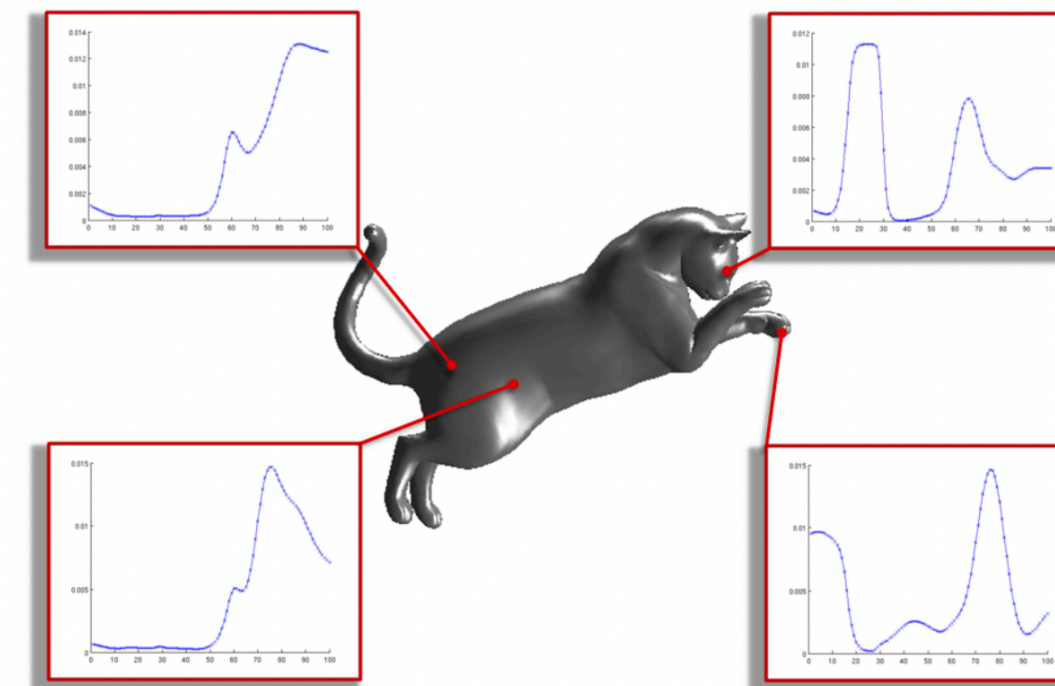
Haghverdi et al., *Bioinformatics* (2015)



Hierarchy of cell types



Eum et al., *Sensors* (2015)



Aubry et al., *ICCV workshop, IEEE* (2011)

## The manifold hypothesis:

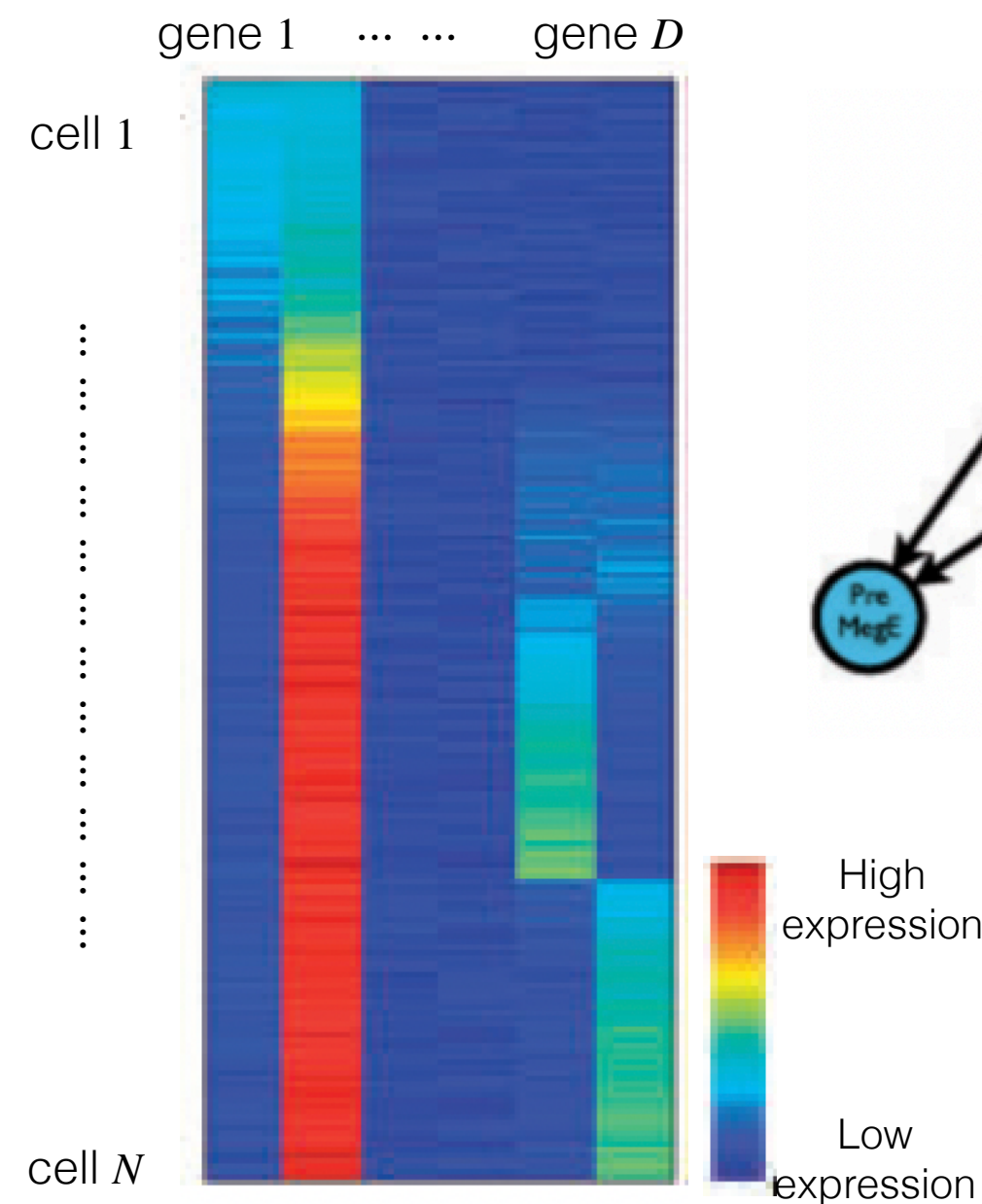
“high dimensional data tend to lie in the vicinity of a low dimensional manifold”.

Fefferman, Mitter, Narayanan. *J. Am. Math. Soc.*, 29, 983 (2016)

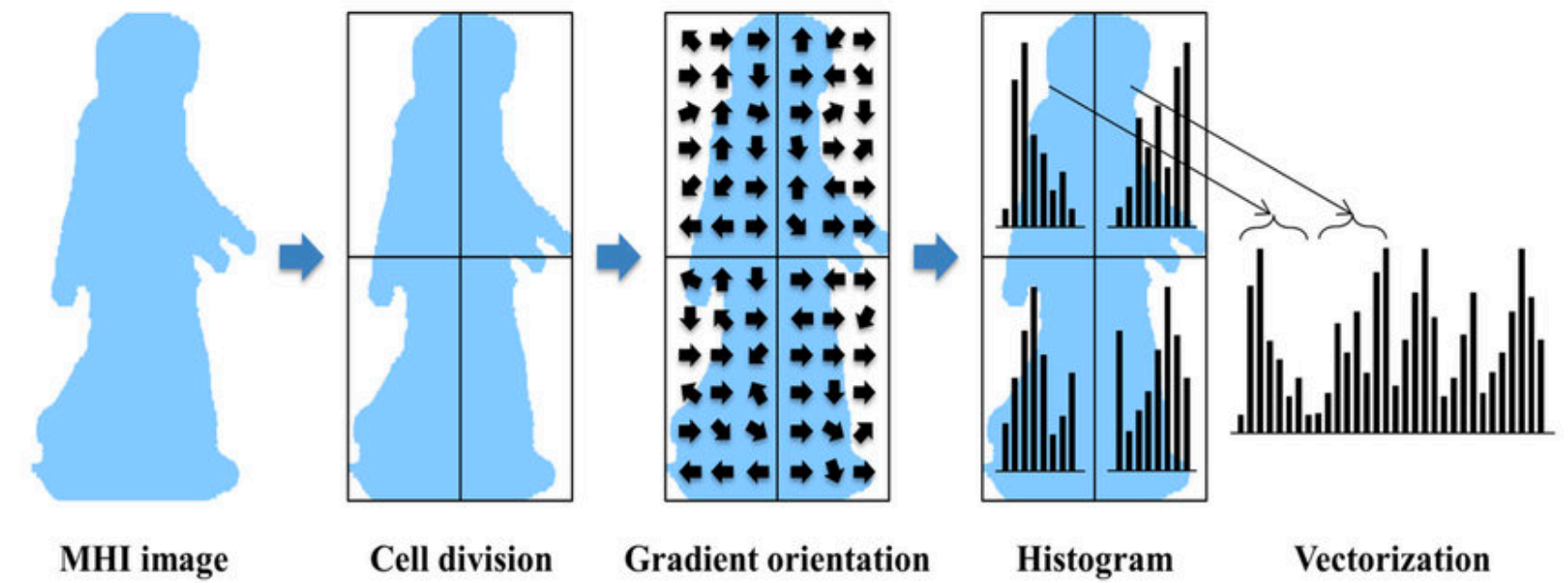
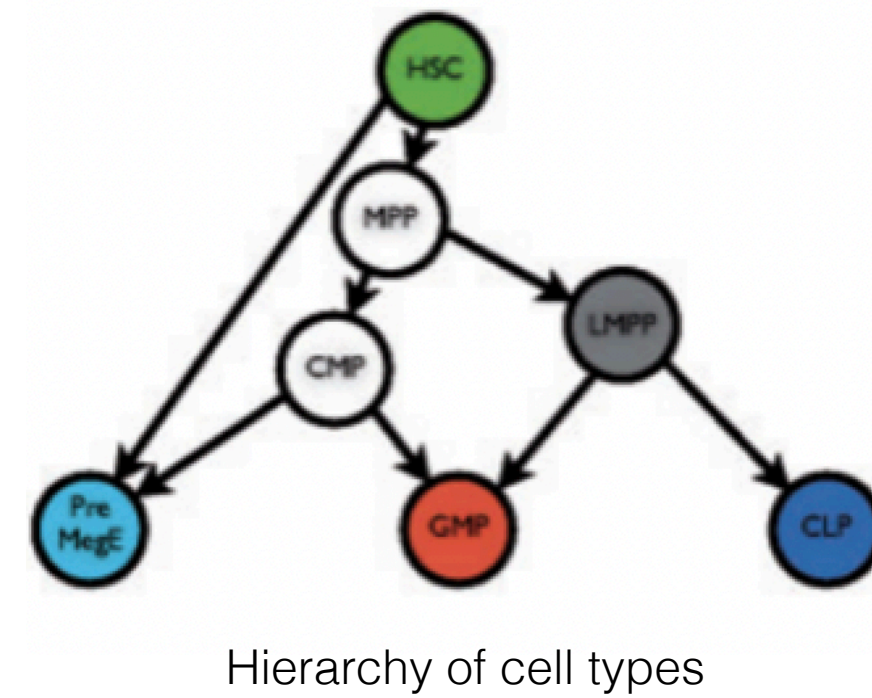


# What is “data”?

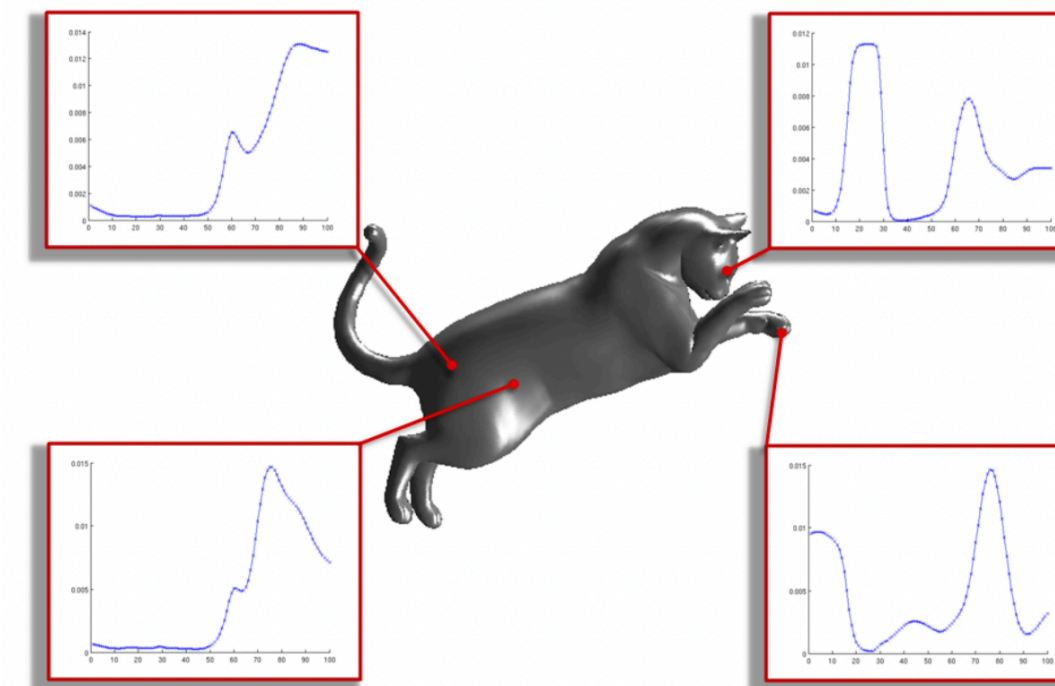
$N$  vectors on low-dim. submanifold



Hagverdi et al., *Bioinformatics* (2015)



Eum et al., *Sensors* (2015)



Aubry et al., *ICCV workshop, IEEE* (2011)

## The manifold hypothesis:

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Fefferman, Mitter, Narayanan. *J. Am. Math. Soc.*, 29, 983 (2016)

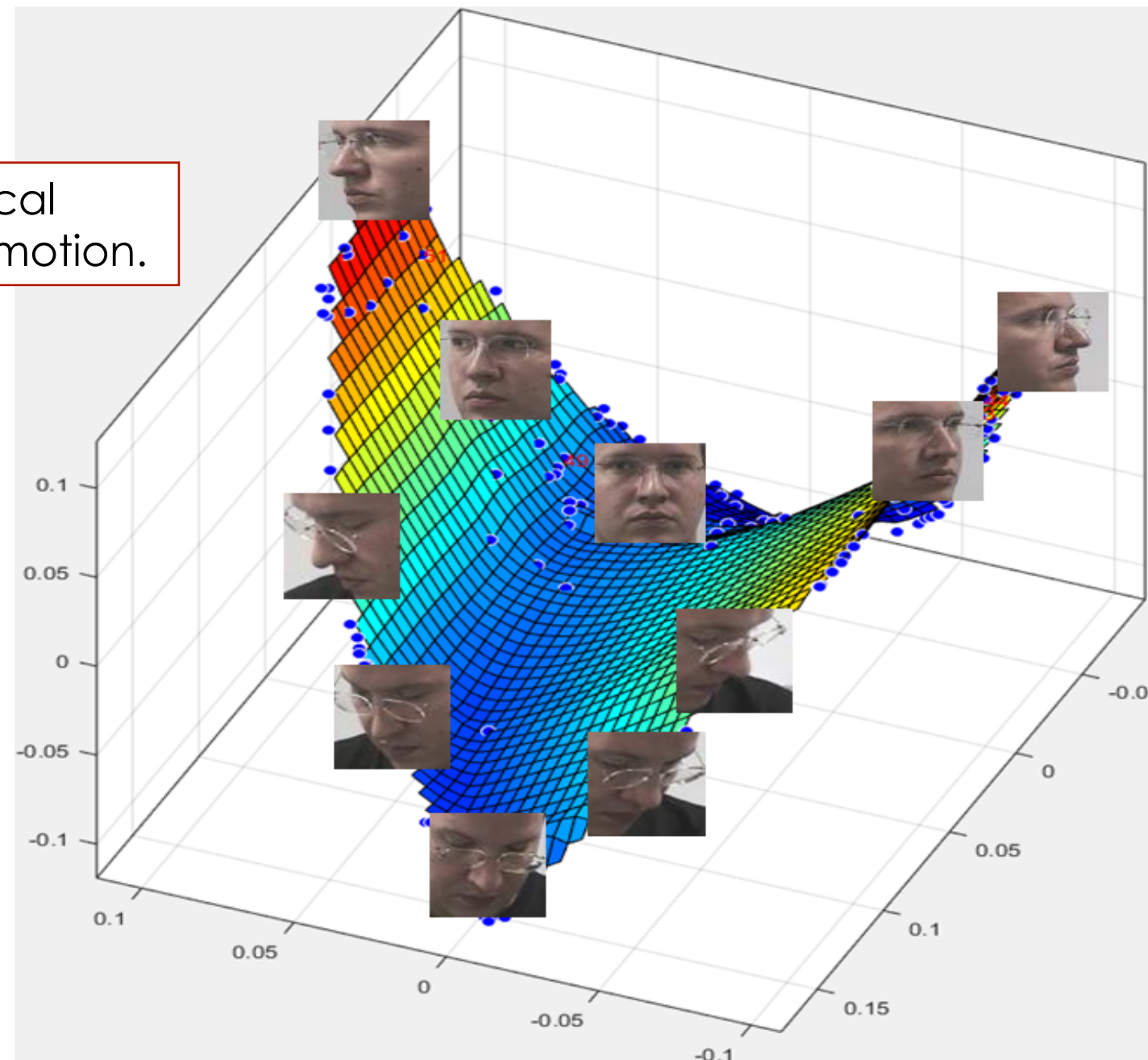
# Real-world data has low-dimensional structure



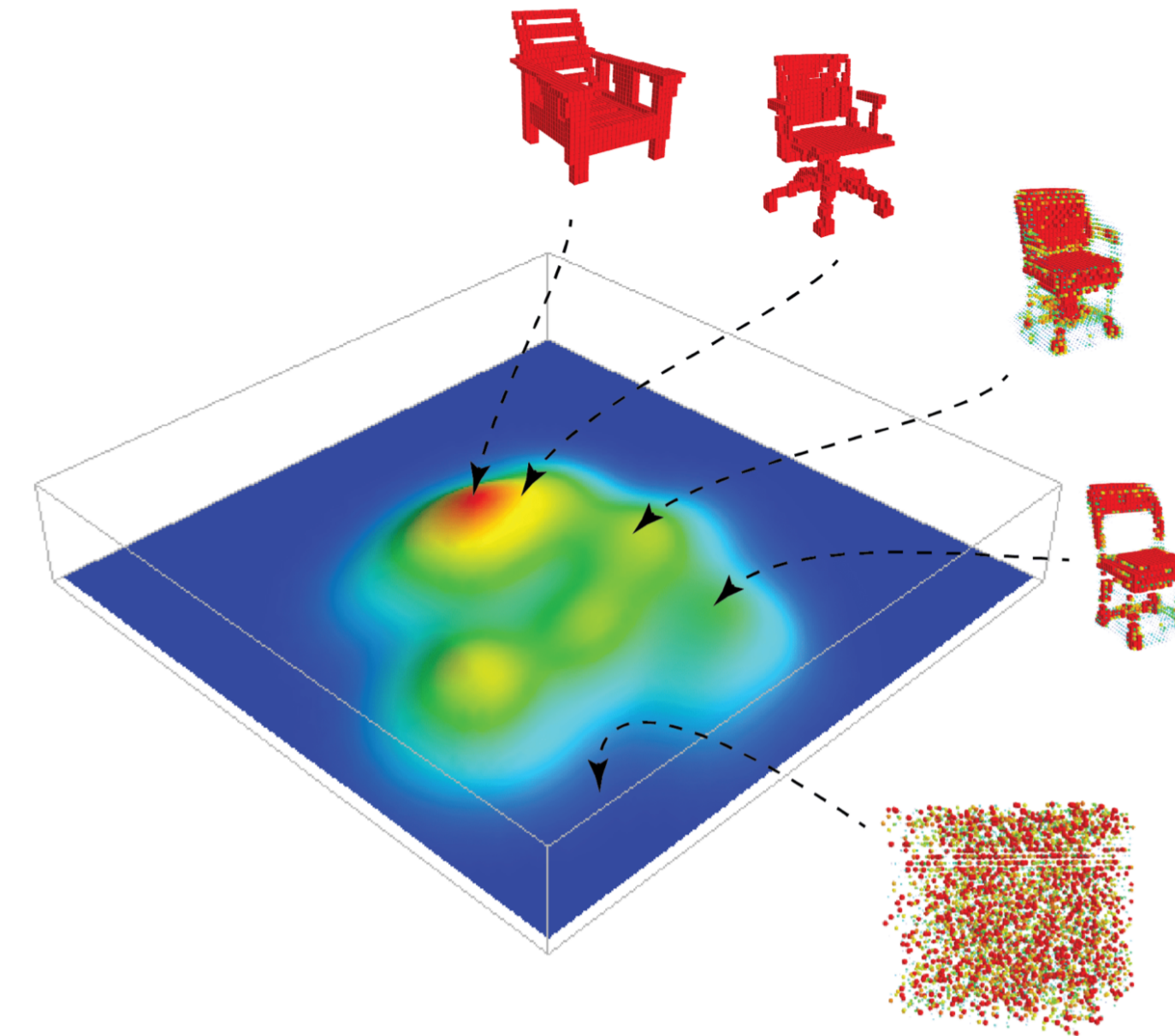
# What is “data”?

$N$  vectors on low-dim. *submanifold*

Data generated by dynamical system follows equations of motion.



<https://www.intechopen.com/books/manifolds-current-research-areas/head-pose-estimation-via-manifold-learning>



Randomly generated image of  $N \times N$  pixels  $\neq$  real world scene.

Gwak et al. *International Conference on 3D Vision (3DV)*, IEEE (2017).

**The manifold hypothesis:**

“high dimensional data tend to lie in the vicinity of a low dimensional manifold”.

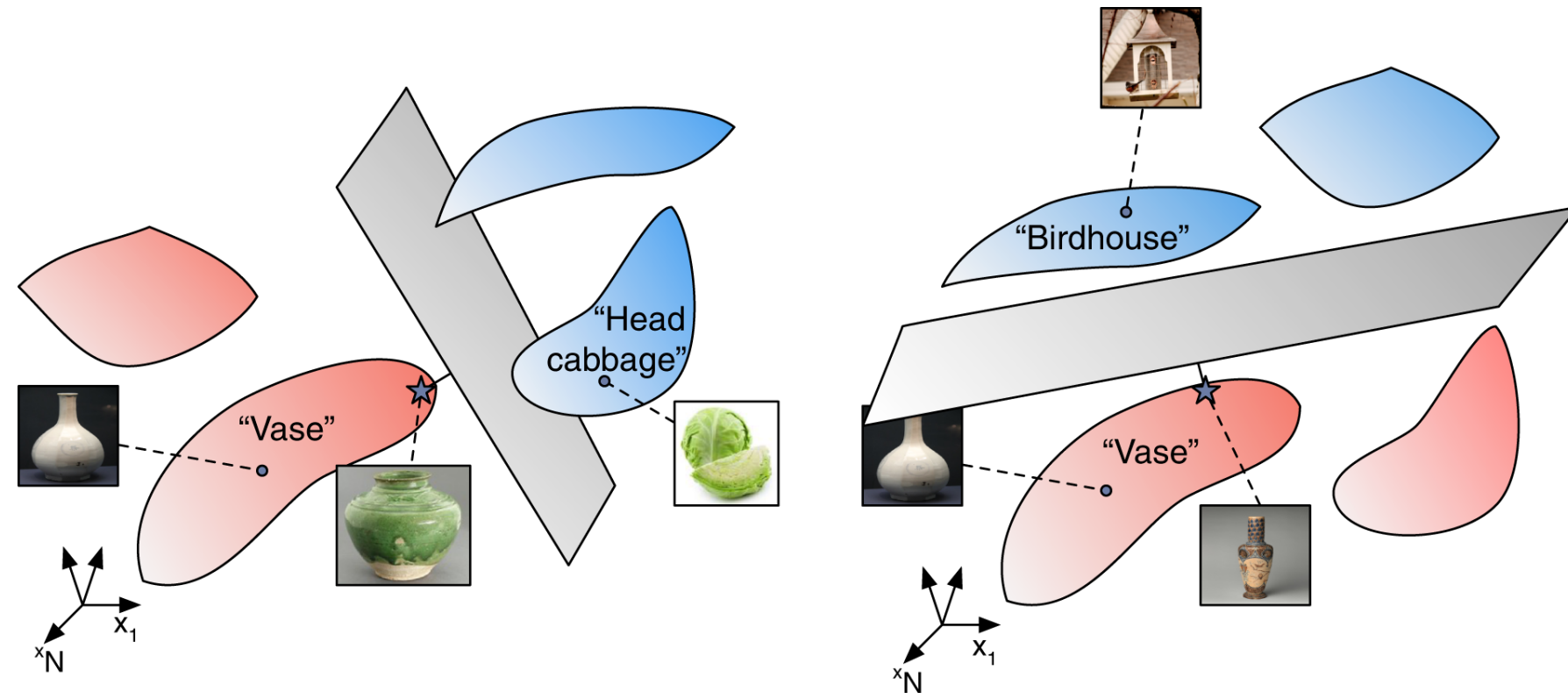
Fefferman, Mitter, Narayanan. *J. Am. Math. Soc.*, 29, 983 (2016)

**Real-world data has low-dimensional structure**

**Data analysis  $\approx$  Recovering geometry of data**



Classification within neural network's *concept space*:



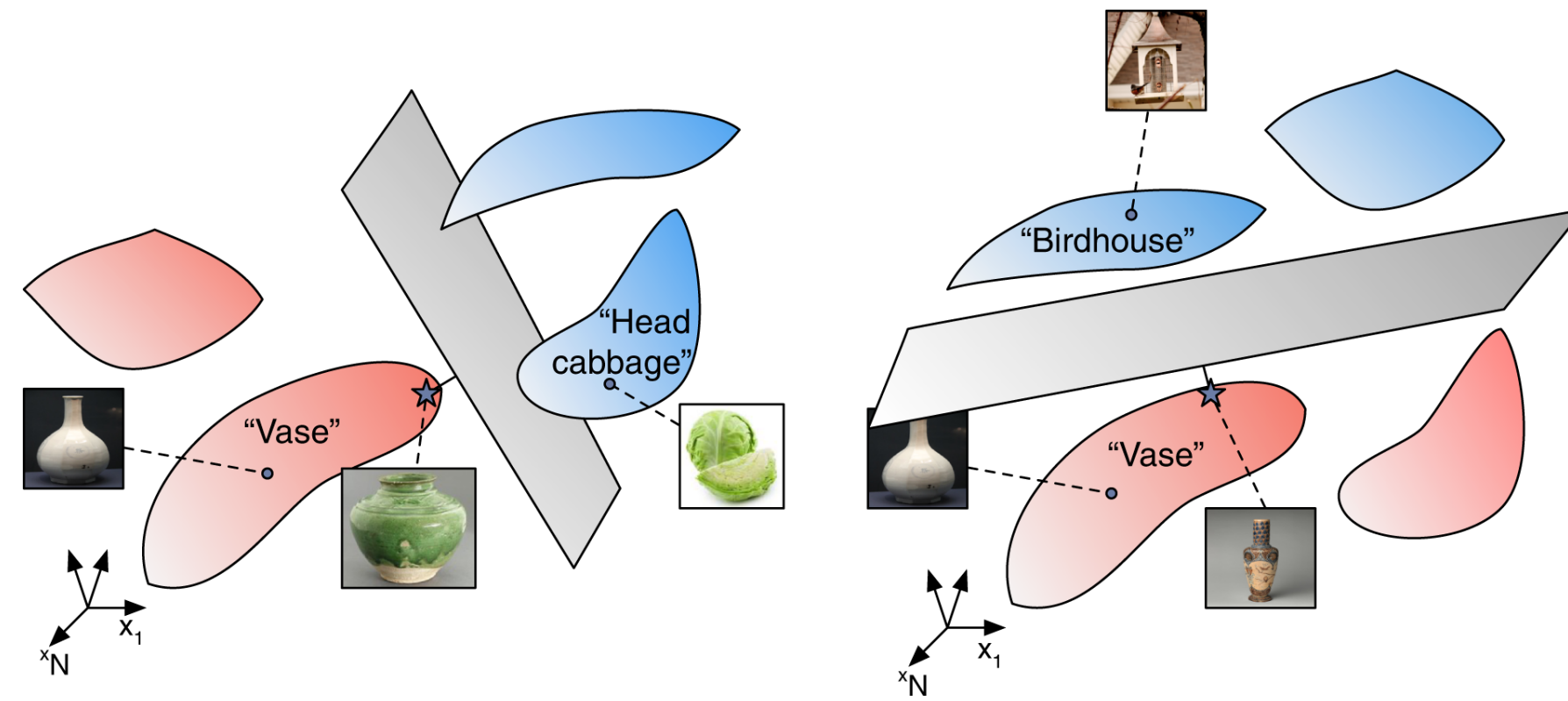
Cohen et al. *Nat Commun* 11, 746 (2020).

- Classification

**Data analysis  $\approx$  Recovering geometry of data**

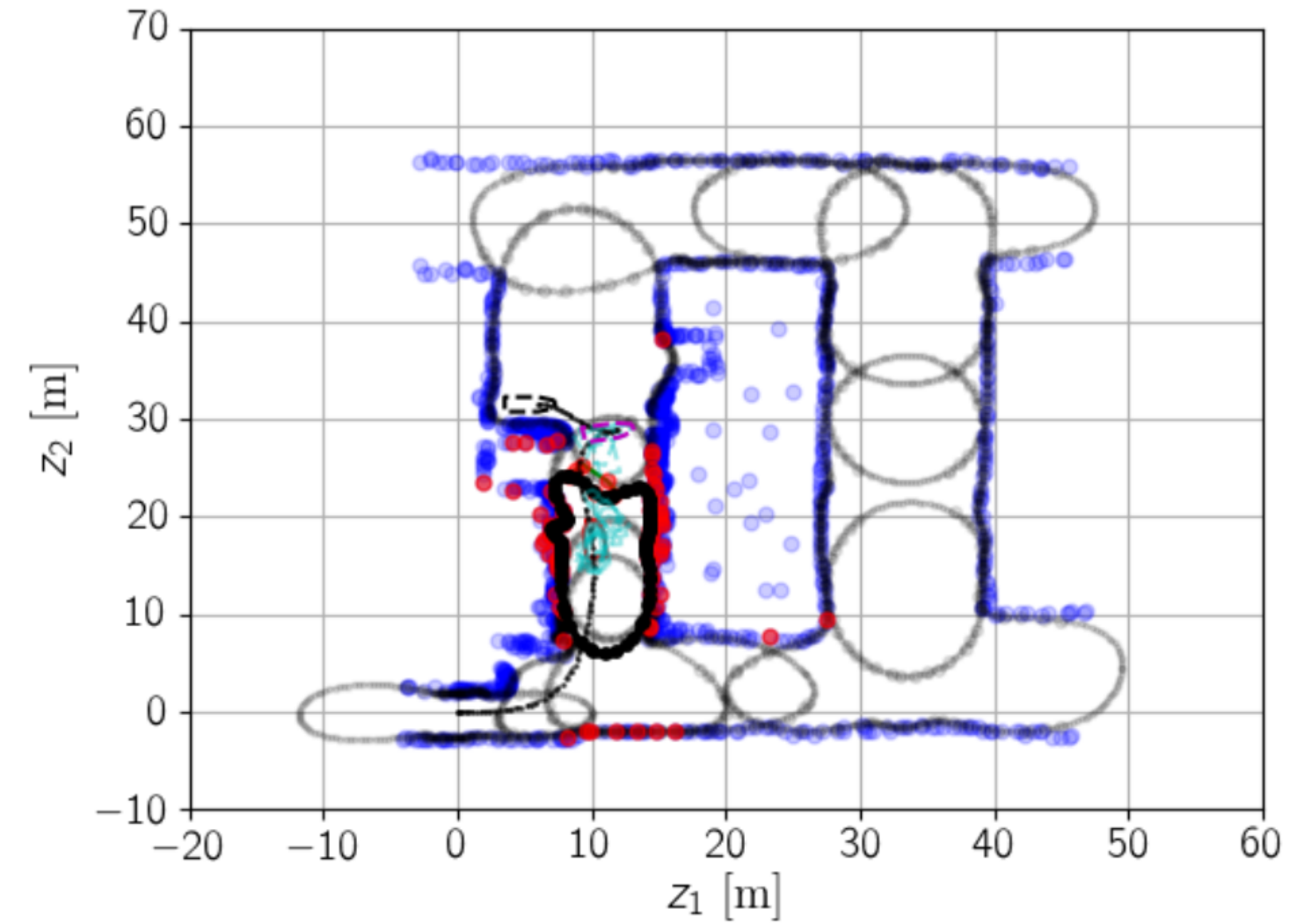


Classification within neural network's *concept space*:



Cohen et al. *Nat Commun* 11, 746 (2020).

Obstacle avoidance in autonomous driving:

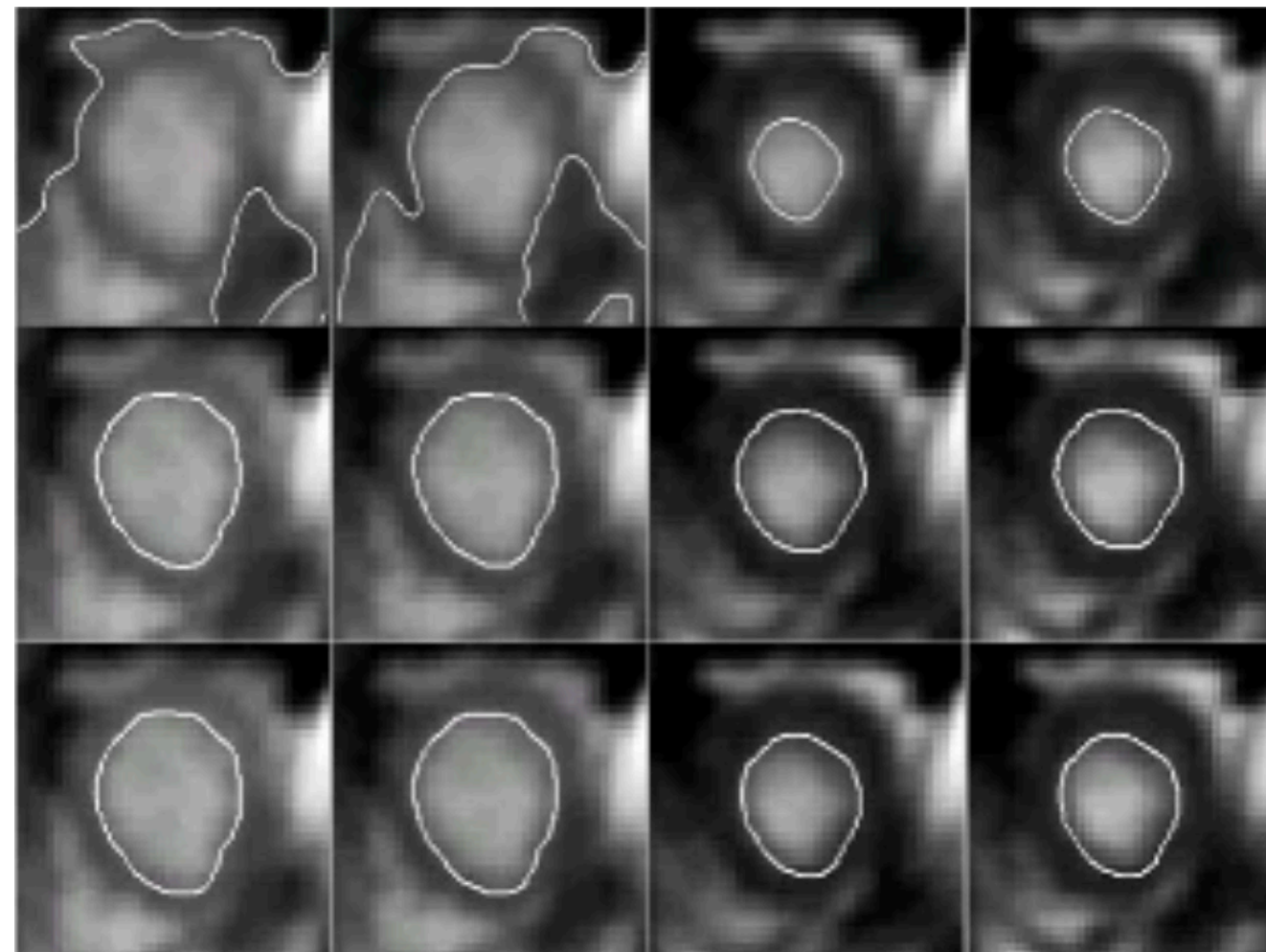


Diwale et al., <https://infoscience.epfl.ch/record/265381>

- Classification
- Route planning

## Data analysis $\approx$ Recovering geometry of data

Image segmentation for medical imaging:

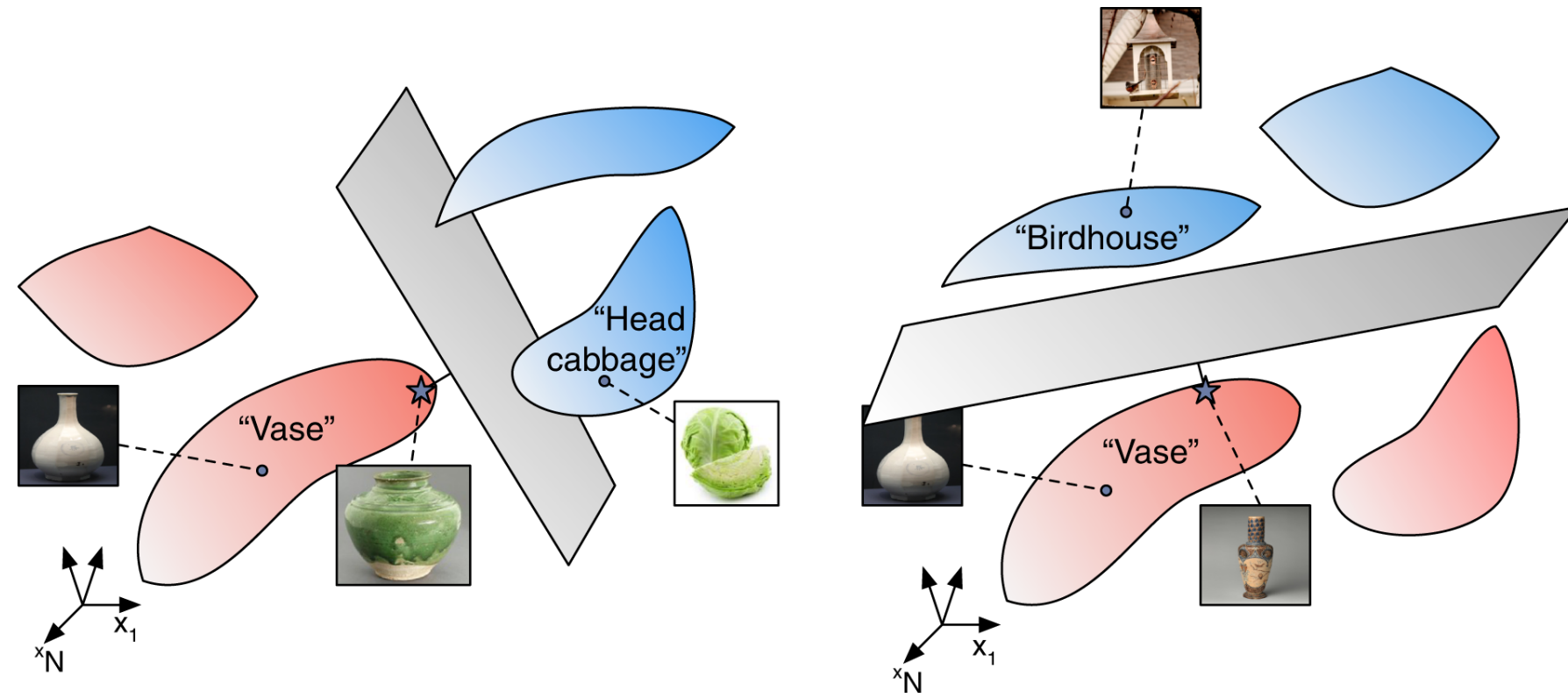


Zhang et al., *IEEE CVPR*, 1092 (2006).

- Image segmentation

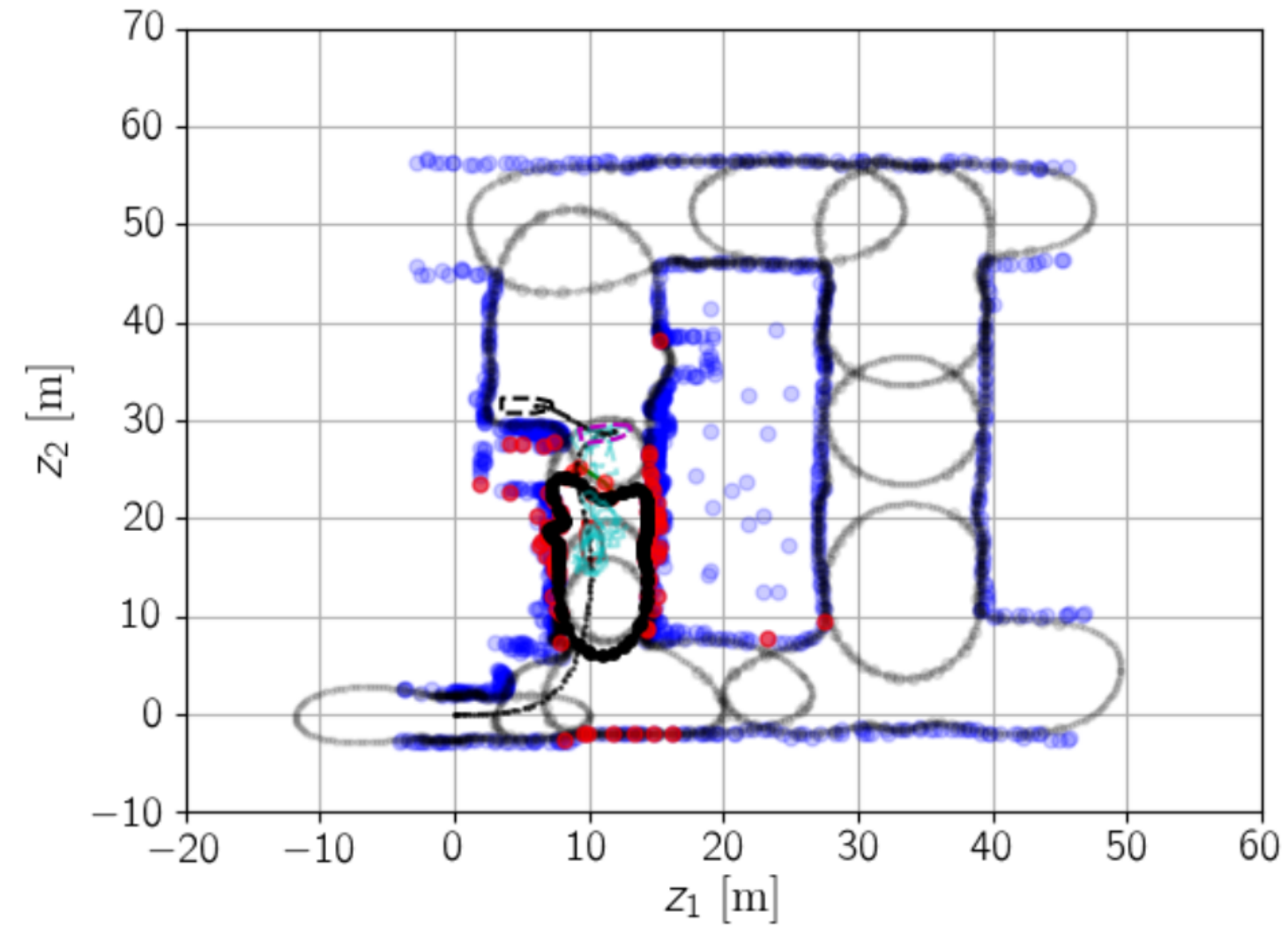


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Obstacle avoidance in autonomous driving:

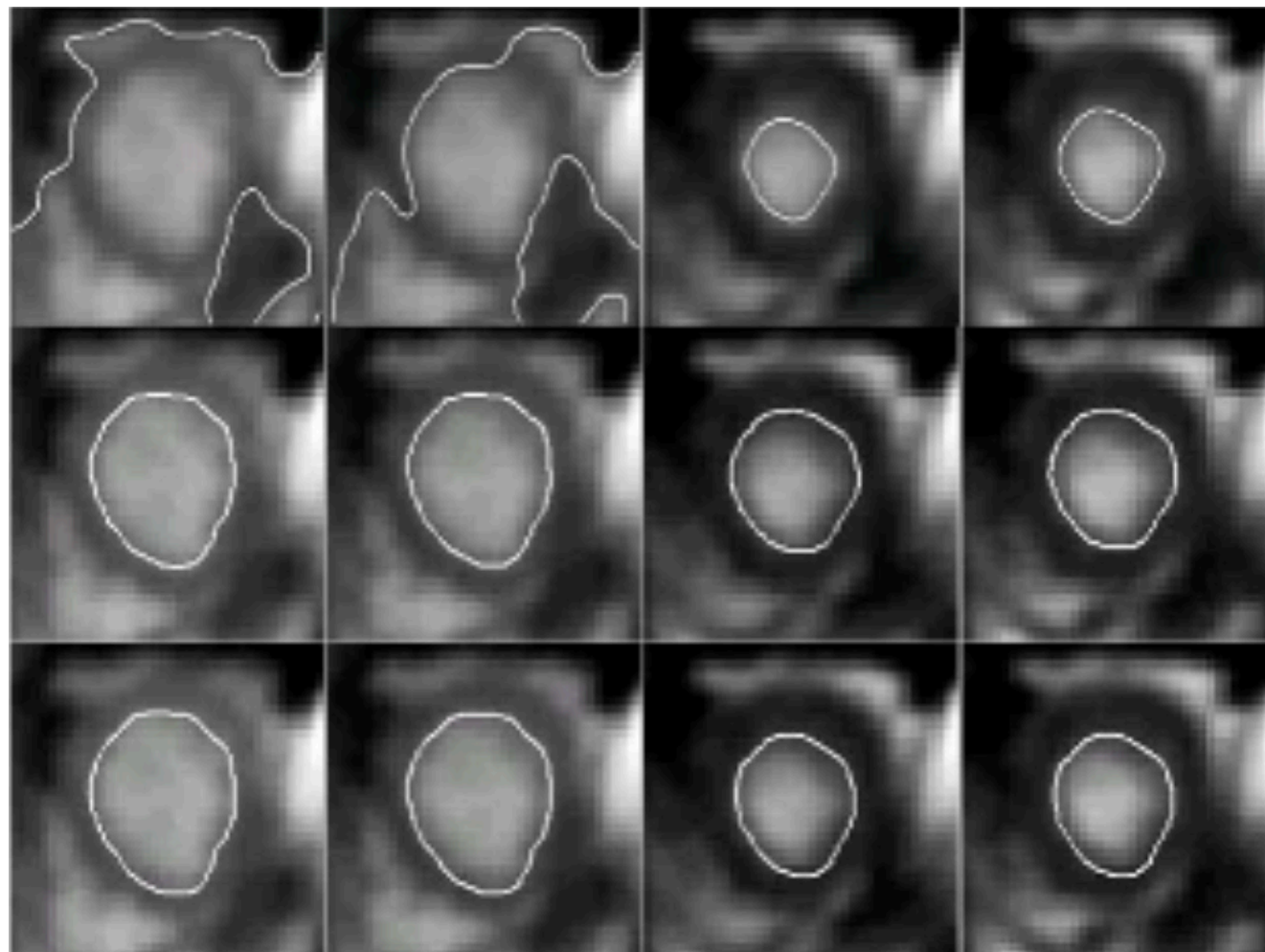


Diwale et al., <https://infoscience.epfl.ch/record/265381>

- Classification
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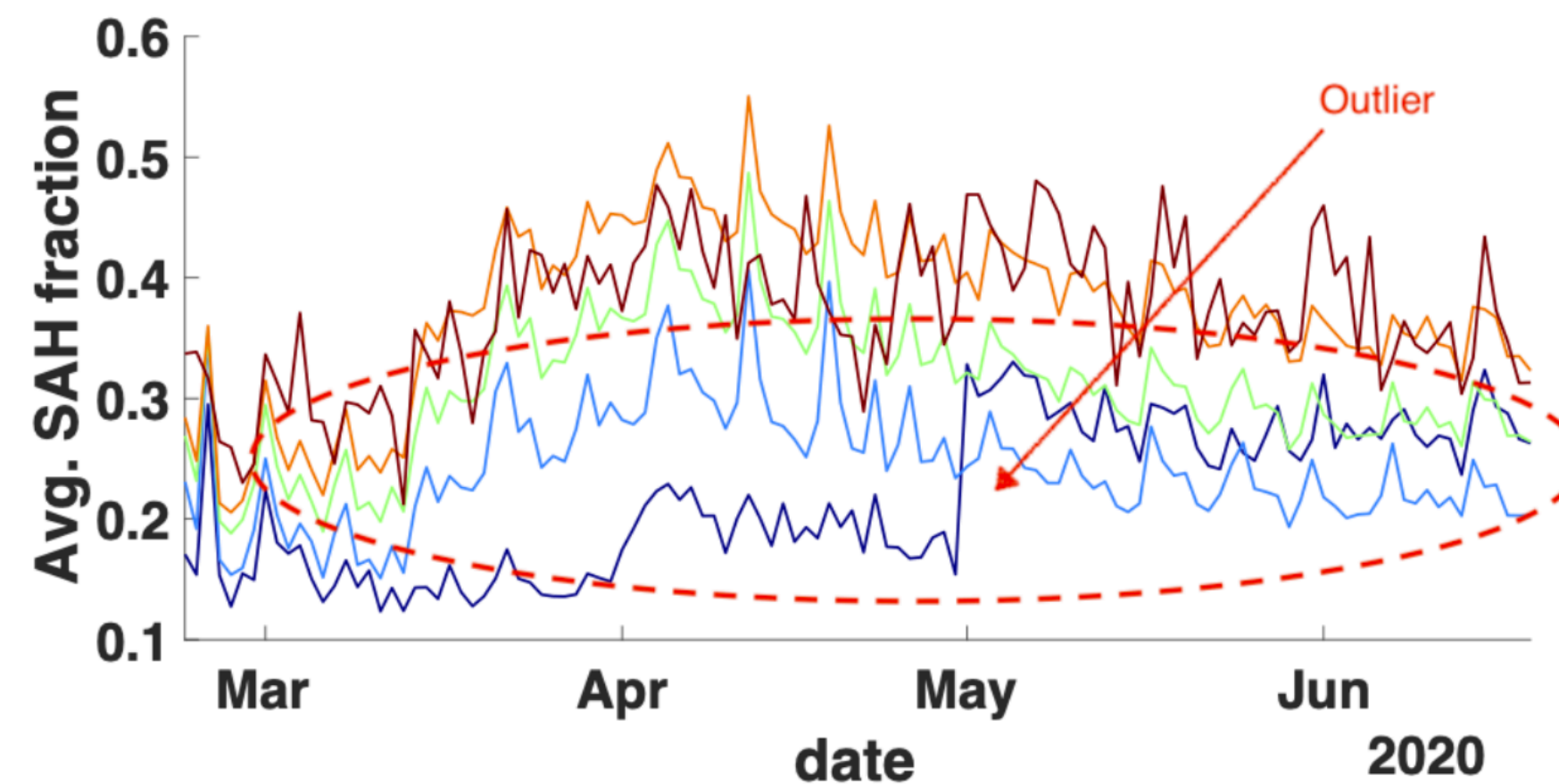
## Data analysis $\approx$ Recovering geometry of data

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Zhang et al., *IEEE CVPR*, 1092 (2006).

Anomaly detection in statistical dataset:

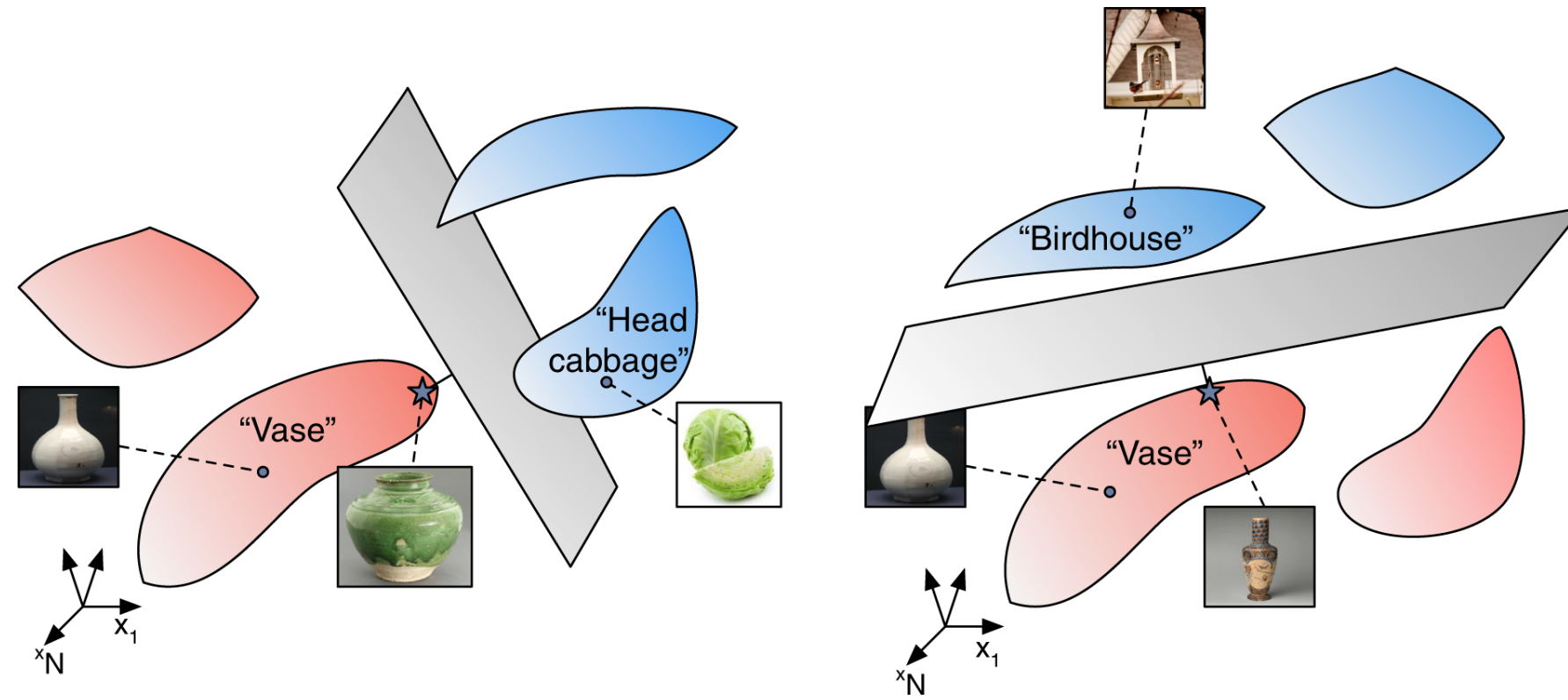


Kumar & Sarovar, *arXiv* (2022).

- Image segmentation
- Outlier detection

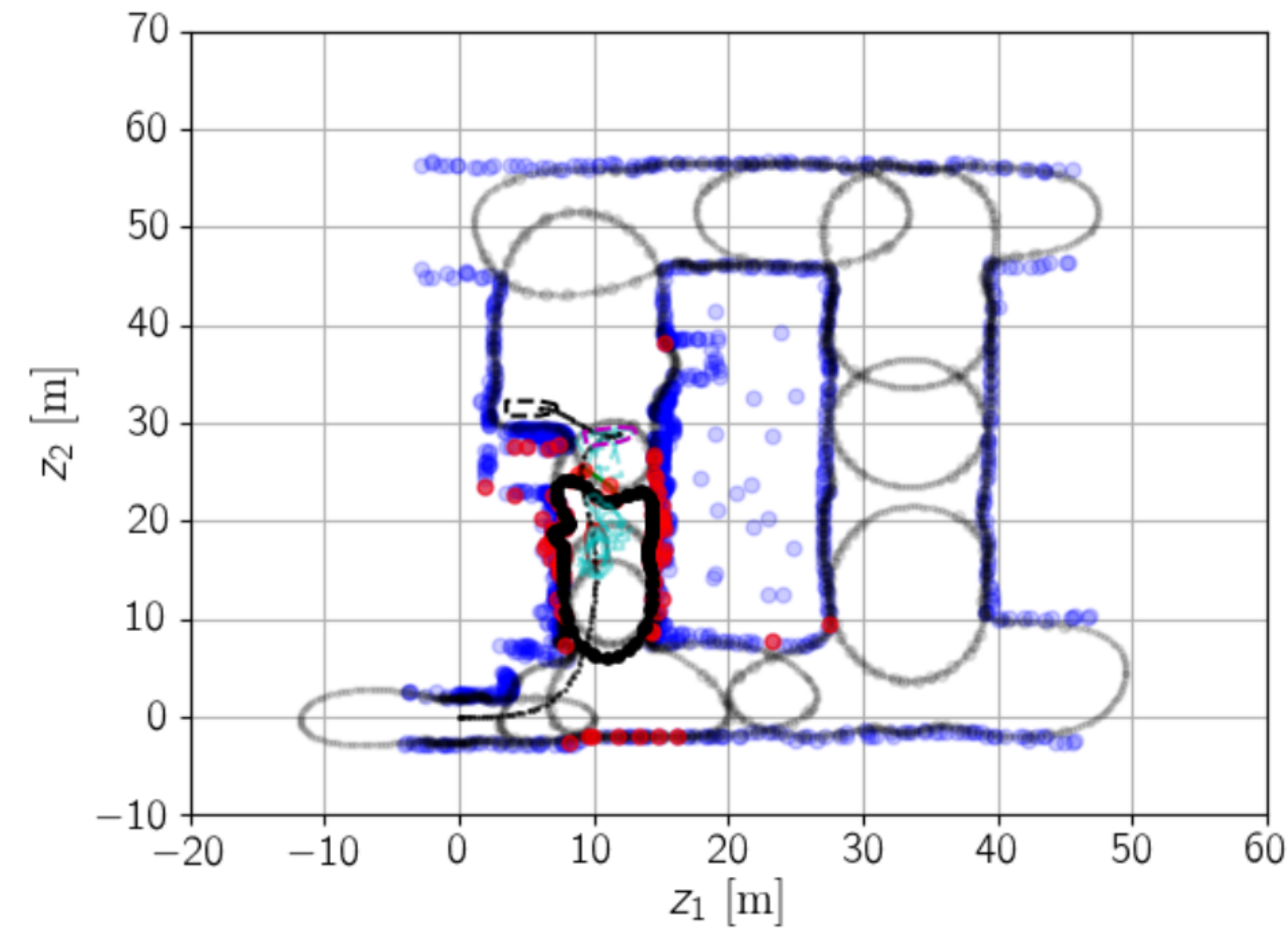


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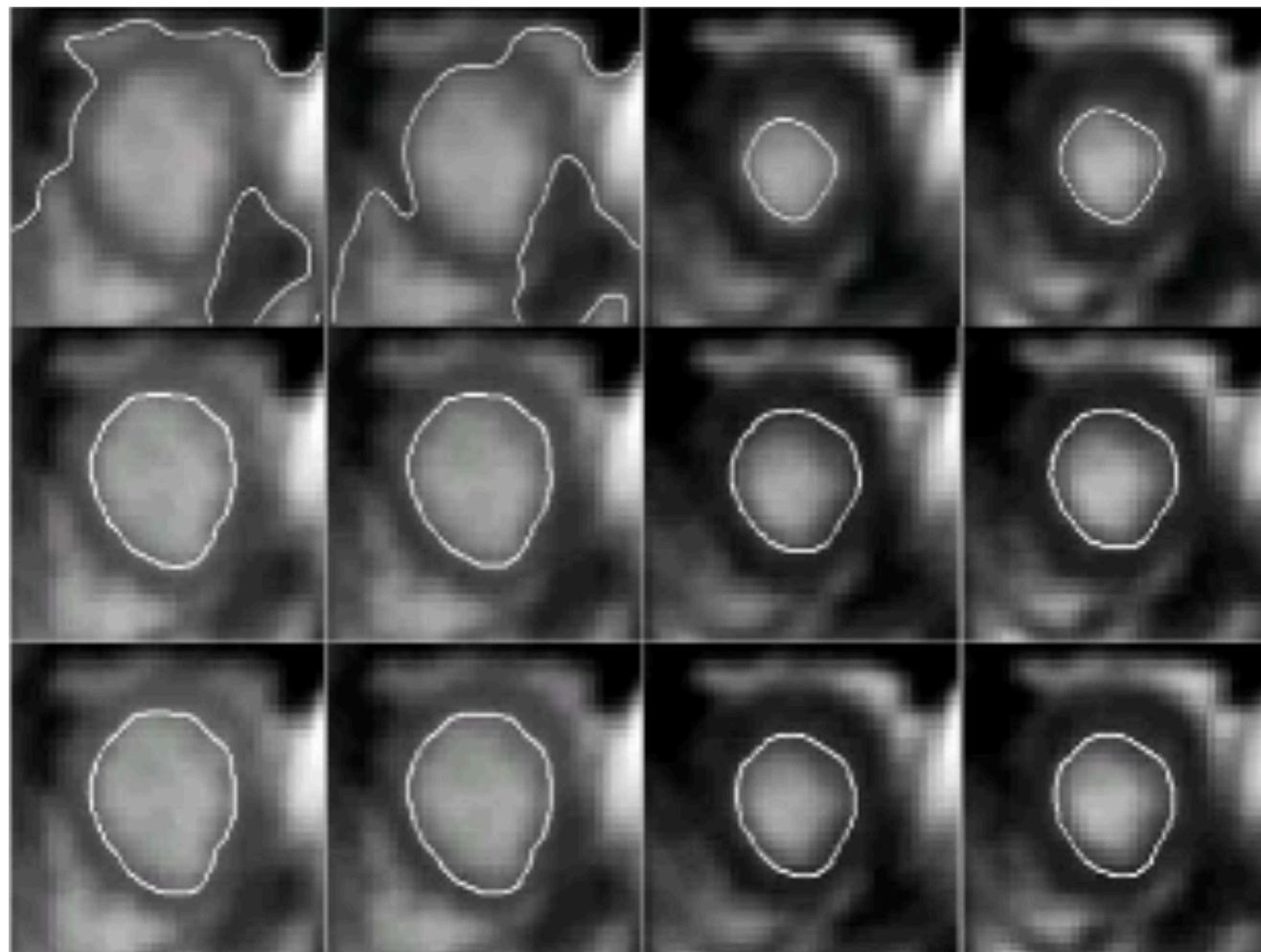
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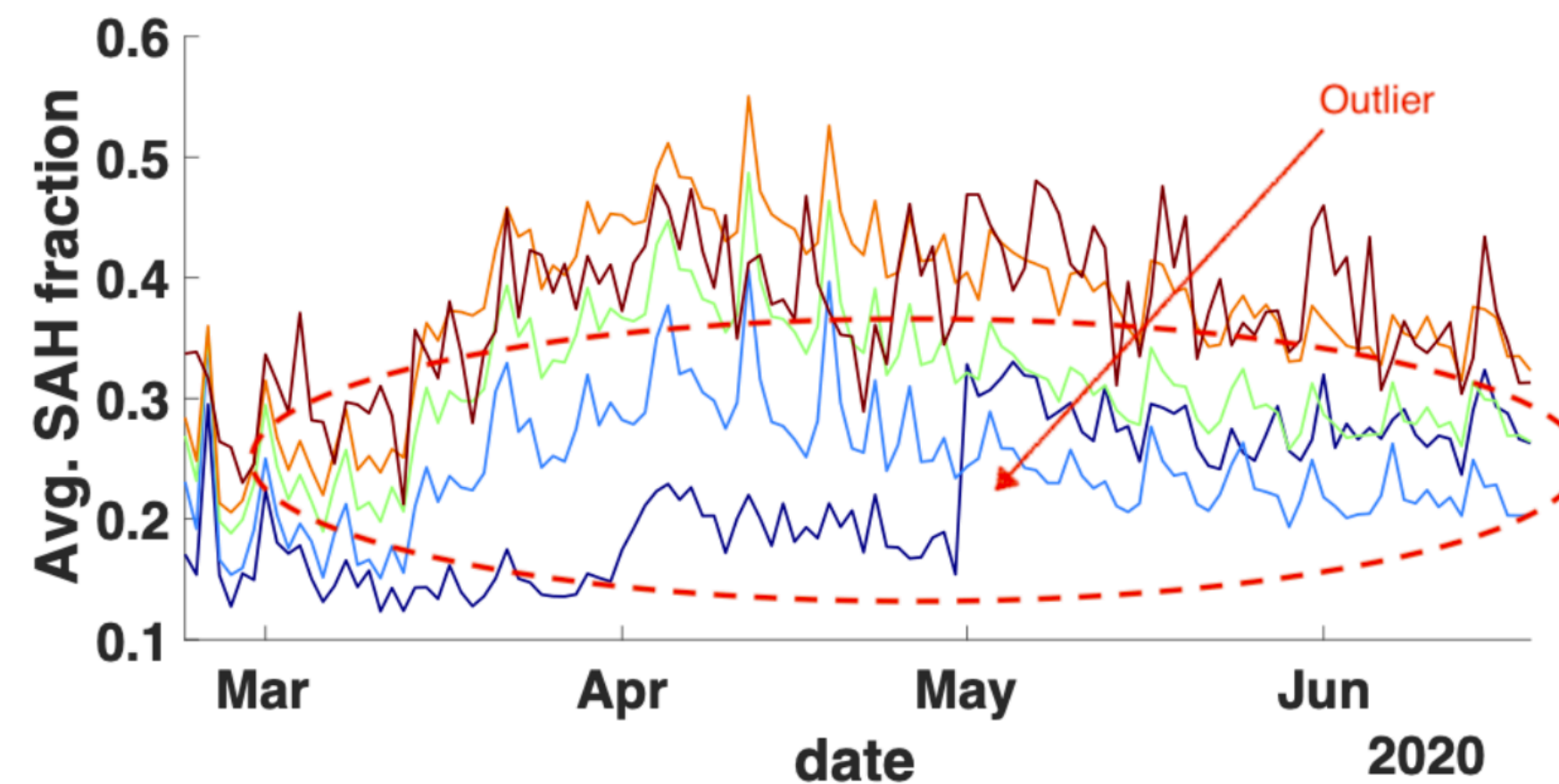
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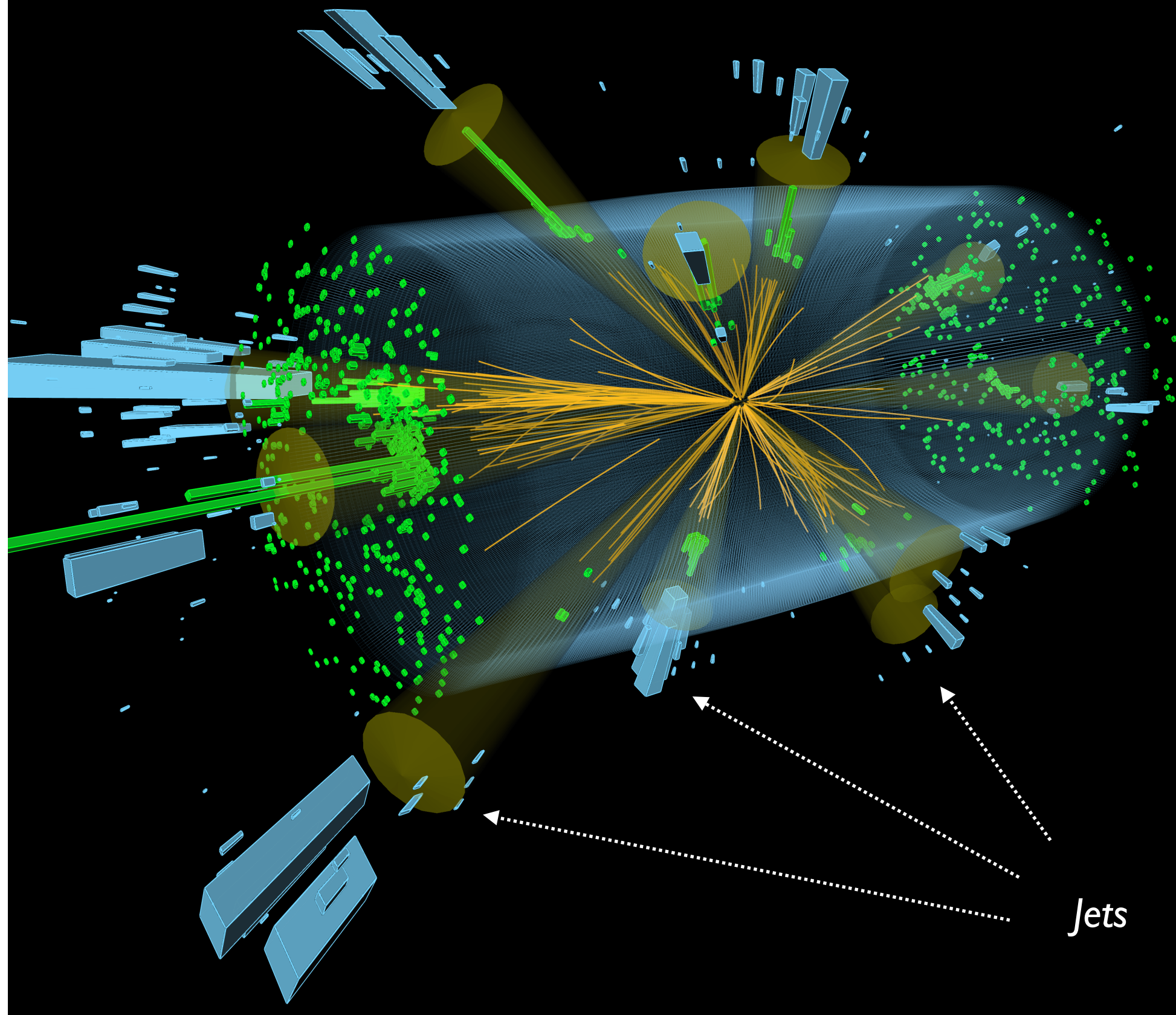
Kumar & Sarovar, *arXiv* (2022).

- Classification
- Route planning
- Dimensionality reduction, clustering, augmented reality, regularization of learning methods, visualization, ...
- Image segmentation
- Outlier detection



## Collider Event

Every 25 nanoseconds at the LHC

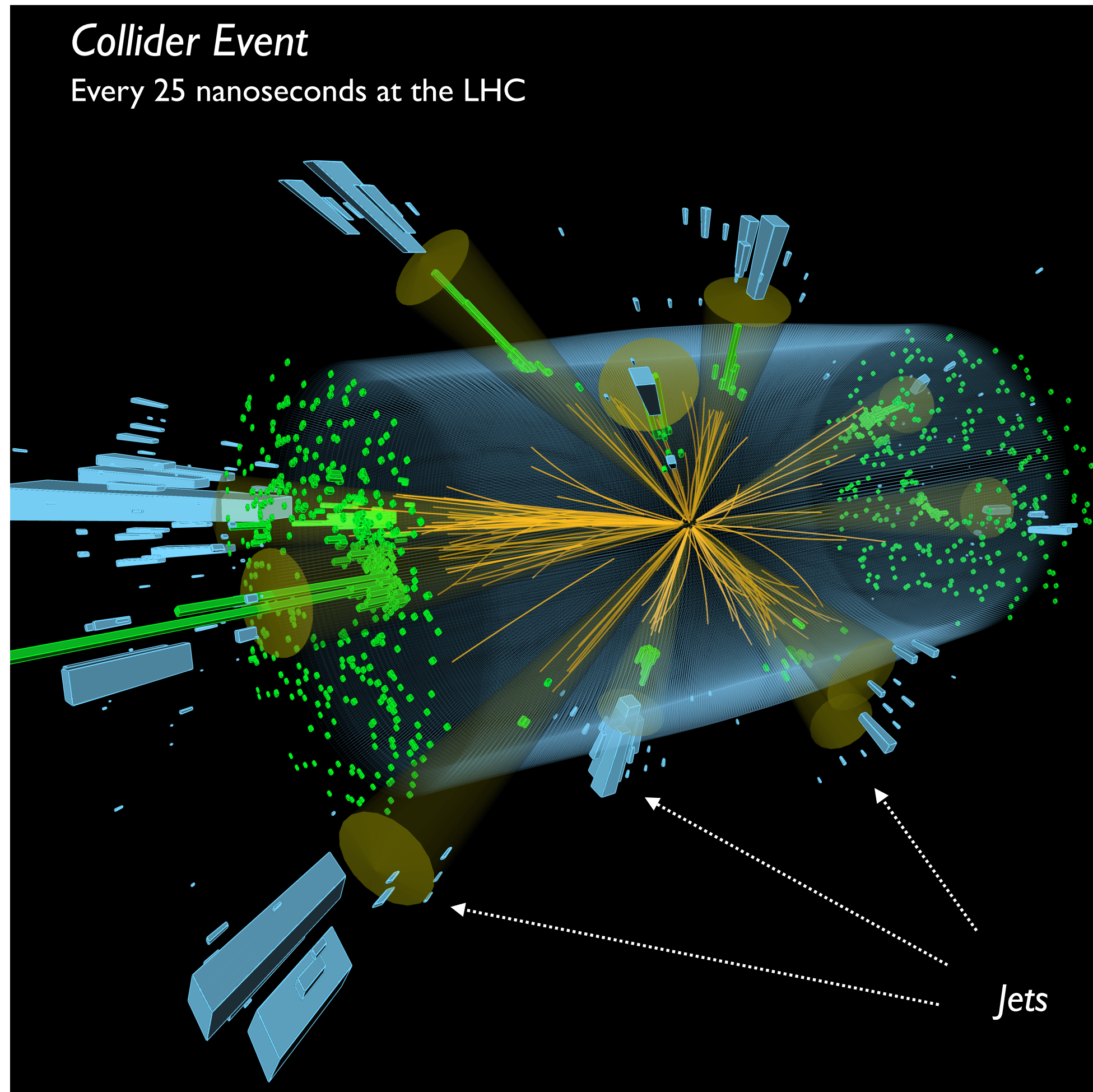


## Collider data has geometric structure

Komiske, Metodiev, Thaler, **The hidden geometry of particle collisions**,  
J. HEP, 6 (2020)



# Collider data has geometric structure

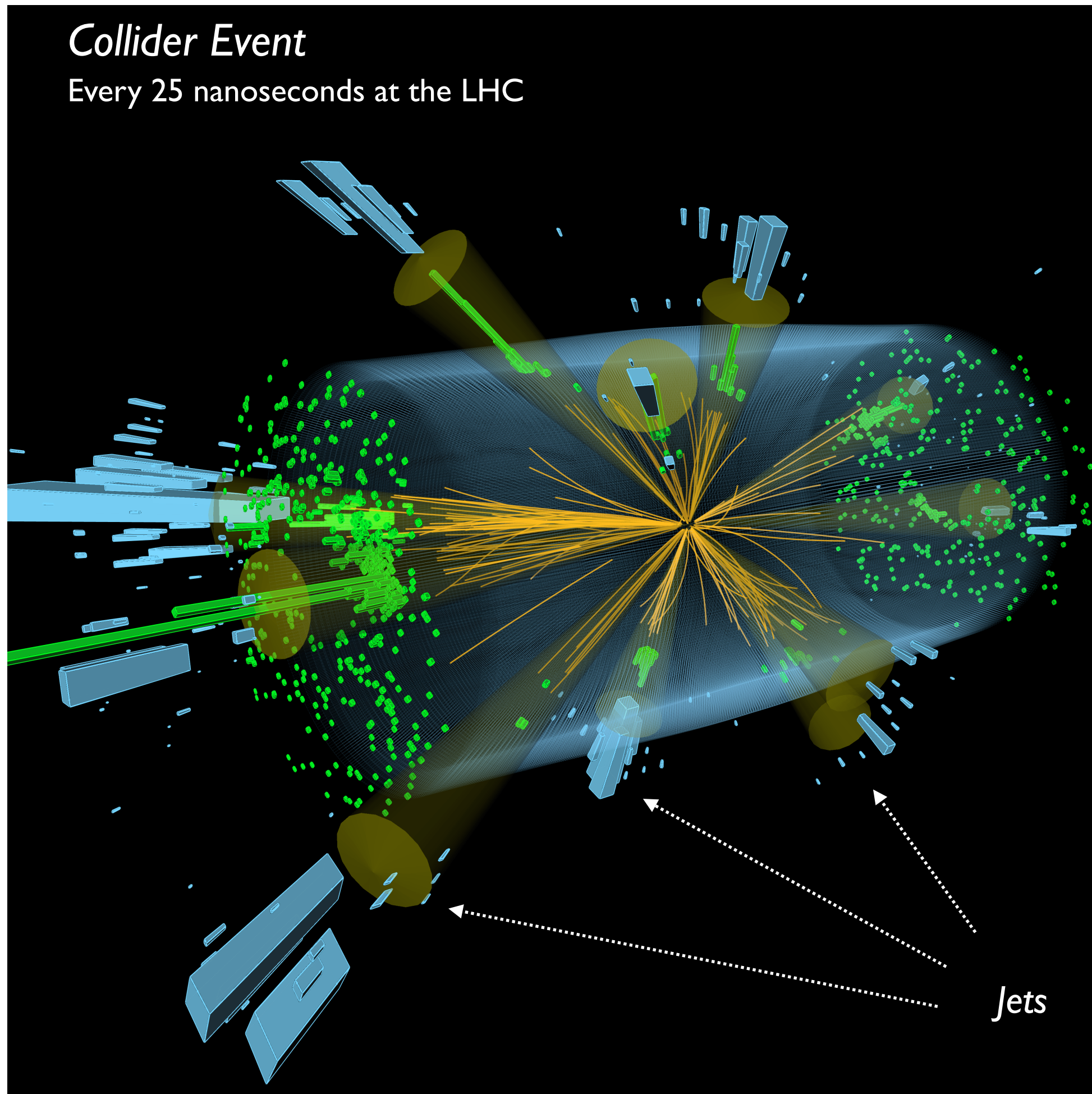


Energy flow  
(or Event):

$$\mathcal{E}(\hat{n}) = \sum_{j=1}^N E_j \delta(\hat{n} - \hat{n}_j)$$



# Collider data has geometric structure



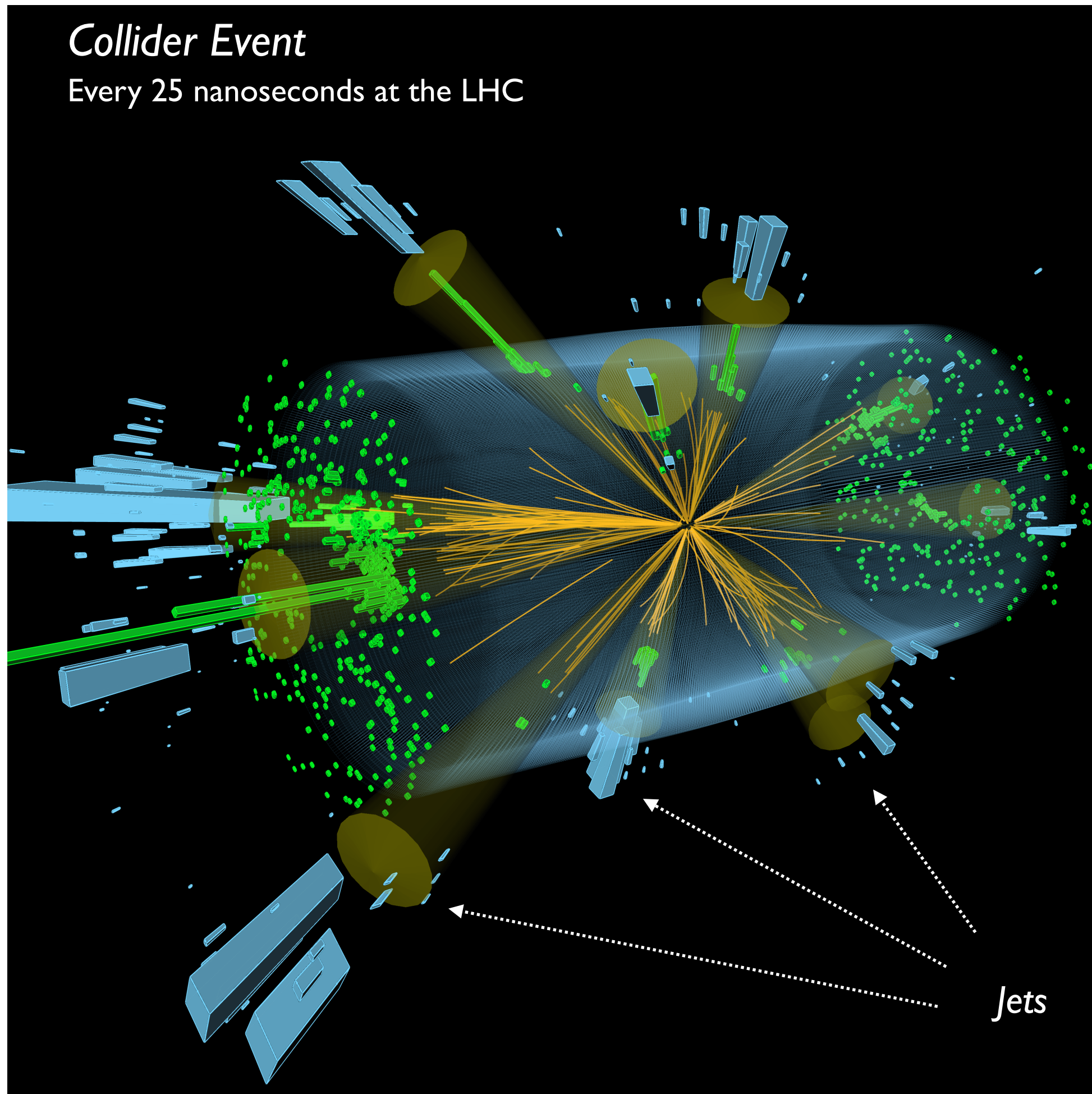
Energy flow  
(or Event):

#particles  
↓  
 $N$

$$\mathcal{E}(\hat{n}) = \sum_{j=1}^N E_j \delta(\hat{n} - \hat{n}_j)$$



# Collider data has geometric structure



Energy flow  
(or Event):

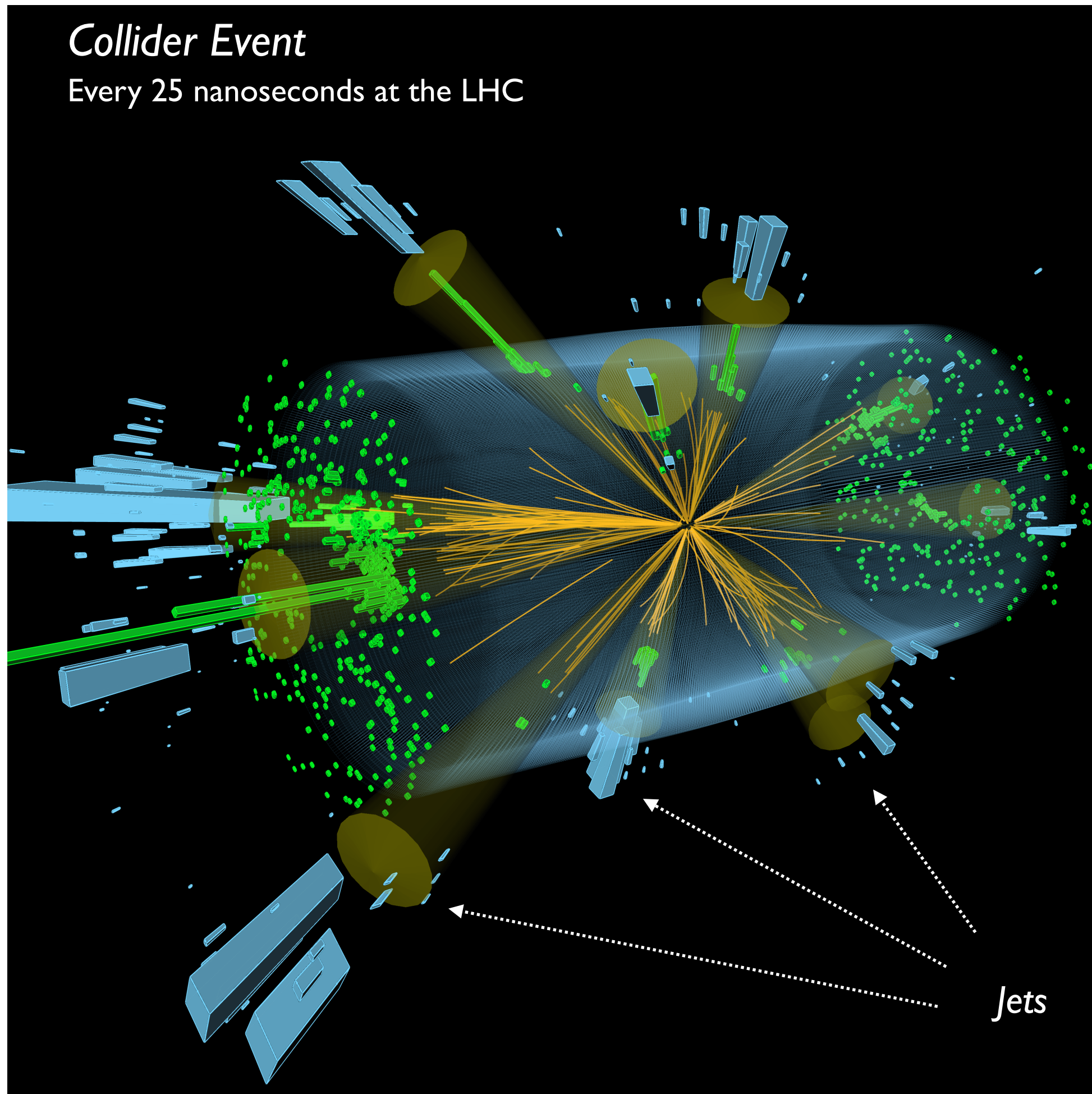
$$\mathcal{E}(\hat{n}) = \sum_{j=1}^N E_j \delta(\hat{n} - \hat{n}_j)$$

#particles  
↓  
 $N$   
energies\*  
↙

\* or particle transverse momenta



# Collider data has geometric structure



Energy flow  
(or Event):

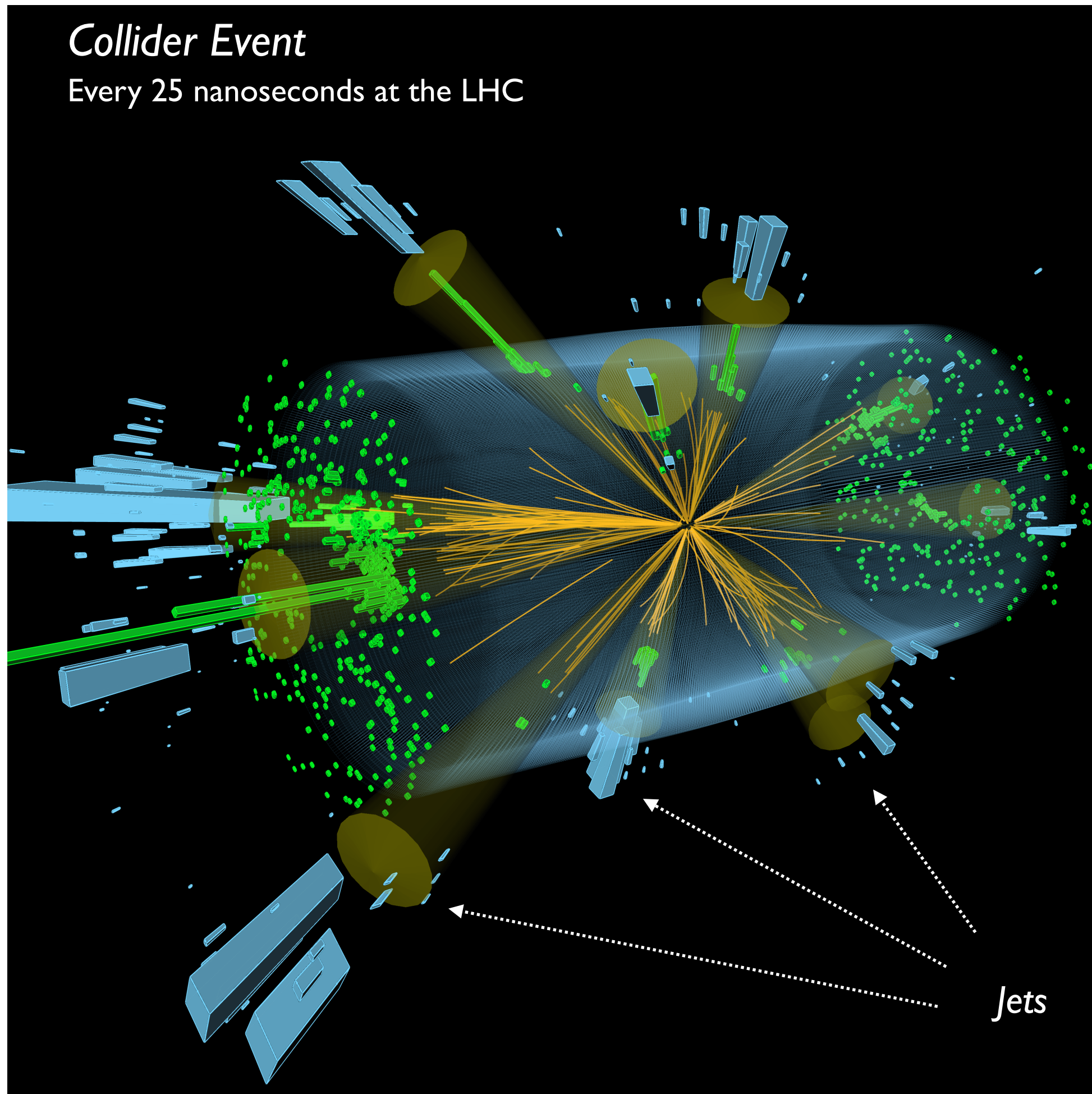
$$\mathcal{E}(\hat{n}) = \sum_{j=1}^N E_j \delta(\hat{n} - \hat{n}_j)$$

#particles  
↓  
 $N$   
energies\*  
∠directions

\* or particle transverse momenta



# Collider data has geometric structure



Energy flow  
(or Event):

$$\mathcal{E}(\hat{n}) = \sum_{j=1}^N E_j \delta(\hat{n} - \hat{n}_j)$$

#particles  $\downarrow$   $N$

energies\*  $\swarrow$   $E_j$

$\uparrow$   $\hat{n}_j$

$\angle$  directions

Energy-weighted  
point cloud:

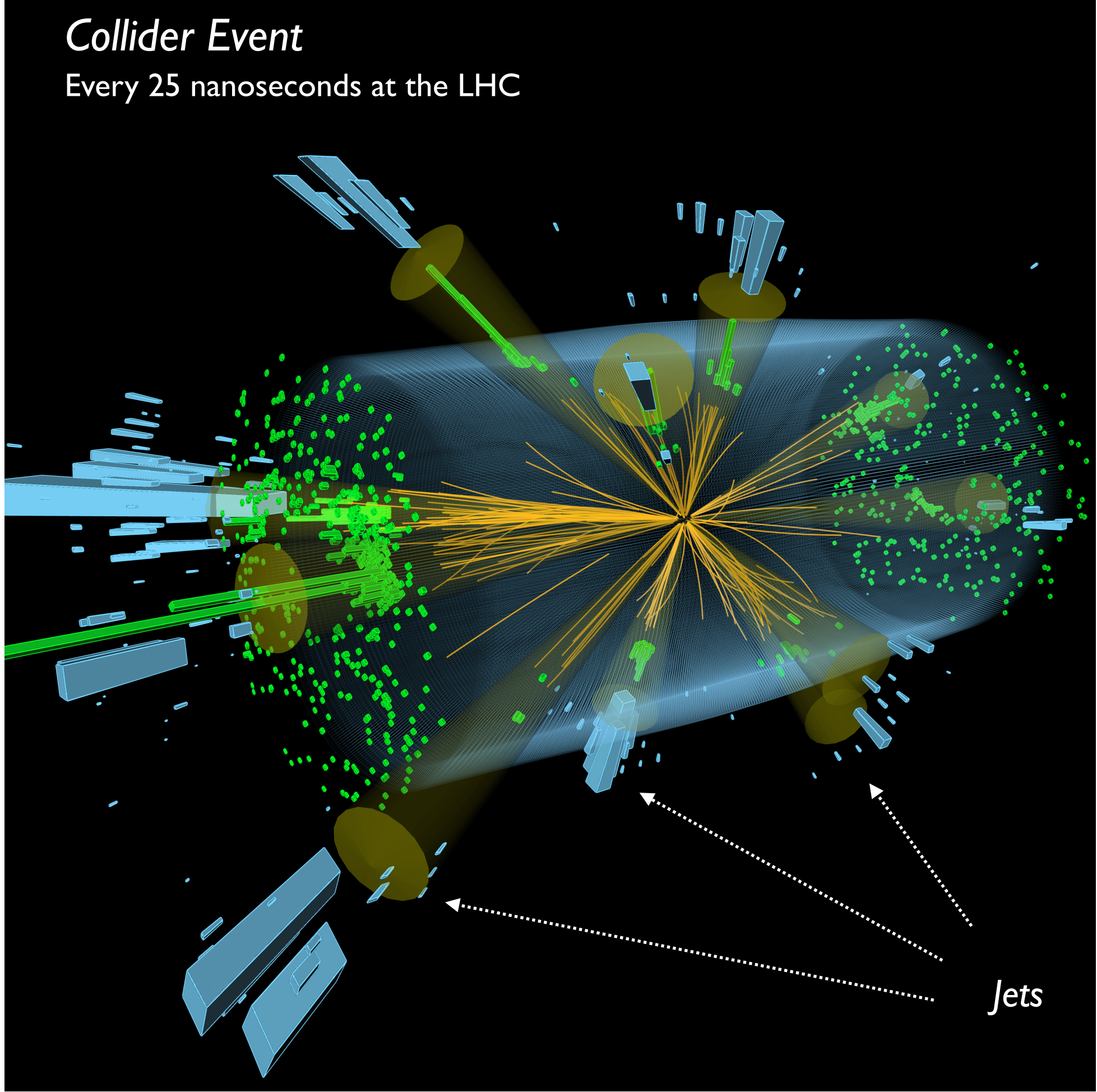
$$\left( E_j, \hat{n}_{x,j}, \hat{n}_{y,j}, \hat{n}_{z,j} \right)_{j=1}^N$$

$$\cap \mathbb{R}_+ \times S^2$$

\* or particle transverse momenta

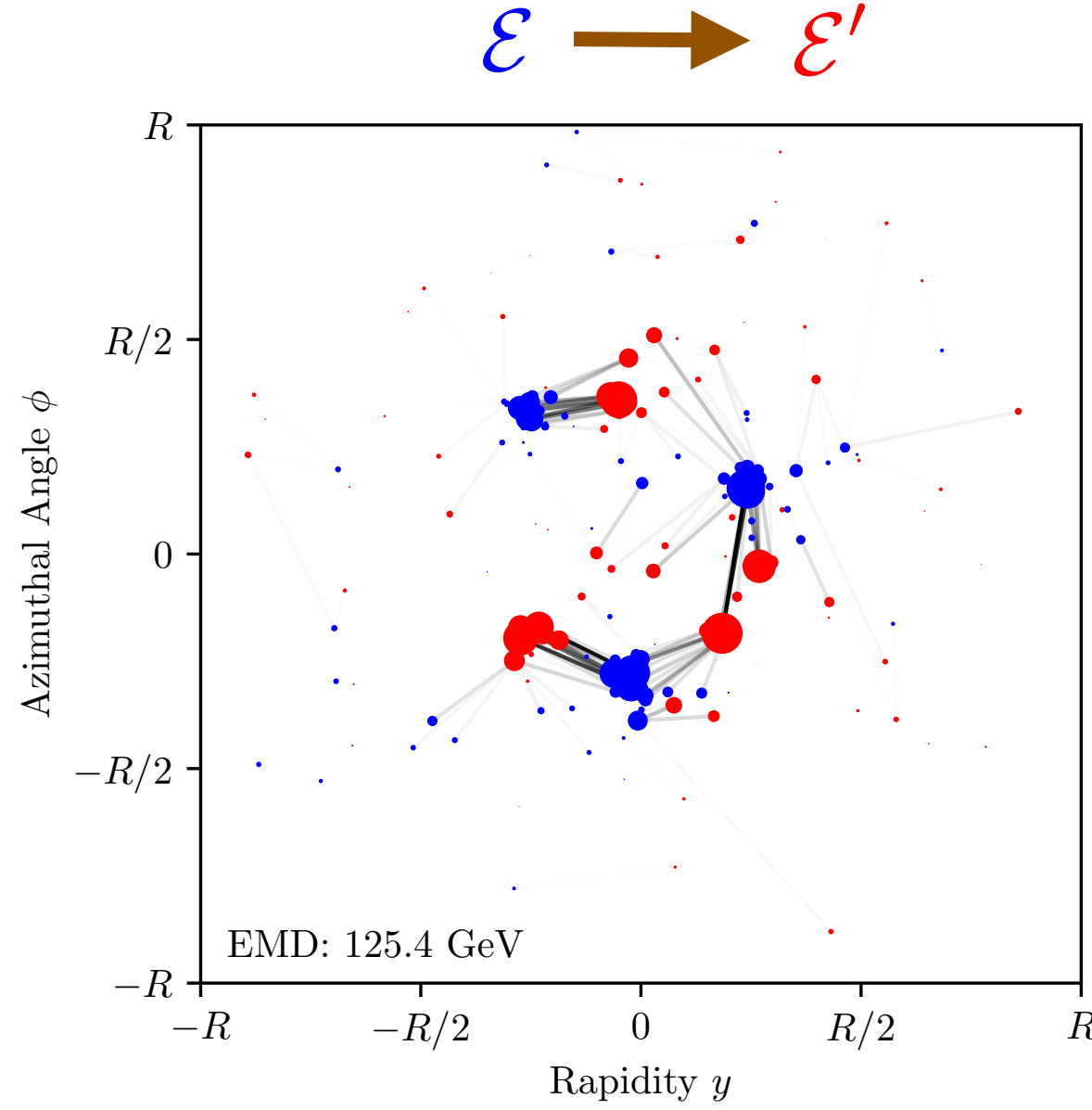
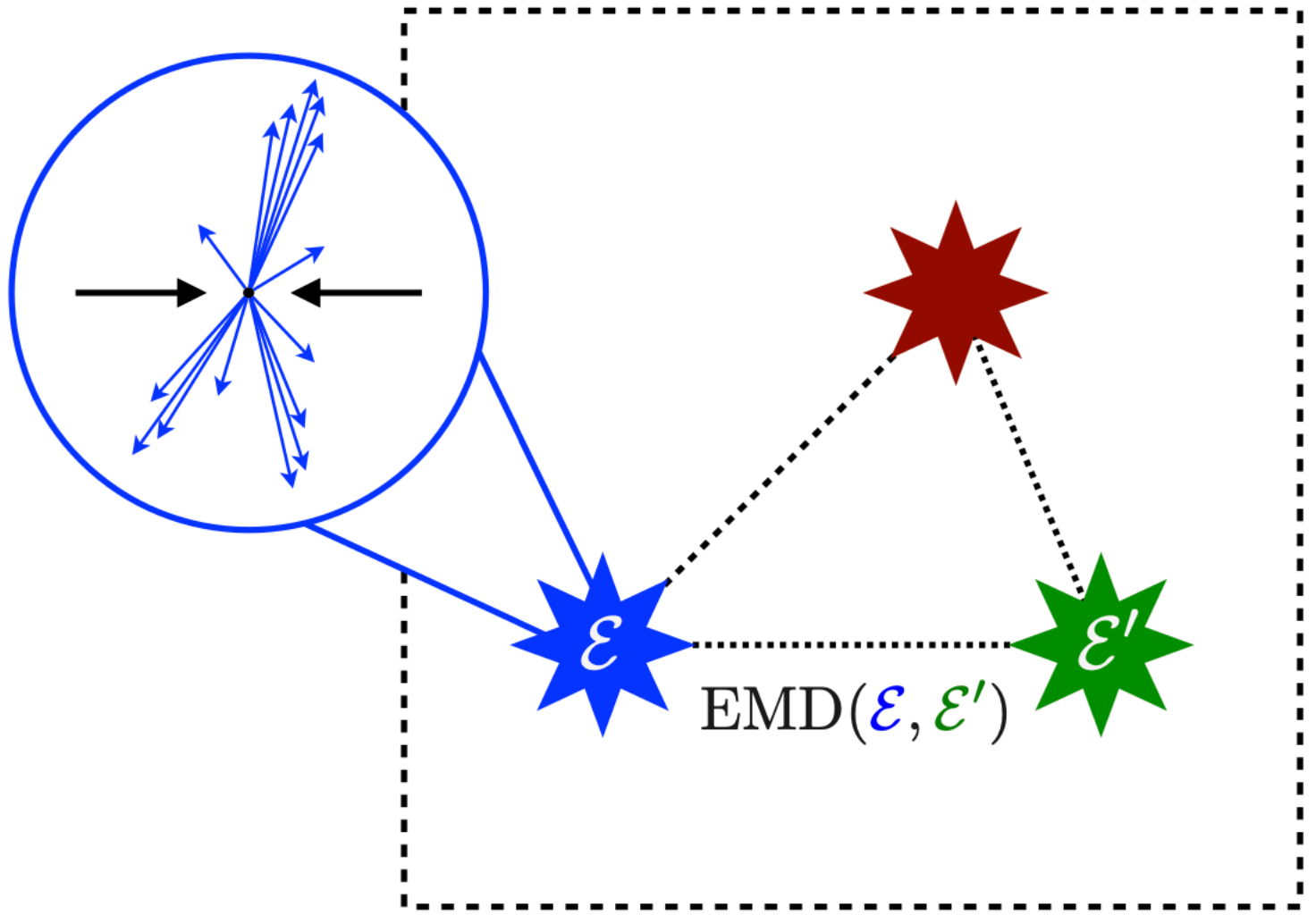


# Collider data has geometric structure



$$\text{EMD}(\mathcal{E}, \mathcal{E}') := \min_{\{f_{i,j} \geq 0\}} \sum_{i=1}^N \sum_{j=1}^{N'} f_{i,j} \frac{\text{dist}(\hat{n}_i, \hat{n}_j)}{R} + \left| \sum_{i=1}^N E_i - \sum_{j=1}^{N'} E_j \right|$$

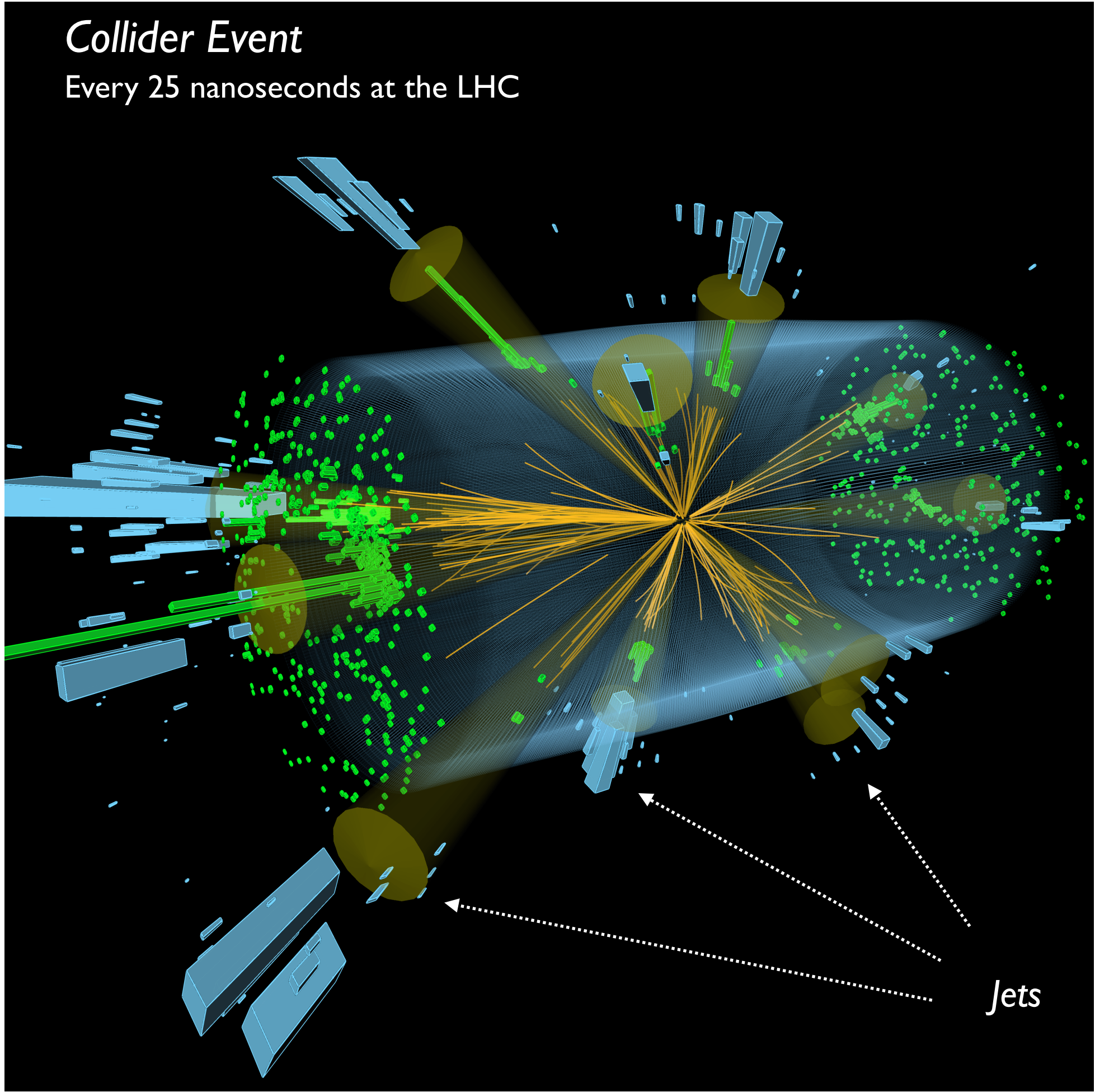
Metric\* space of possible events



Figures from talk by Jesse Thaler, University of Chicago and Caltech AI+Science: <https://www.youtube.com/watch?v=BMBSAWUxBn4>



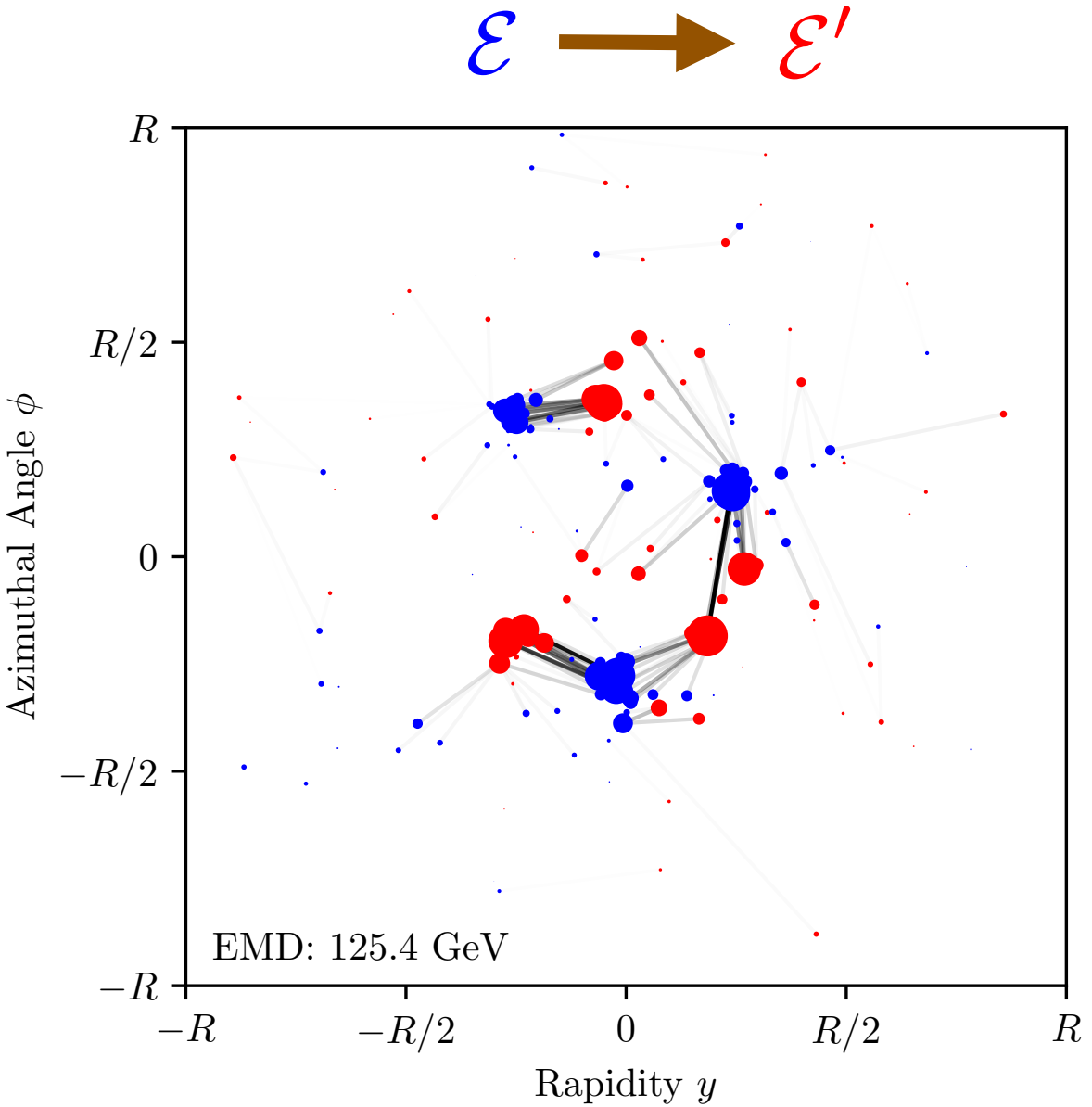
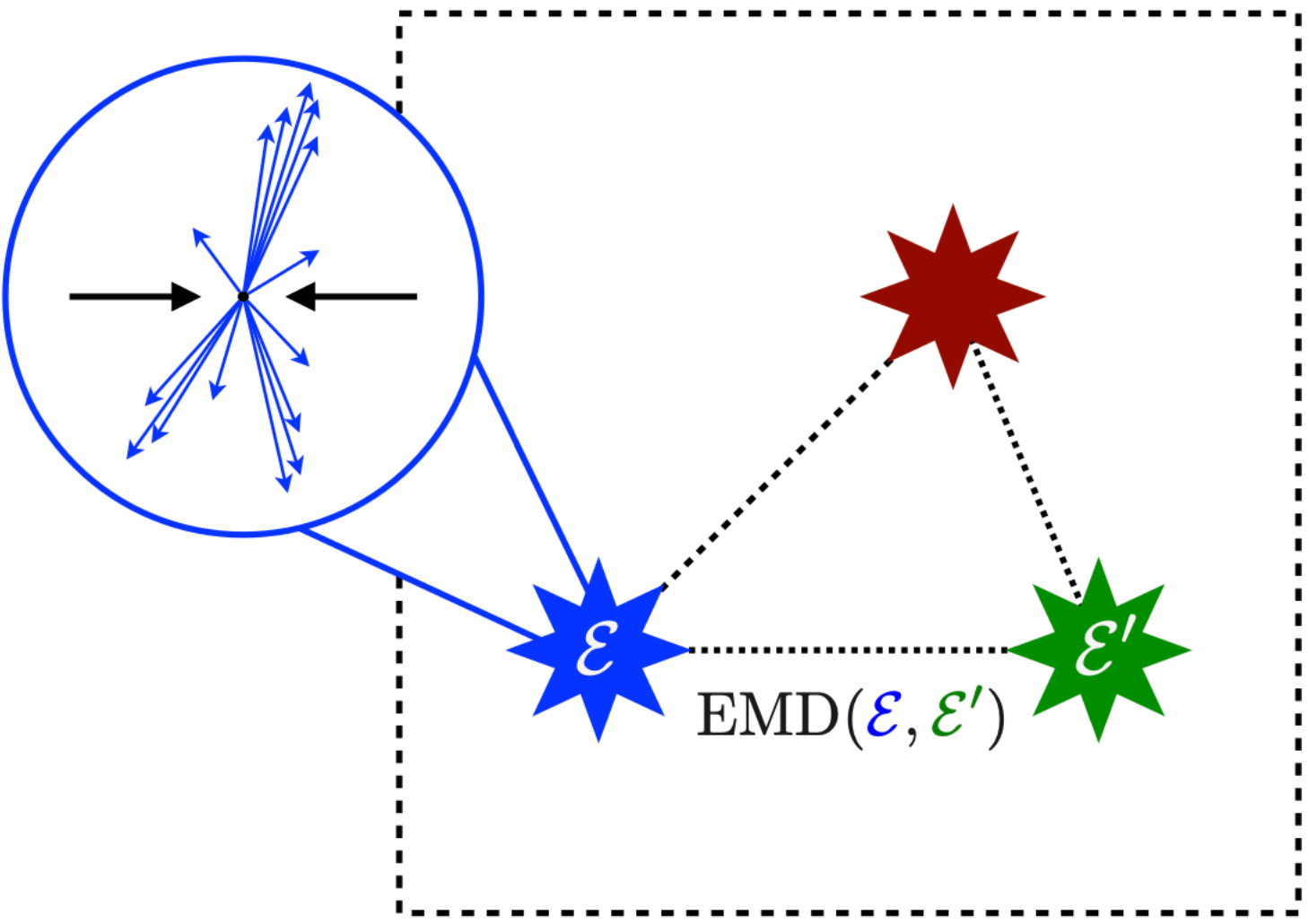
# Collider data has geometric structure



energy (GeV)

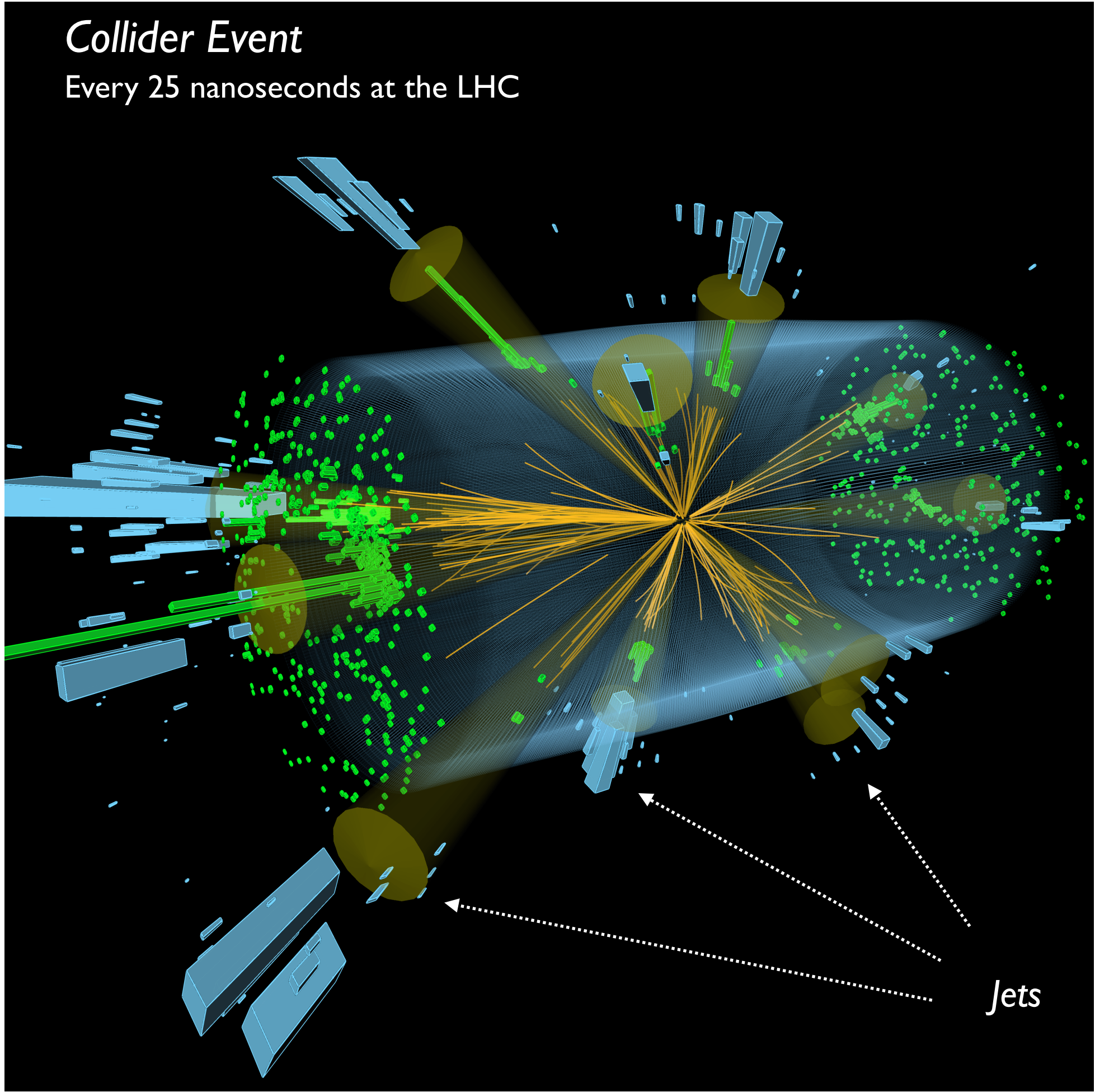
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Metric\* space of possible events





# Collider data has geometric structure

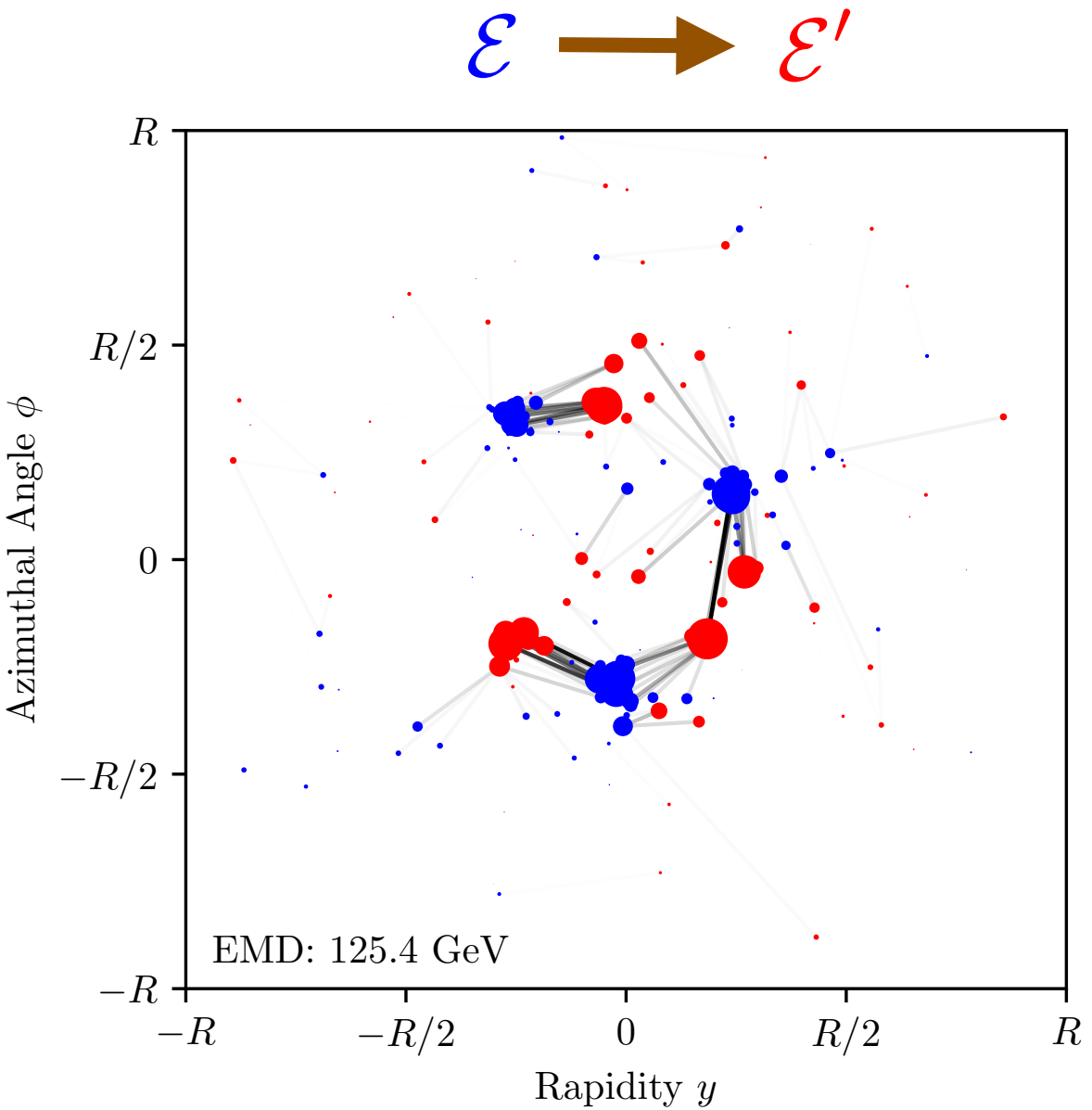
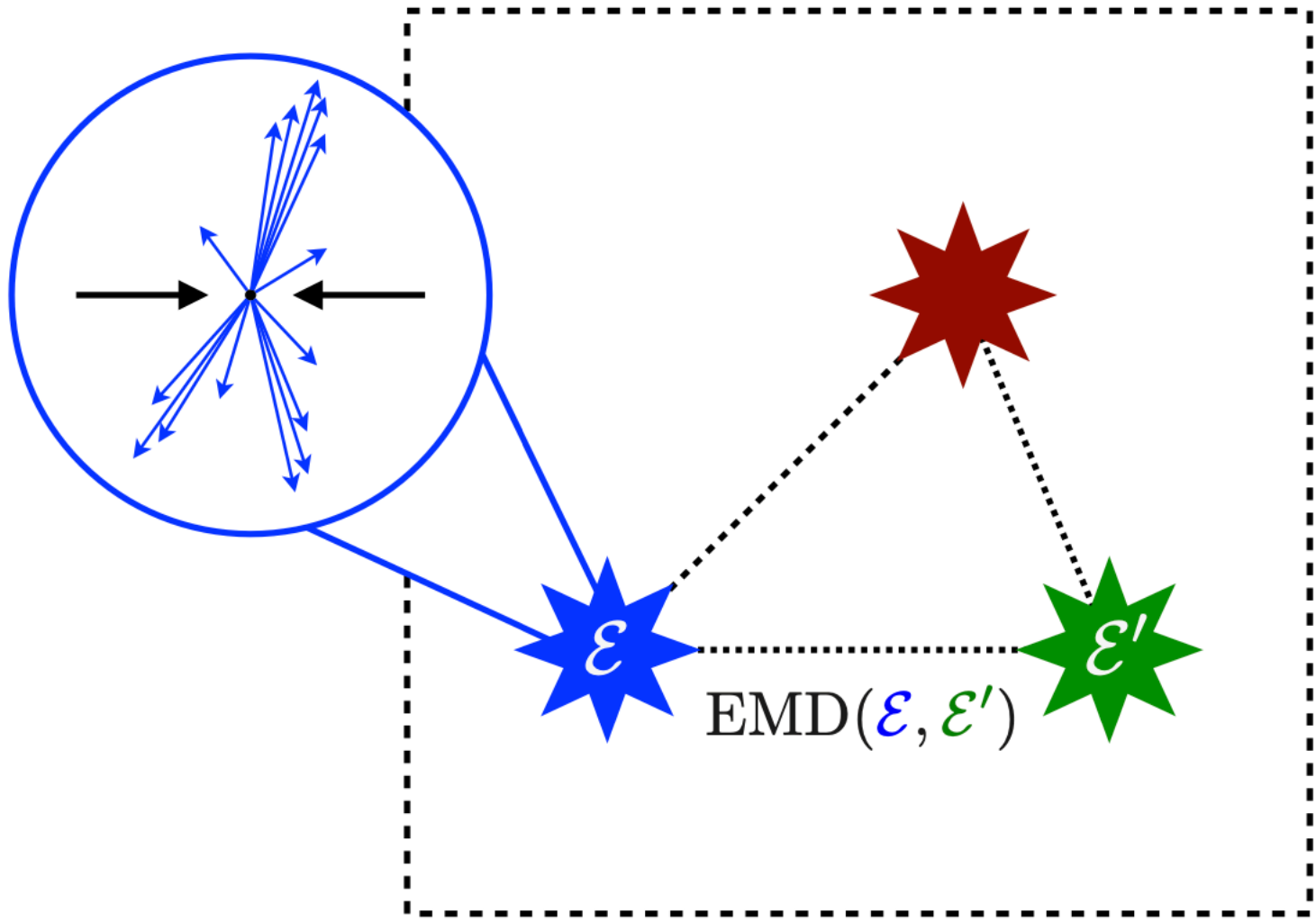


energy (GeV)

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↓
cost to move energy

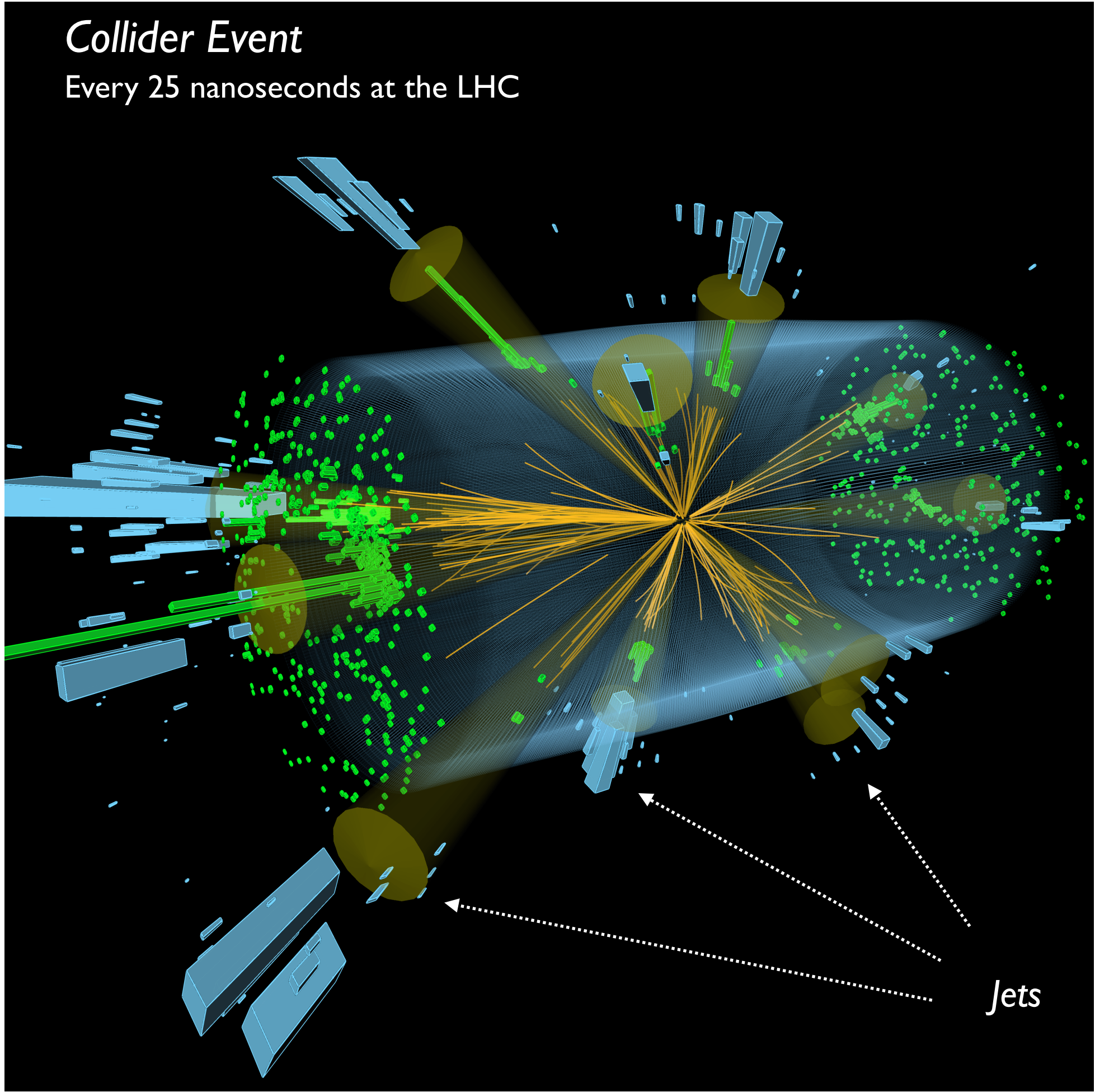
Metric\* space of possible events



\* for R sufficiently large  
i.e.,  $R \geq \text{jet radius}$  for conical jets



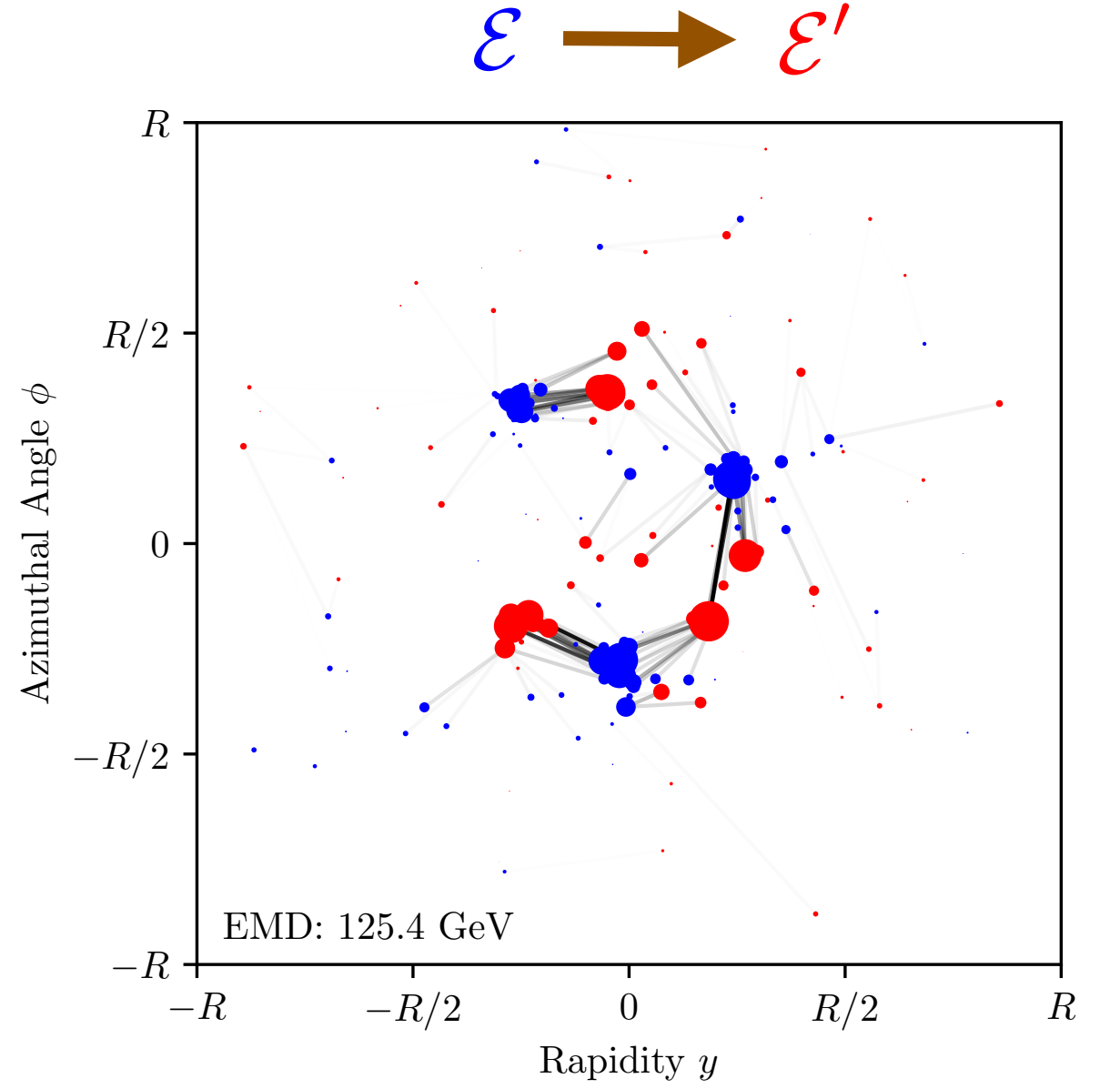
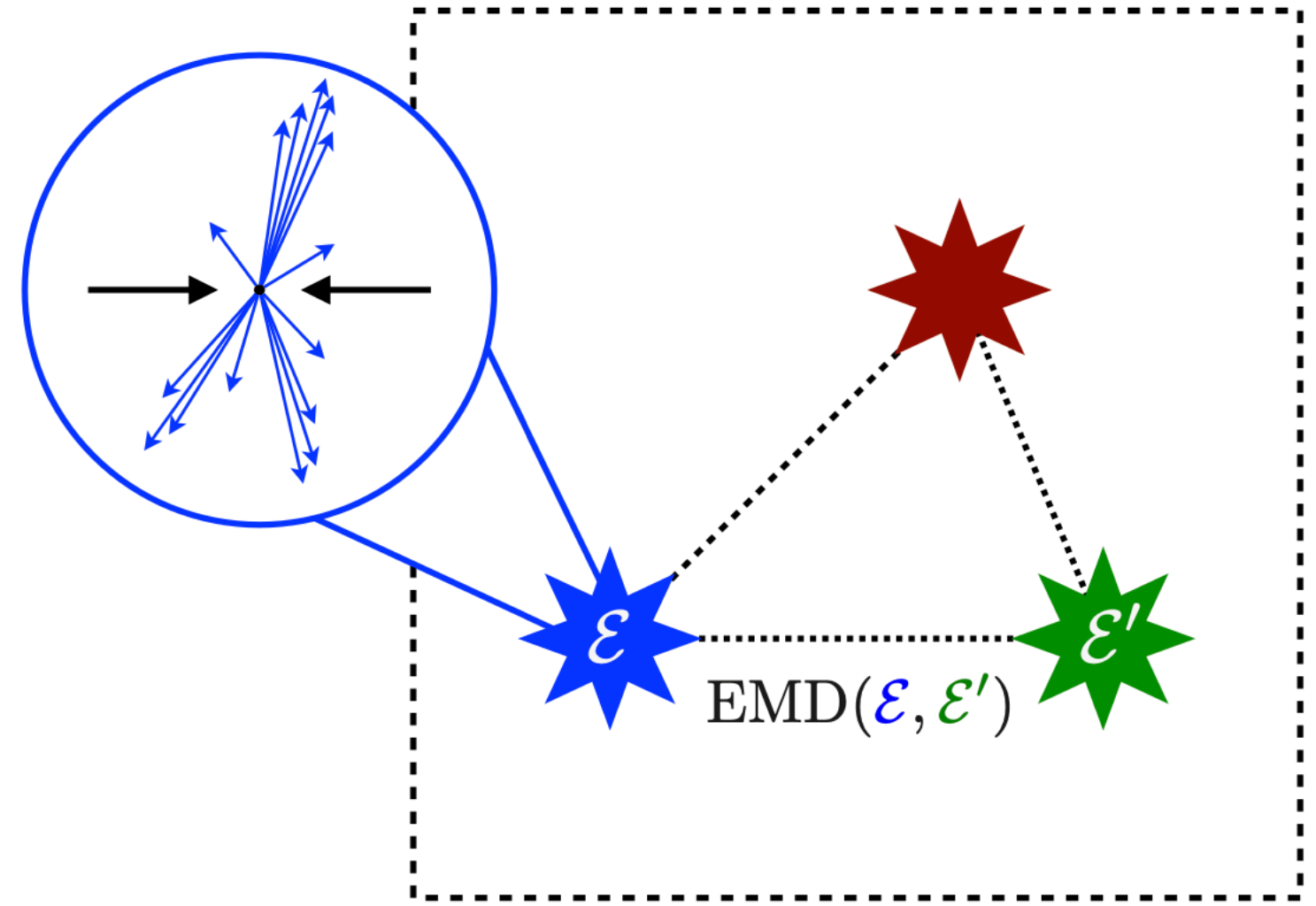
# Collider data has geometric structure



energy (GeV)

$$\text{EMD}(\mathcal{E}, \mathcal{E}') := \min_{\{f_{i,j} \geq 0\}} \underbrace{\sum_{i=1}^N \sum_{j=1}^{N'} f_{i,j} \frac{\text{dist}(\hat{n}_i, \hat{n}_j)}{R}}_{\text{cost to move energy}} + \underbrace{\left| \sum_{i=1}^N E_i - \sum_{j=1}^{N'} E_j \right|}_{\text{cost to create energy}}$$

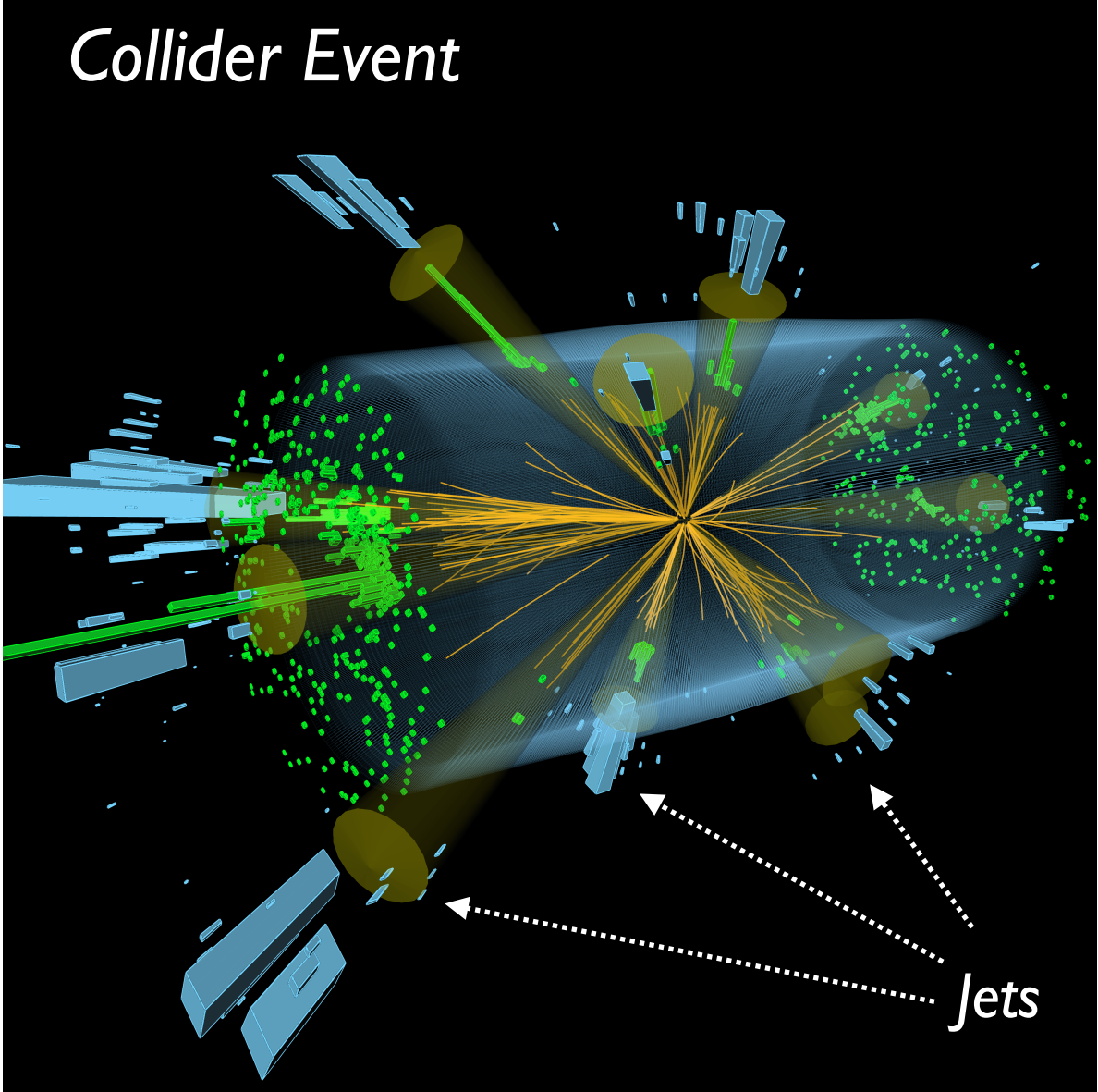
Metric\* space of possible events



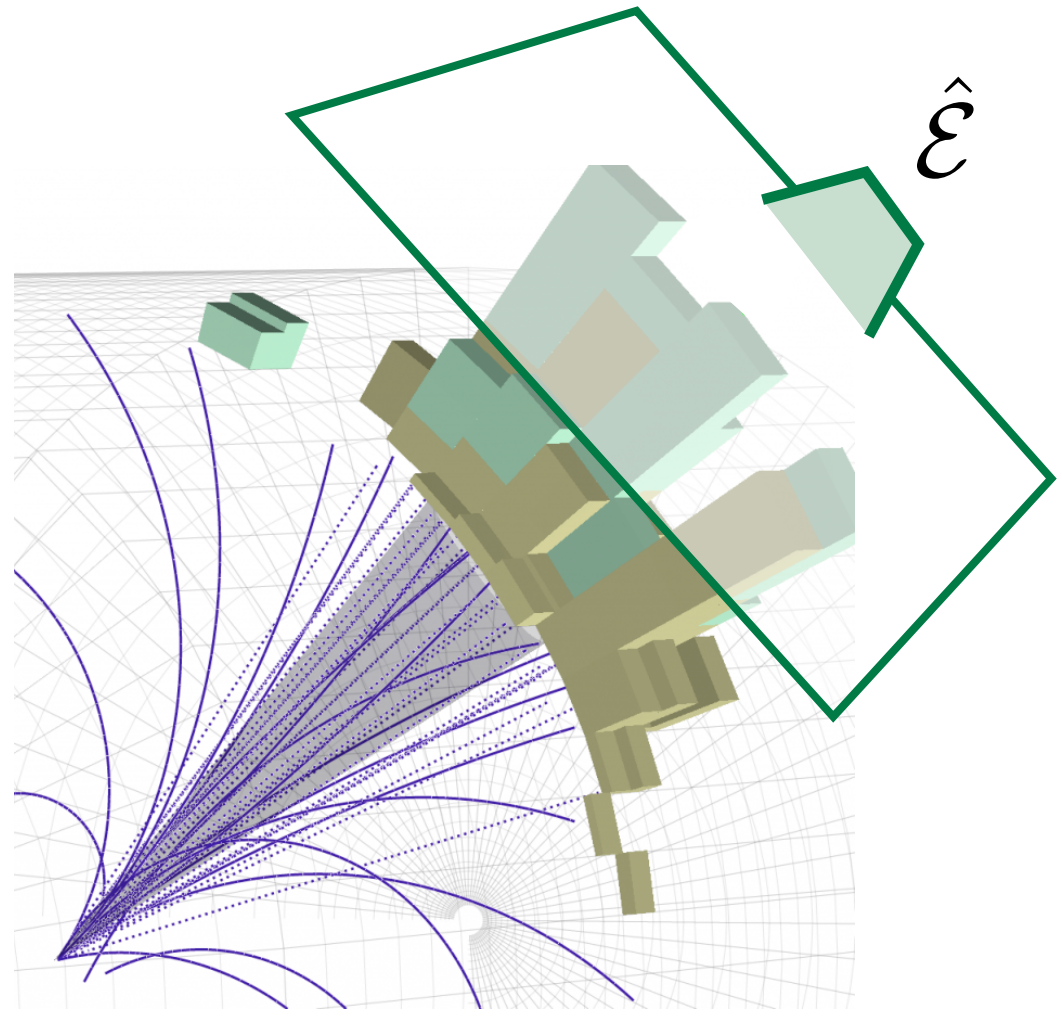
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# Collider data has geometric structure

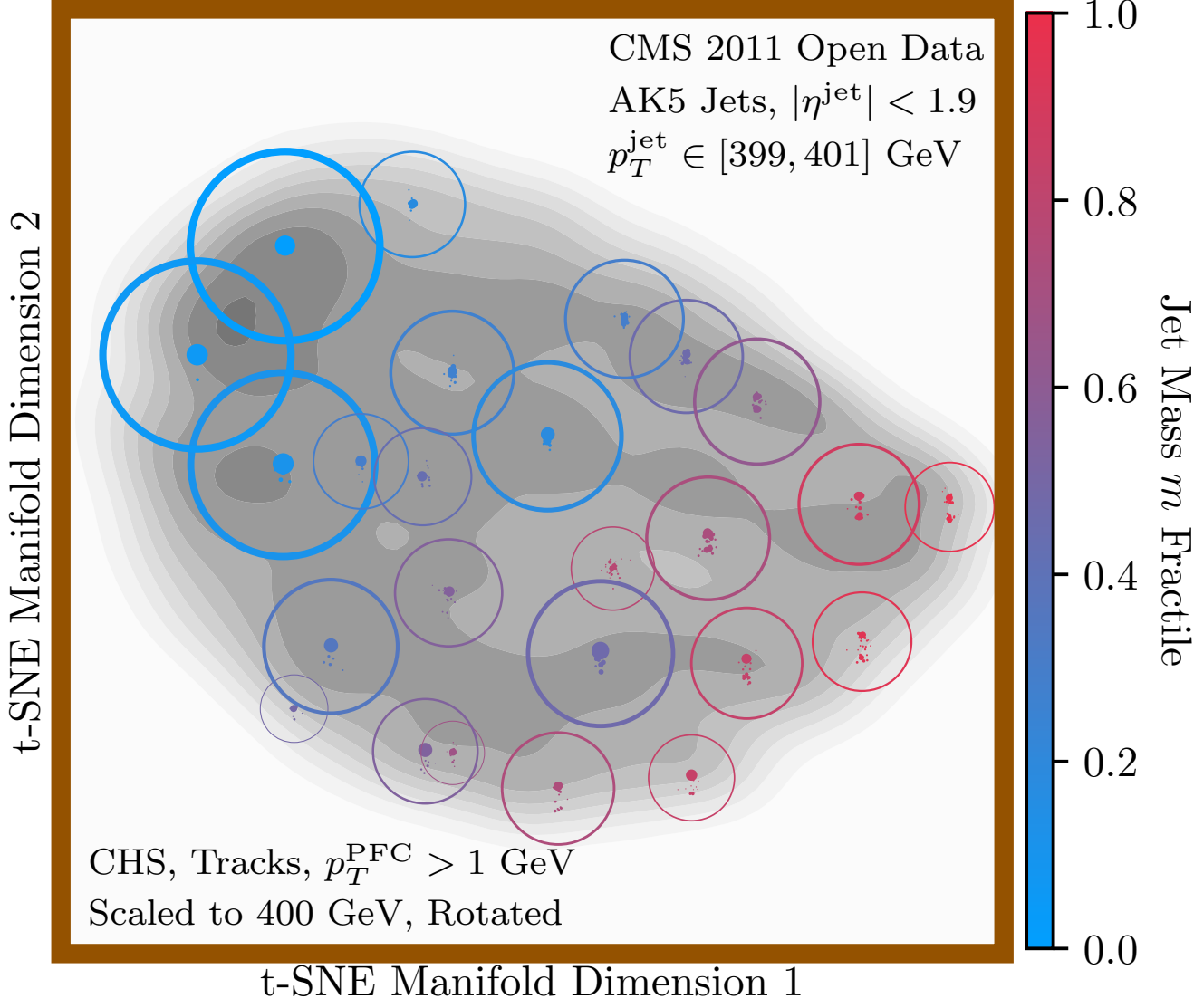


Events summarized by "energy flow"

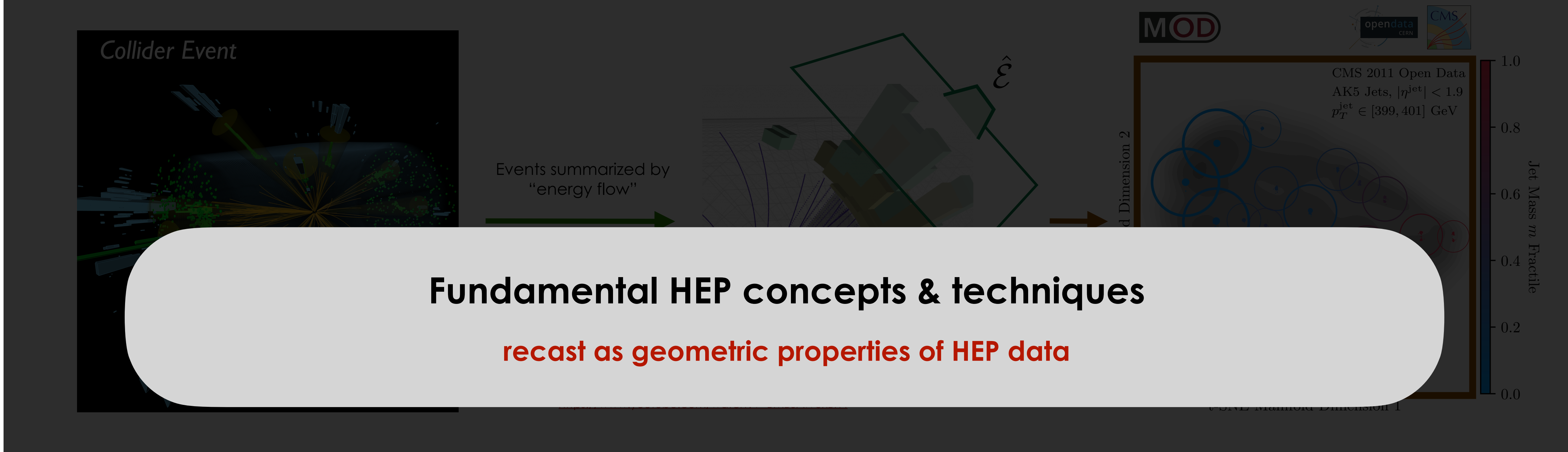


Figures from talk by Jesse Thaler, University of Chicago and Caltech AI+Science: <https://www.youtube.com/watch?v=BMBSAWUxBn4>

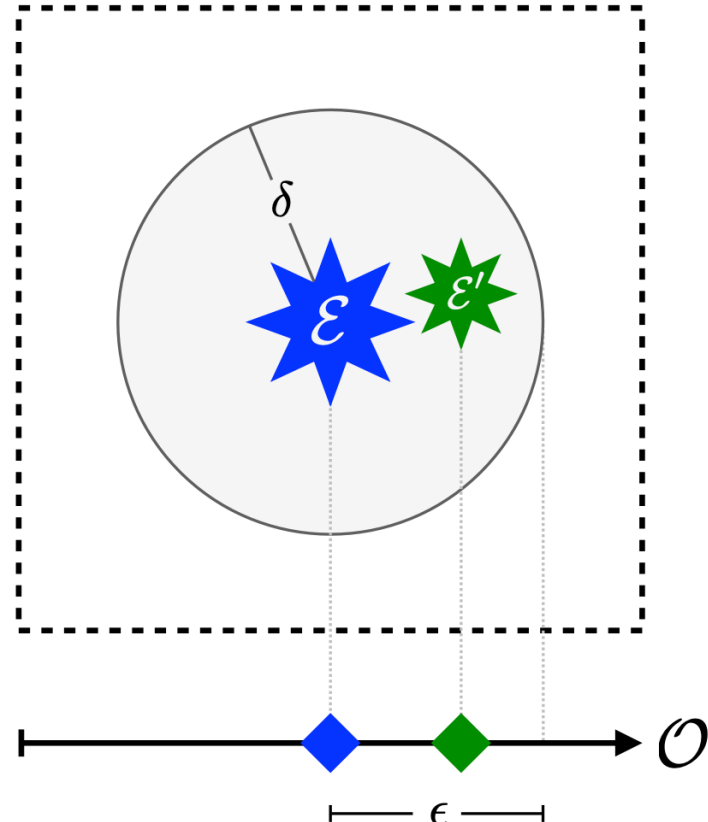
MOD



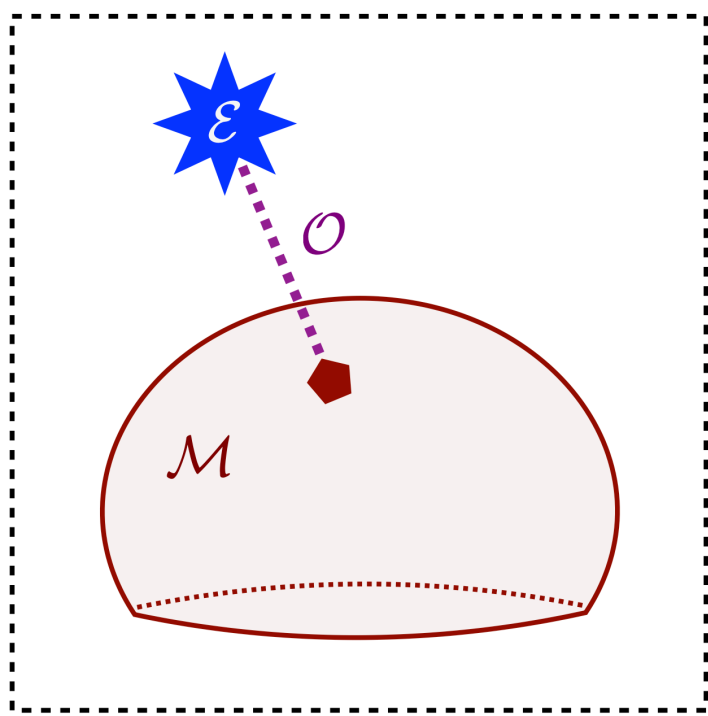
# Collider data has geometric structure



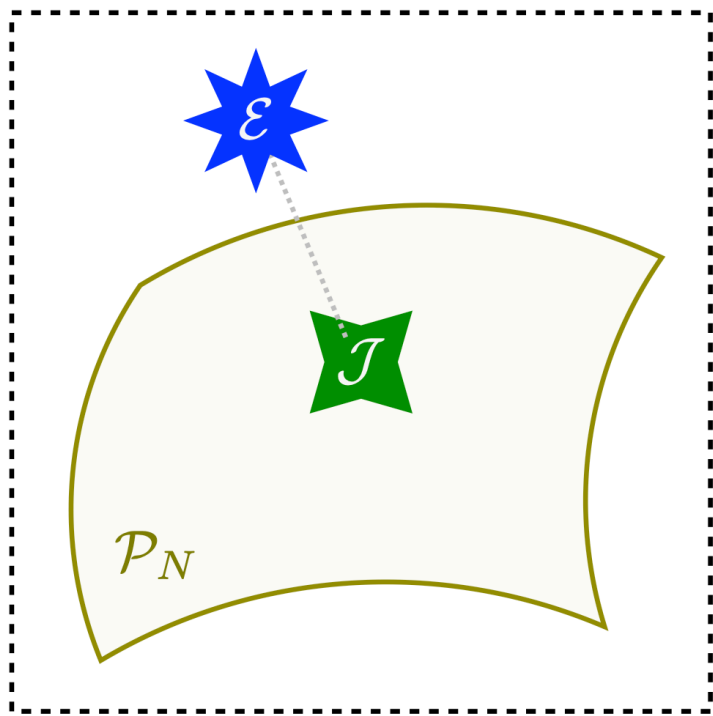
Infrared & Collinear Safety



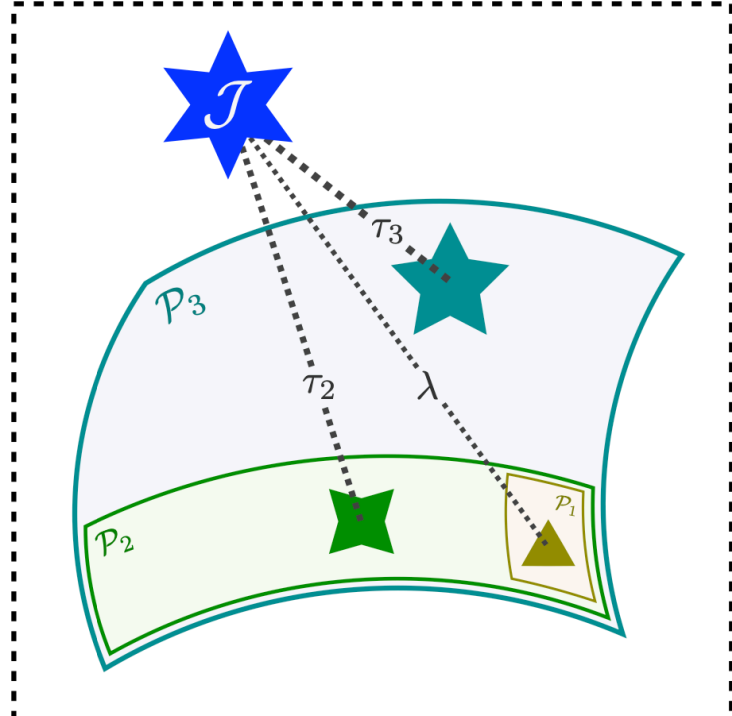
Observables



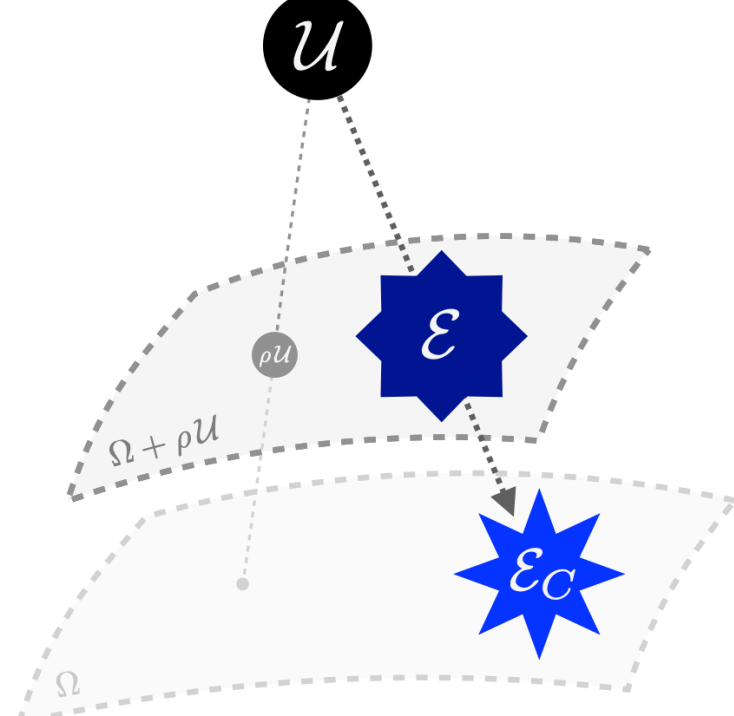
Jets



Jet substructure observables



Pileup subtraction



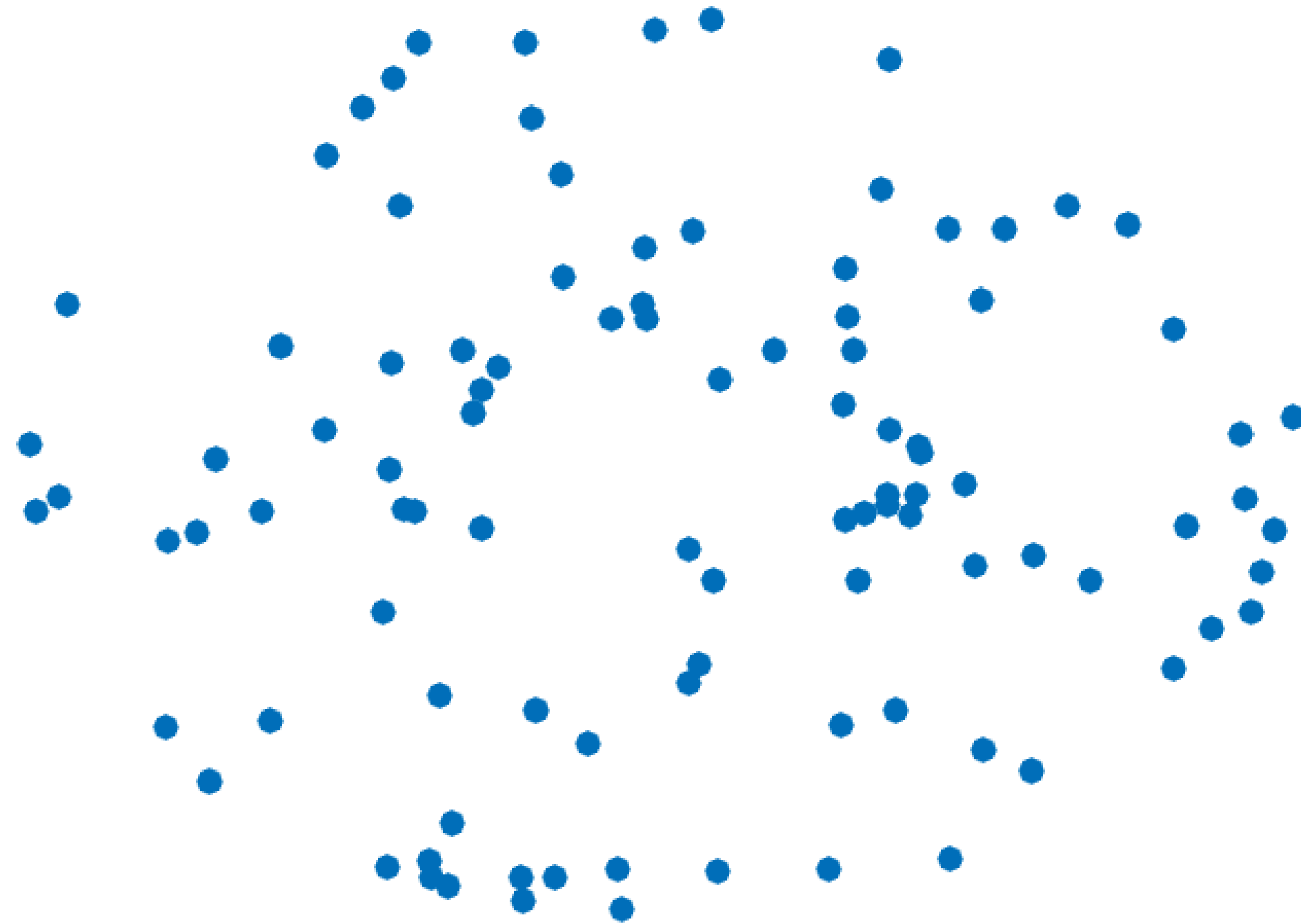
Komiske, Metodiev, Thaler, The hidden geometry of particle collisions, J. HEP, 6 (2020)



Recovering geometry of data:  
problem of **connecting data in the *right* way**

What do you see?

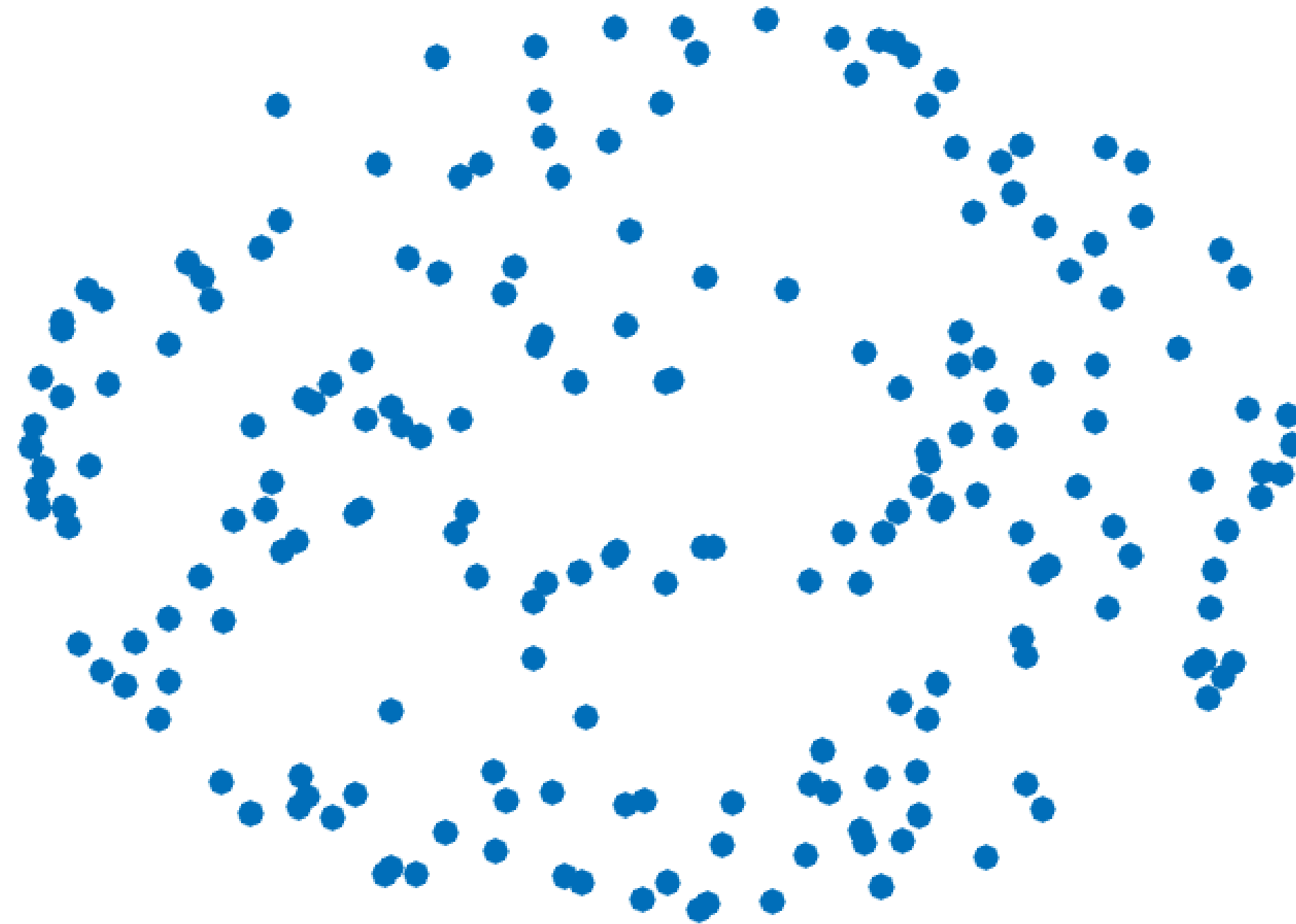
$N = 100$





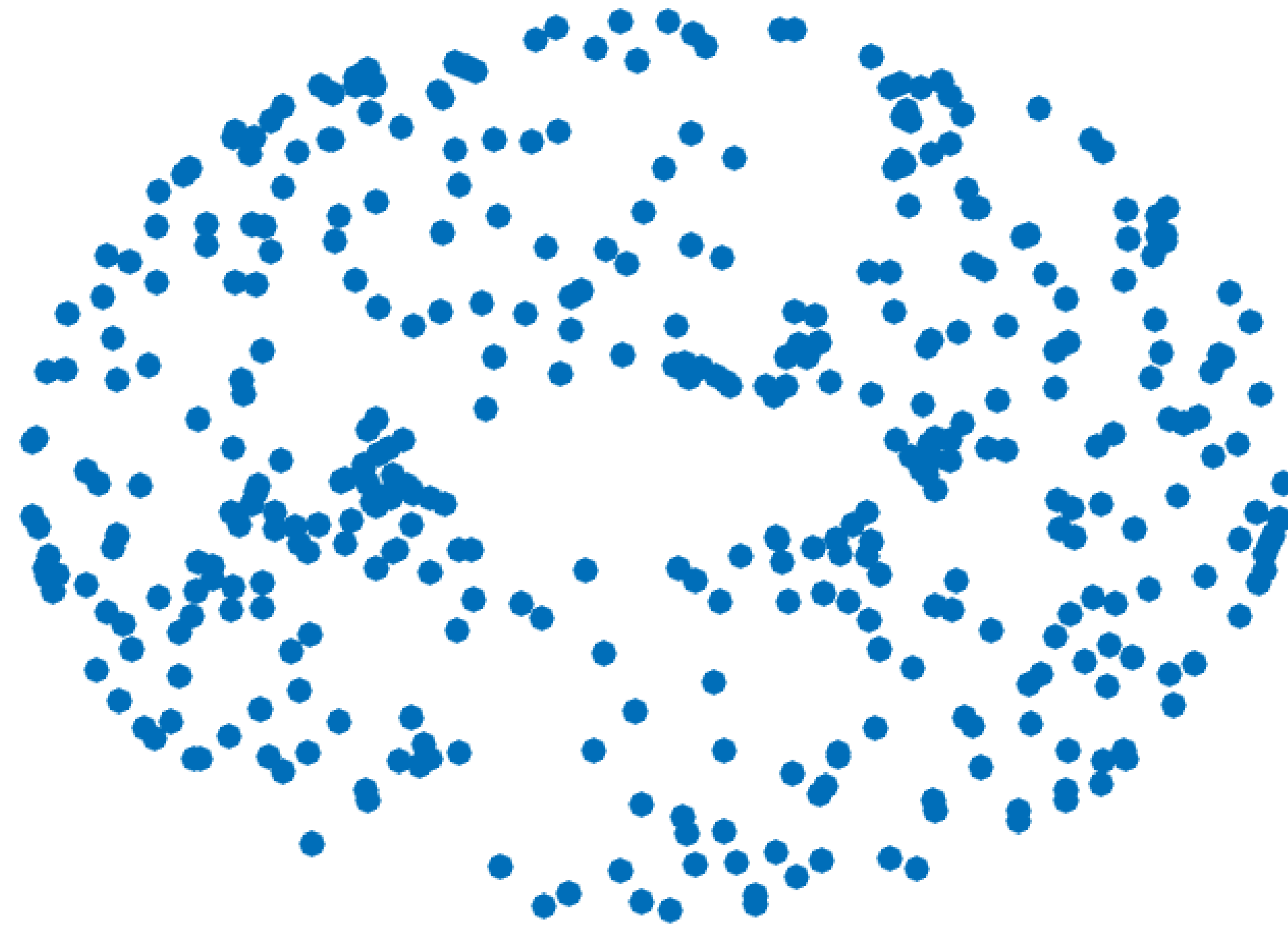
What do you see?

$N = 200$



What do you see?

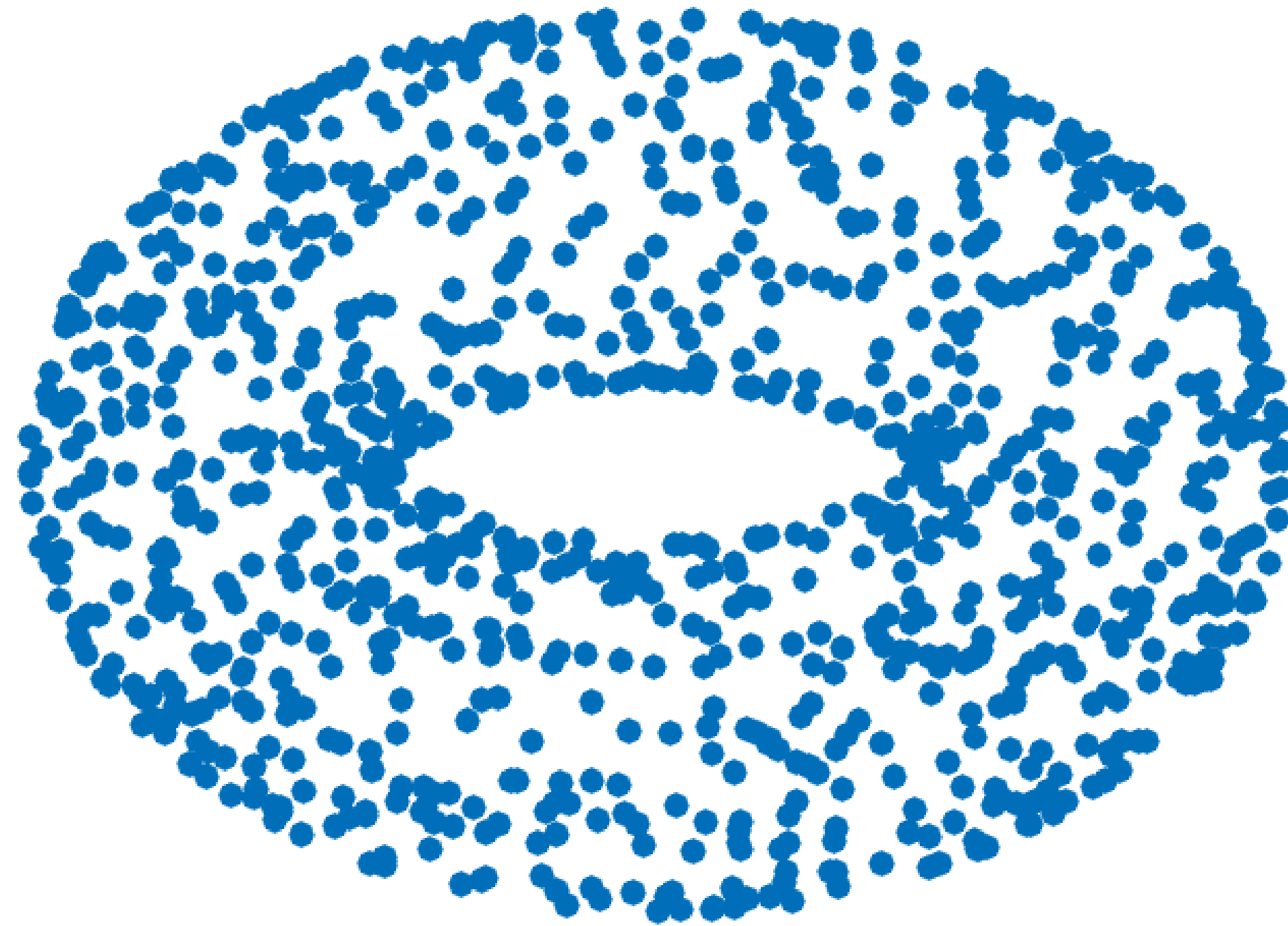
$N = 400$





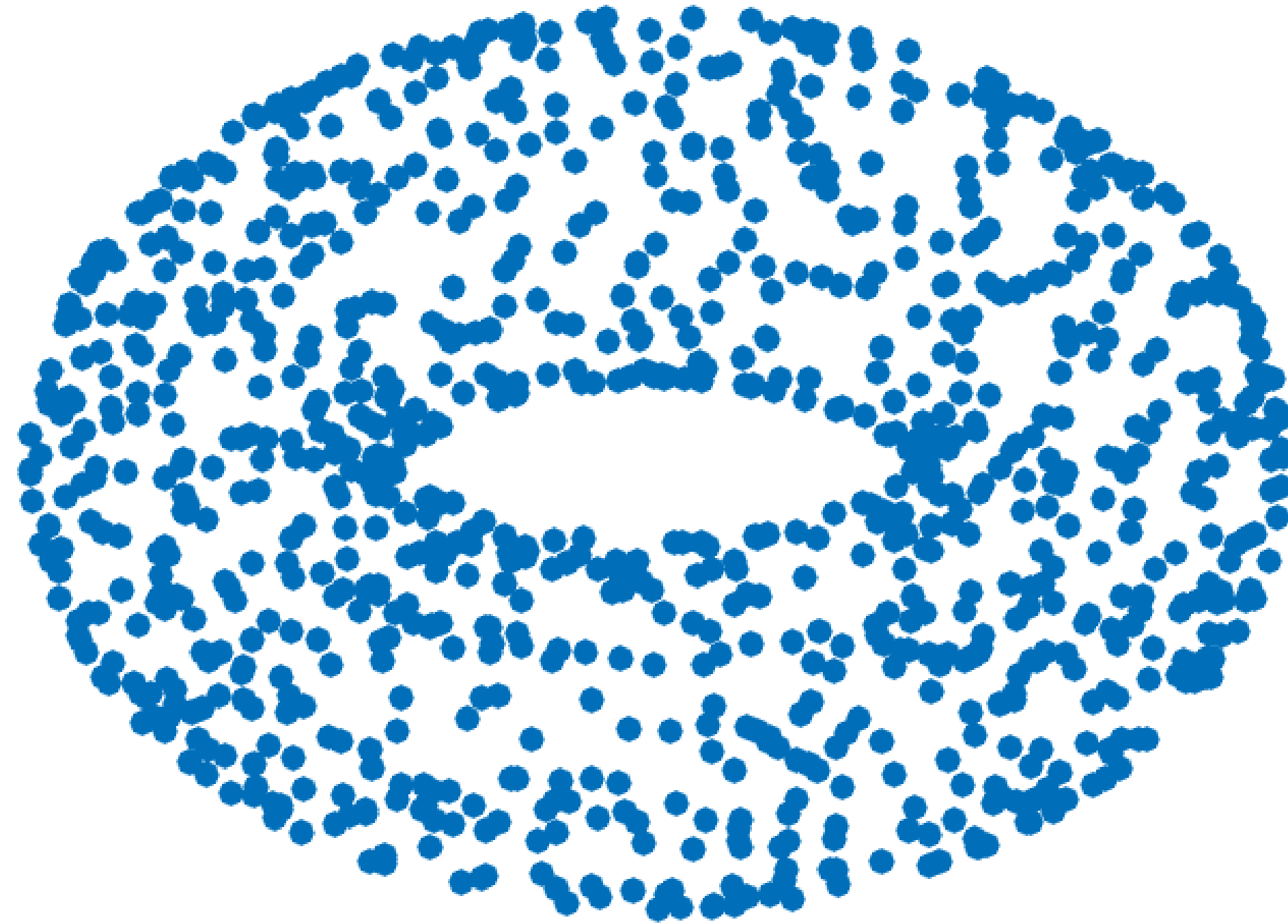
What do you see?

$N = 1000$



What do you see?

$N = 1000$

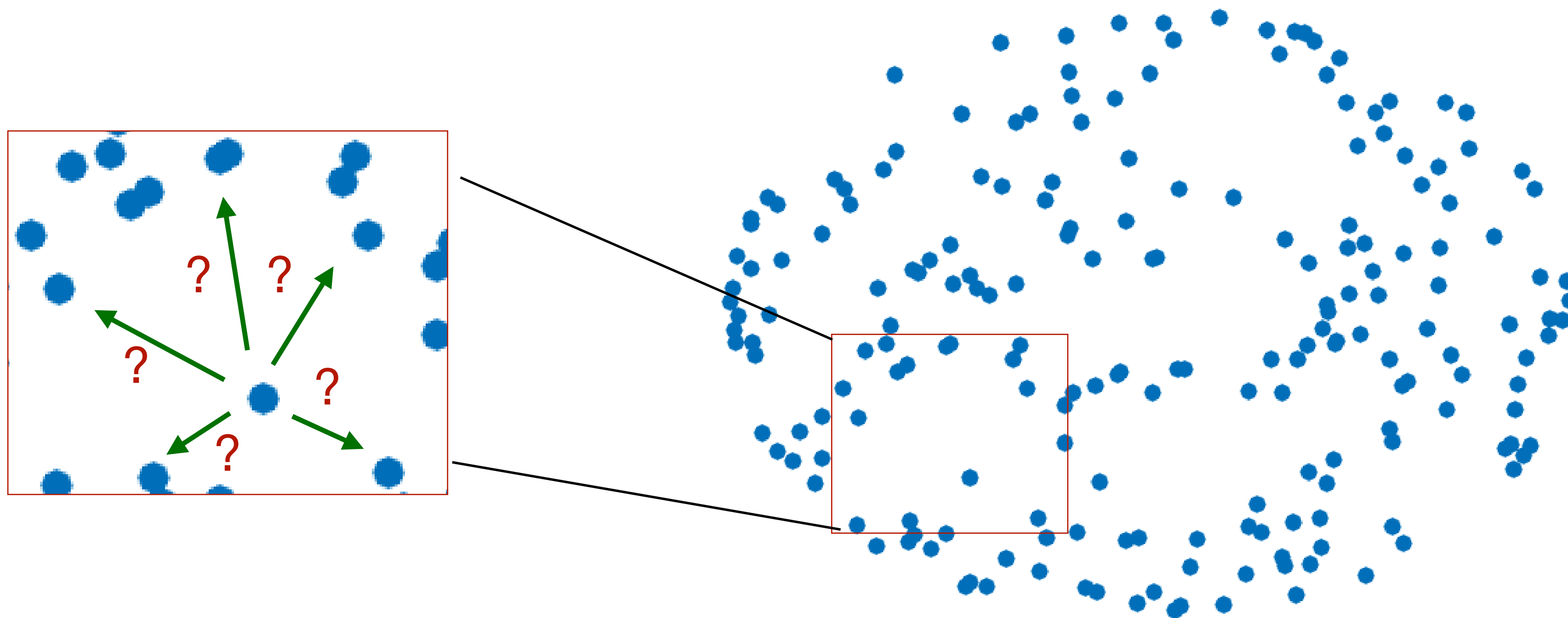


$N$  data points in  $\mathbb{R}^3$  sampled from a distribution constrained to a *submanifold*  $T^2 \subset \mathbb{R}^3$

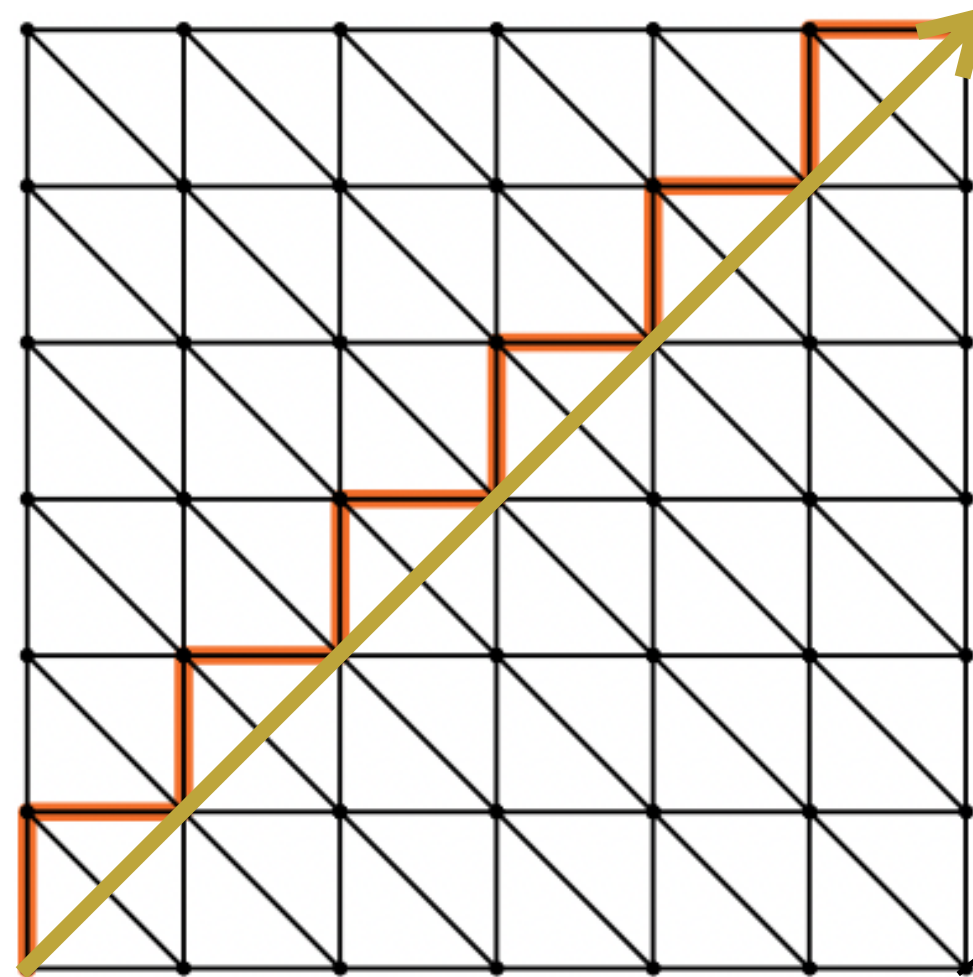


# How is data **interconnected**?

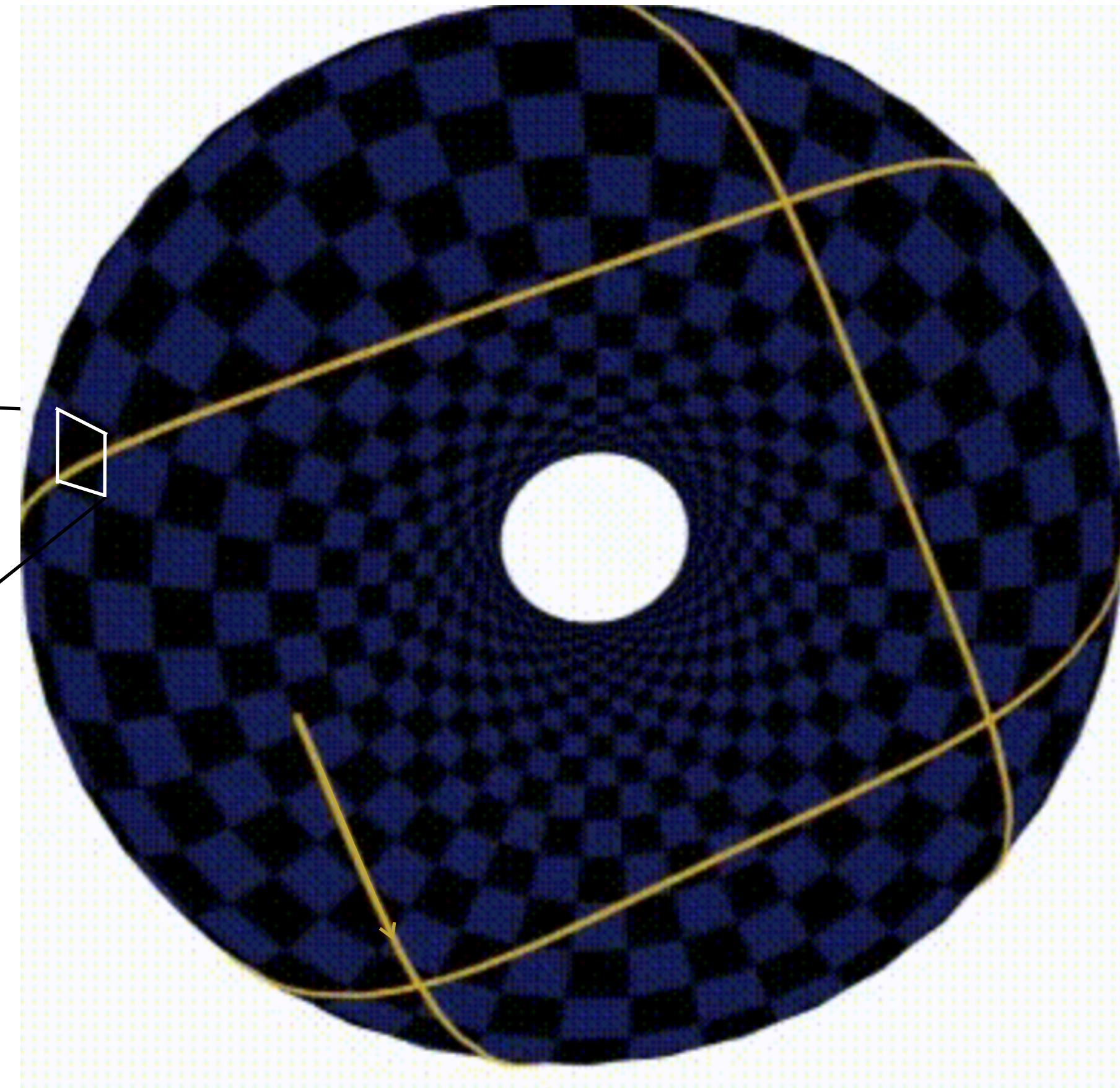
$N = 200$



# How is data **interconnected**?



Crane et al., *Comm. ACM* (2017)



Wikipedia: Geodesics

*intrinsic* local and **non-local** relationships between data points

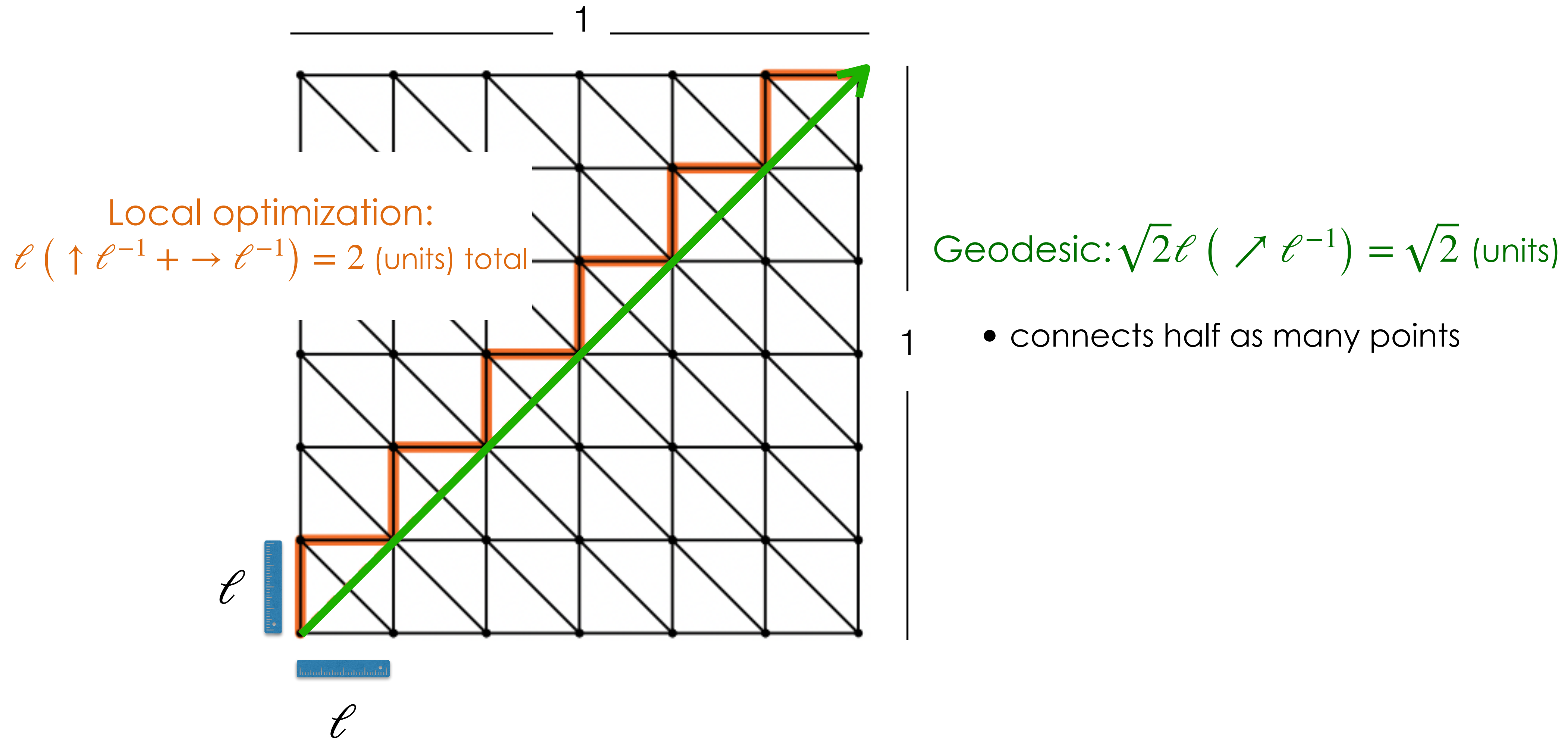








# How is data **interconnected**?



*intrinsic* local and **non-local** relationships between data points

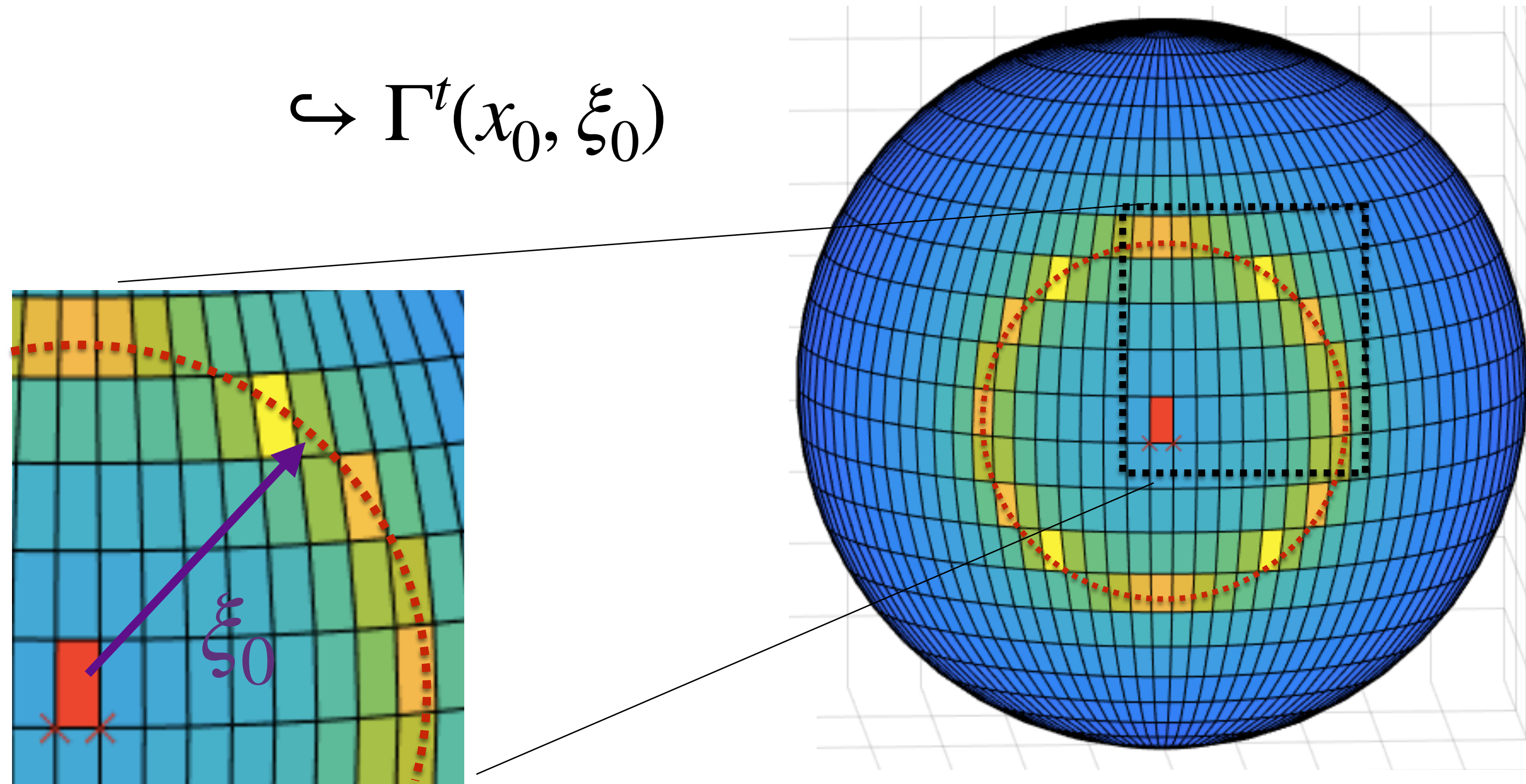




# How is data **interconnected**?

**Geodesic flow:** 
$$\begin{cases} \partial_t x_j &= \partial_{\xi_j} H = (g^{-1}(x) \cdot \xi)_j \\ \text{nonlinear in } x, \xi & \partial_t \xi_j &= -\partial_{x_j} H = \langle \partial_{x_j} g^{-1}(x) \cdot \xi, \xi \rangle \end{cases}$$

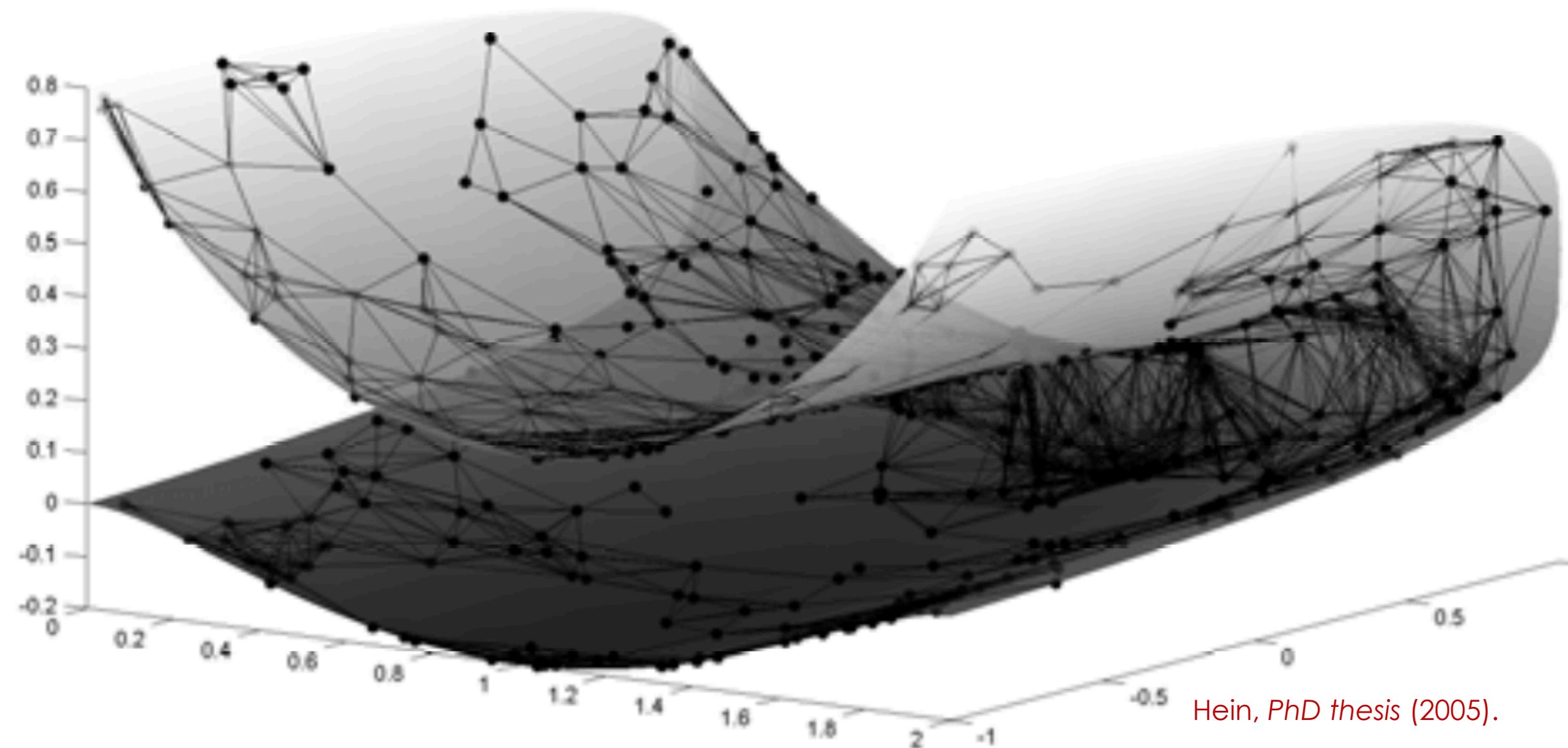
$\hookrightarrow \Gamma^t(x_0, \xi_0)$



The flow moves the point  $x_0$  to the geodesic neighbour  $x(t)$  at distance  $t$  in the direction  $\xi_0$

# The problem

**Given** *data*  $X_N := \{v_1, \dots, v_N\} \subset \mathcal{M} \subset \mathbb{R}^D$  sampled from a probability distribution confined to a Riemannian submanifold  $\mathcal{M}$ , **recover** the *intrinsic geometry* of  $\mathcal{M}$



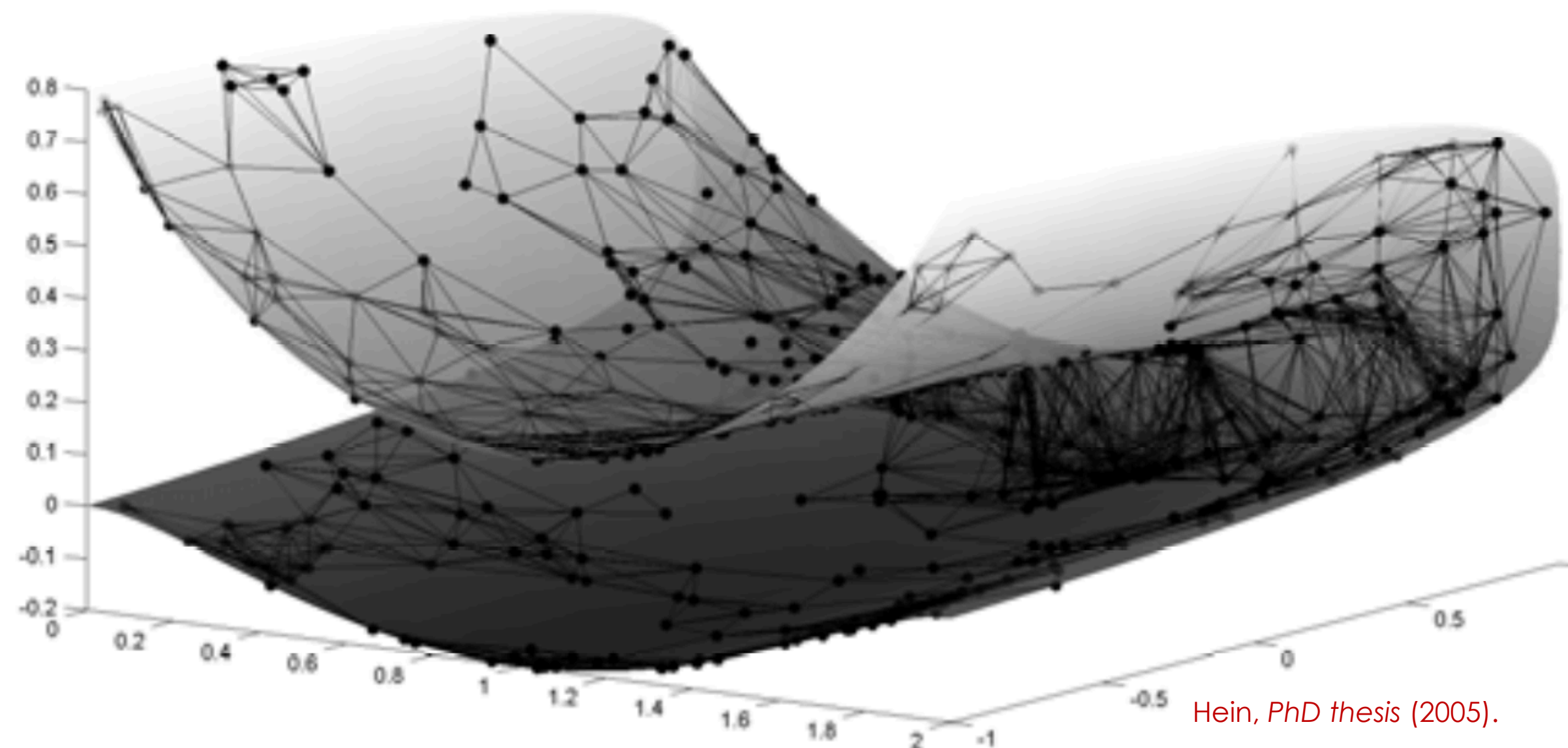


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- intrinsic dimension, Riemannian metric, low-dimensional isometric embedding, heat diffusion,  $\Delta_{\mathcal{M}}$

} *Belkin-Niyogi (2003), Hein (2005),  
Hein-Audibert-von Luxburg (2007),  
Trillos-Gerlach-Hein-Slepčev (2020)*

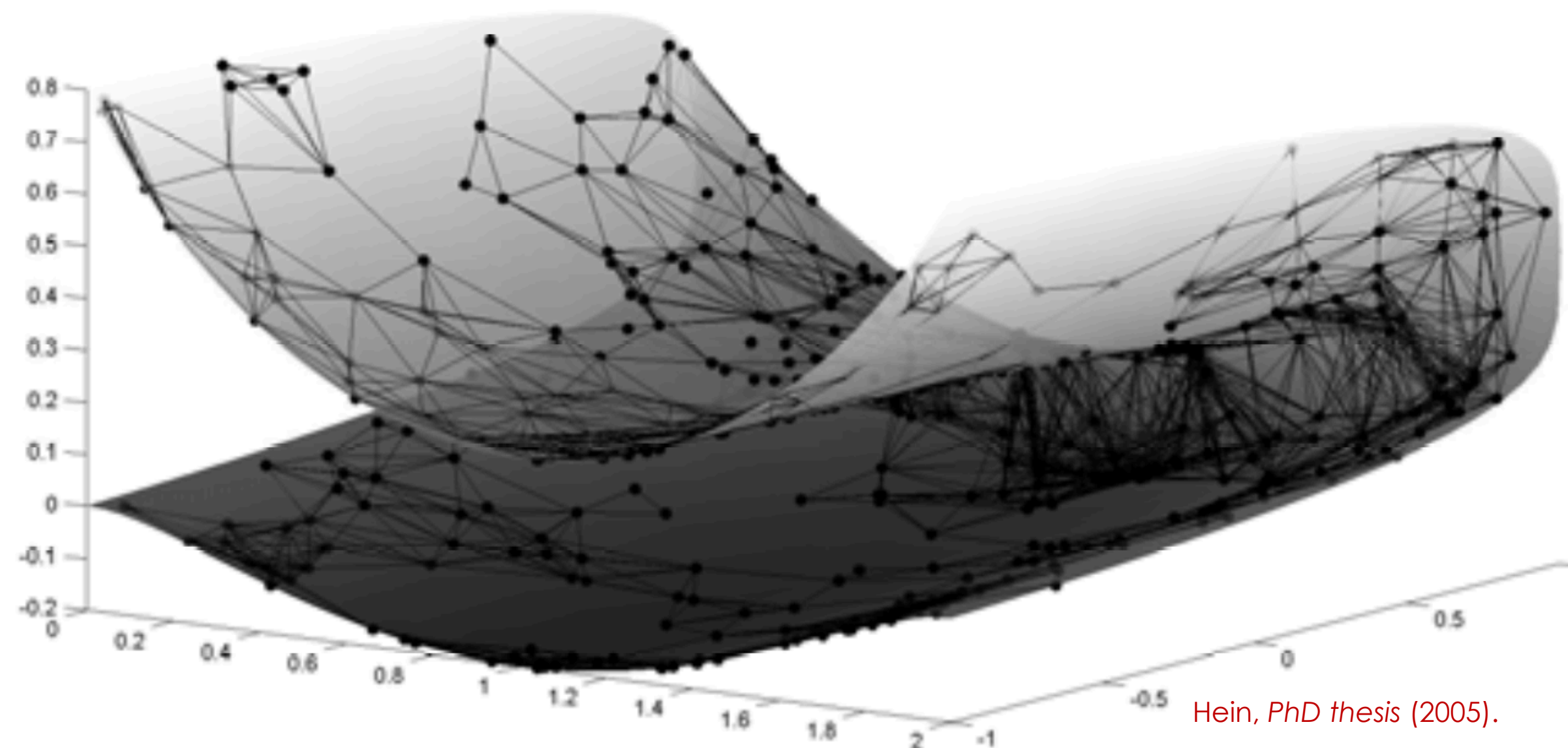


Hein, PhD thesis (2005).

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- **This talk:** Geometry-encoding quantum dynamics, geodesics ♦ **Much harder!**



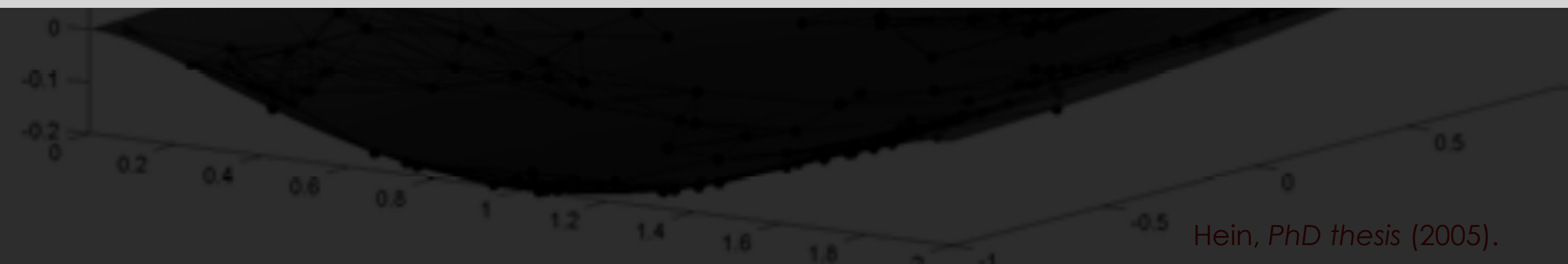


# The problem

Given *data*  $X_N := \{v_1, \dots, v_N\} \subset \mathcal{M} \subset \mathbb{R}^D$  sampled from a probability distribution confined to a Riemannian manifold  $\mathcal{M}$ .

State of the art is to deploy *local* dynamics on data, *i.e.*, **Markov processes**  
These yield **low-frequency** features of data, but miss **high-frequency**  
components (*i.e.*, geodesics)

*Hein (2005),  
Luxburg (2007),  
Slepčev (2020)*



## The solution

Graph Laplacian  
construction

Discrete quantized  
propagation:  
taking the position  
mean gives  $O(h)$   
approx. to  $\iota(t)$

```
1: Inputs:  $X_N = \{v_1, \dots, v_N\}, v^*, \epsilon > 0, \alpha \geq 1, t > 0$ 
2: Output: Propagated state  $[\psi_h^\zeta](t)$ 
3: procedure PROPAGATE
4:   for  $i, j = 1 : N$  do  $[T_\epsilon]_{i,j} \leftarrow k(\|v_i - v_j\|^2 / \epsilon)$ 
5:    $D_\epsilon \leftarrow$  diagonal matrix  $\left( \sum_{j=1}^N [T_\epsilon]_{i,j} \right)_{1 \leq i \leq N}$ 
6:    $\Delta_{\epsilon,N} \leftarrow \frac{4(I_N - D_\epsilon^{-1} T_\epsilon)}{\epsilon}$ 
7:    $U_{\epsilon,N}^t \leftarrow \exp(-it \sqrt{\Delta_{\epsilon,N}})$ 
8:    $h \leftarrow \epsilon^{\frac{1}{2+\alpha}}$ 
9:    $p_0 \leftarrow v_j - v^*$  for  $v_j$  closest to point  $v^*$ 
10:  while  $1 \leq \ell \leq N$  do
11:     $[\psi_h^\zeta]_\ell \leftarrow e^{-\|v_\ell - v^*\|^2 / 2h} e^{\frac{i}{h} (v_\ell - v^*)^\top p_0 / \|p_0\|}$ 
12:  return  $[\psi_h^\zeta](t) = U_{\epsilon,N}^t [\psi_h^\zeta]$ 
```



# The solution

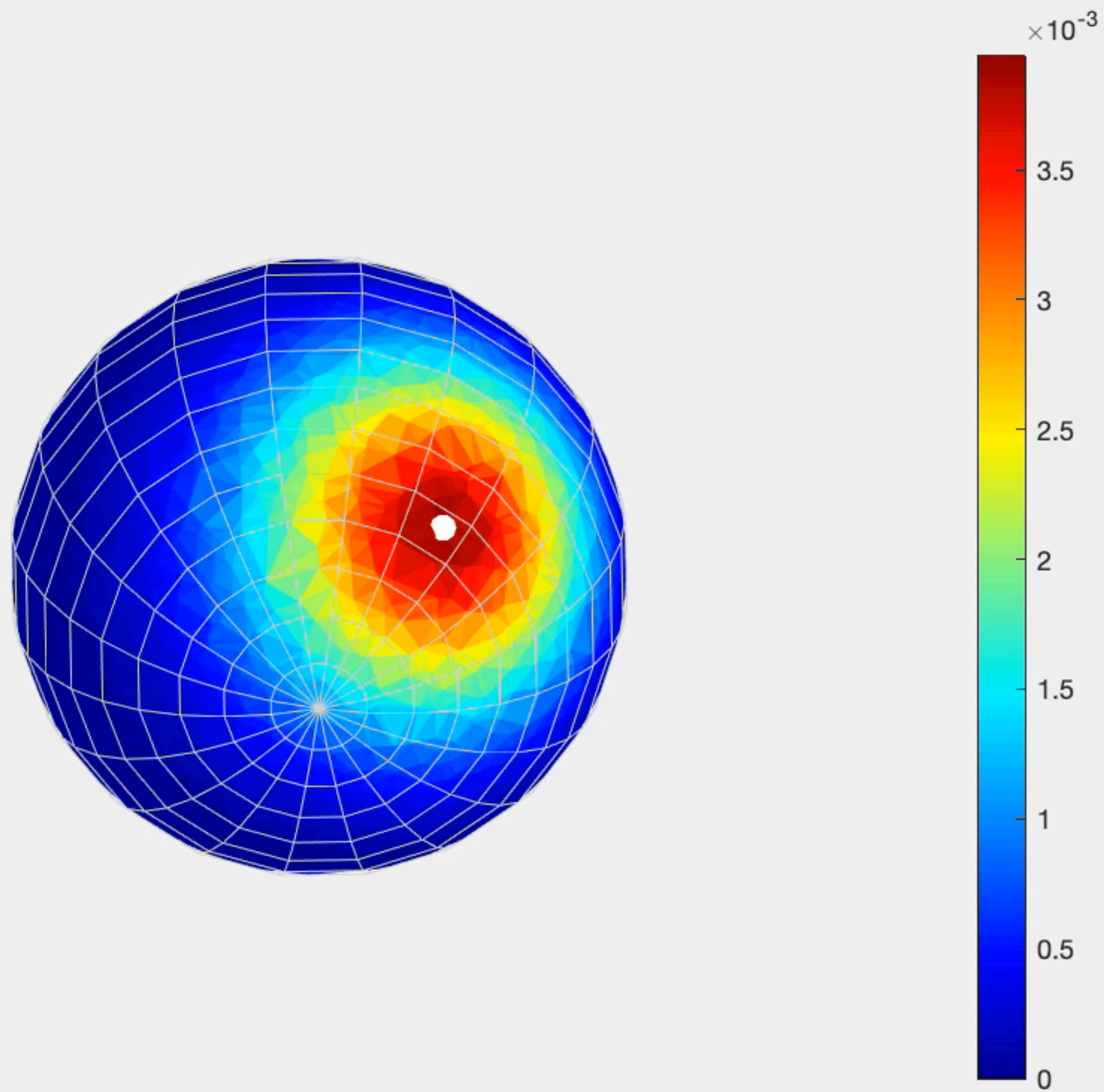
Matrix dynamics  $e^{it\sqrt{\Delta}_{\epsilon,N}} \left| \psi_h^{(x_0, \xi_0)} \right\rangle$  **on dataset**

follows geodesic flow starting at  $x_0$  in direction  $\xi_0$  for distance  $t$   
with  $O(h)$  error

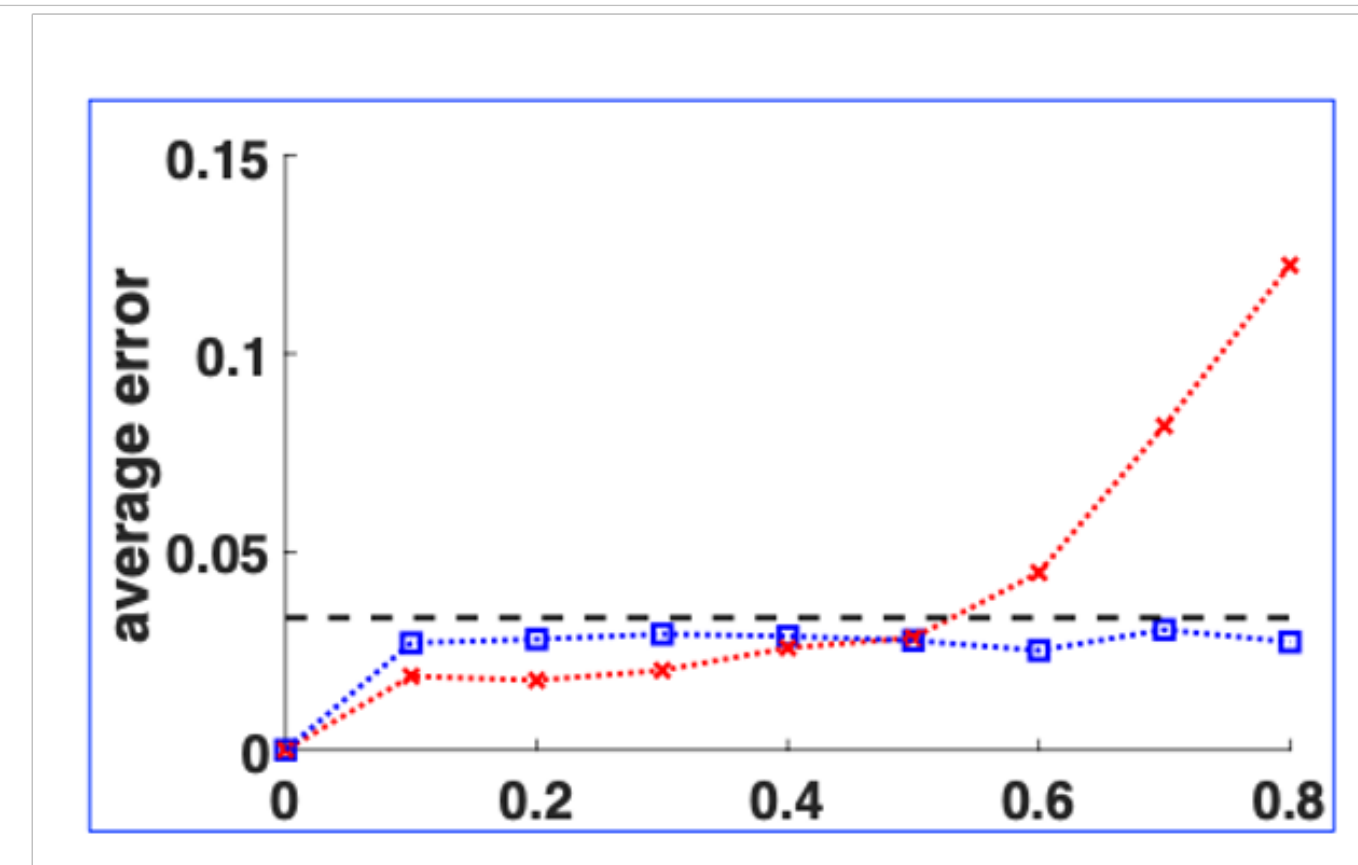
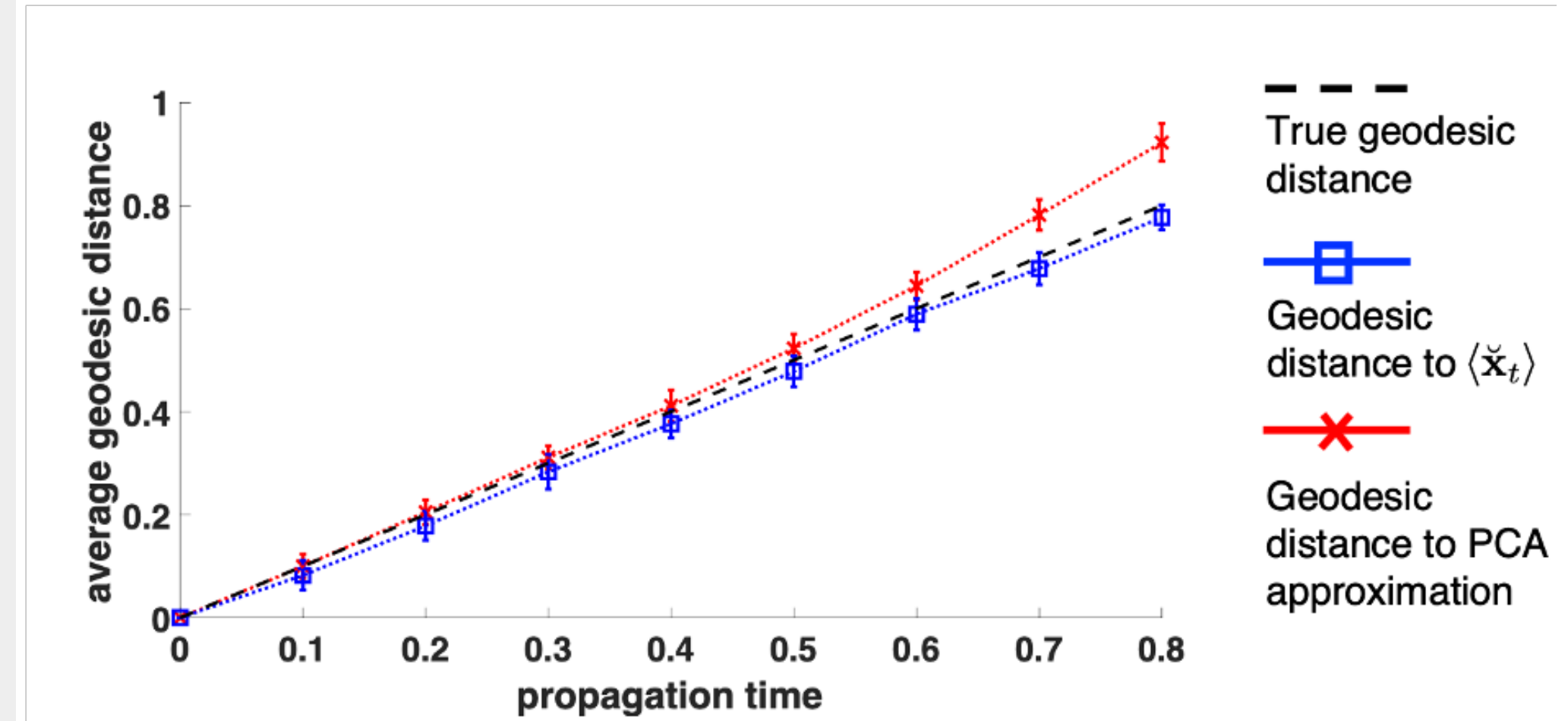
1: **Inputs:**  $X_N = \{v_1, \dots, v_N\}, v^*, \epsilon > 0, \alpha \geq 1, t > 0$

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# The solution

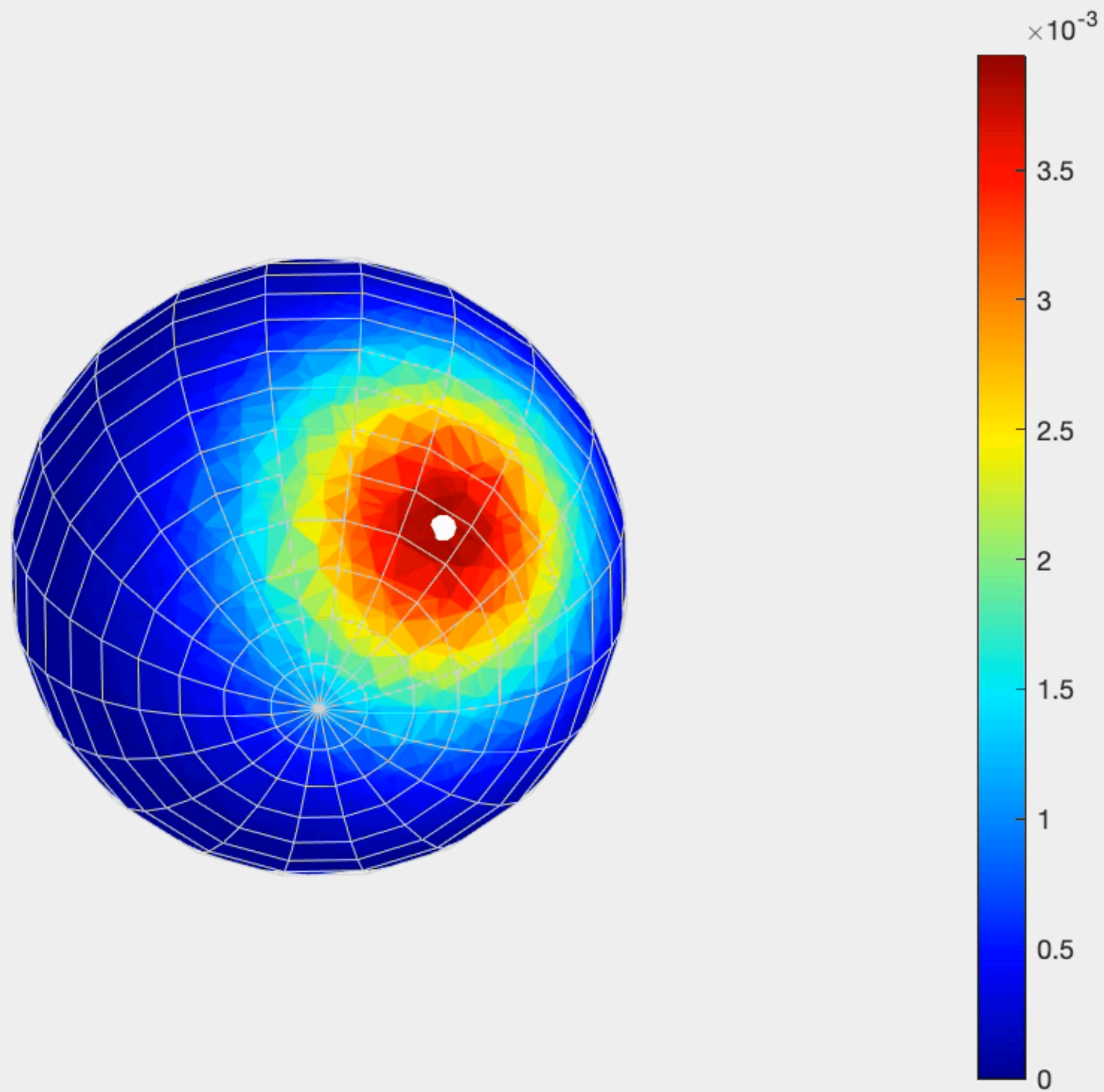


$N = 3000$  points  
uniformly sampled on unit sphere

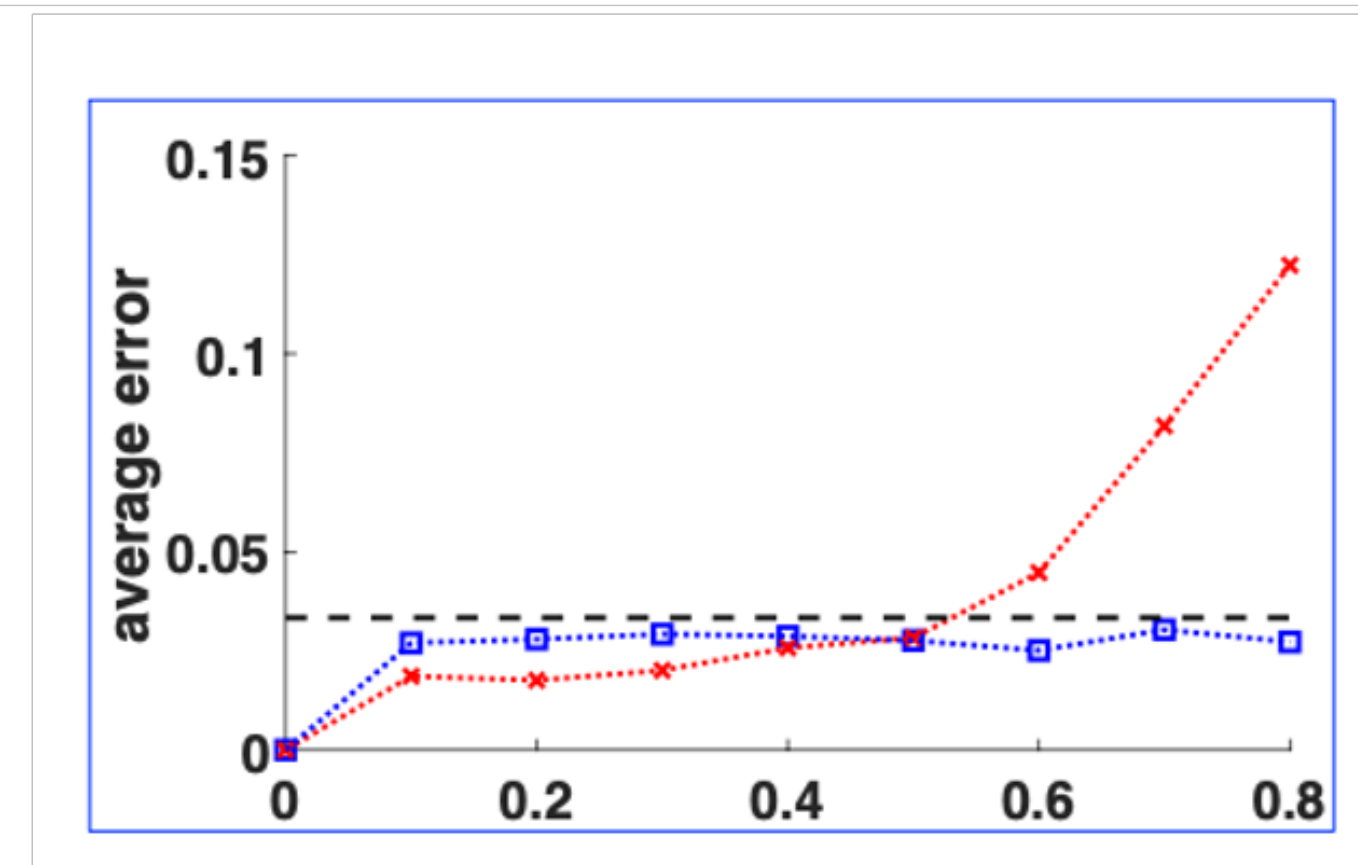
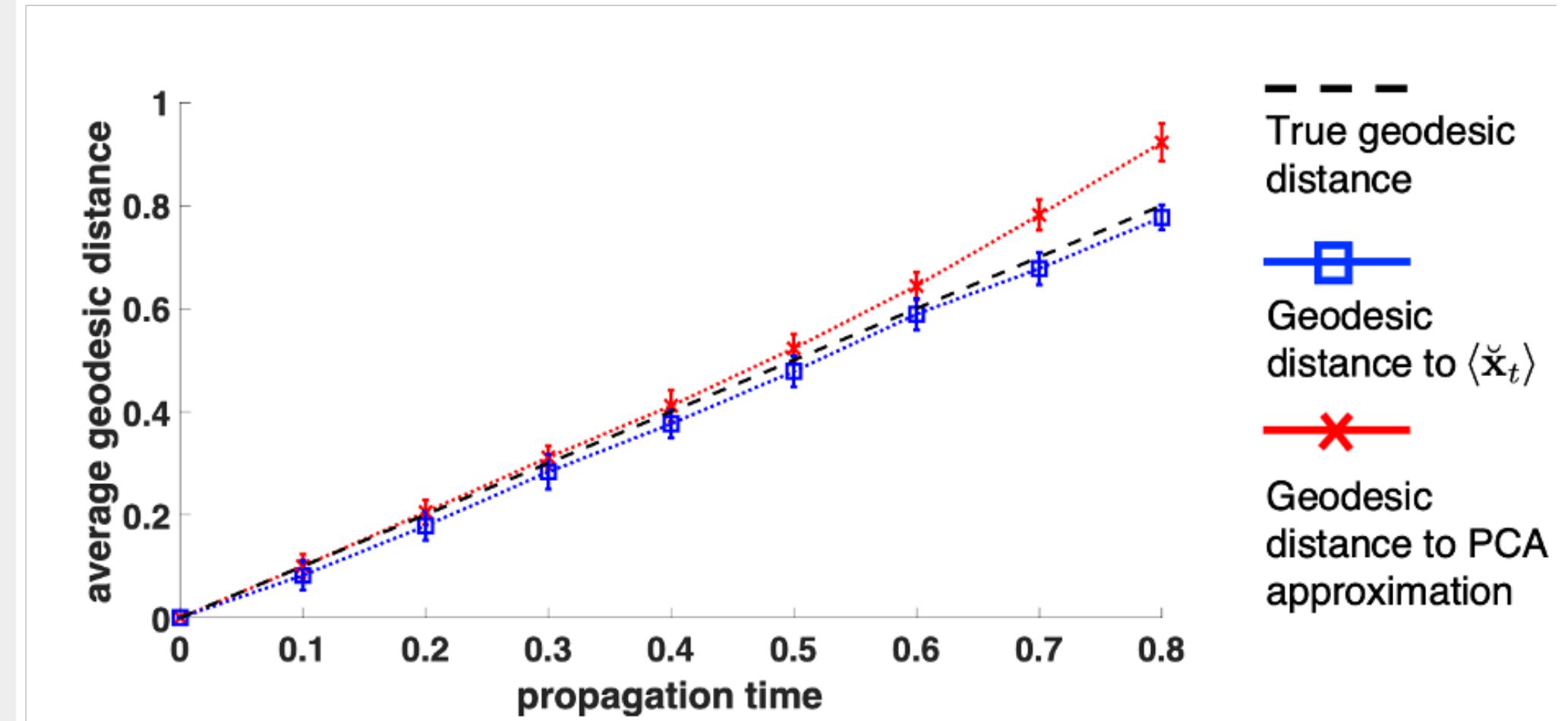




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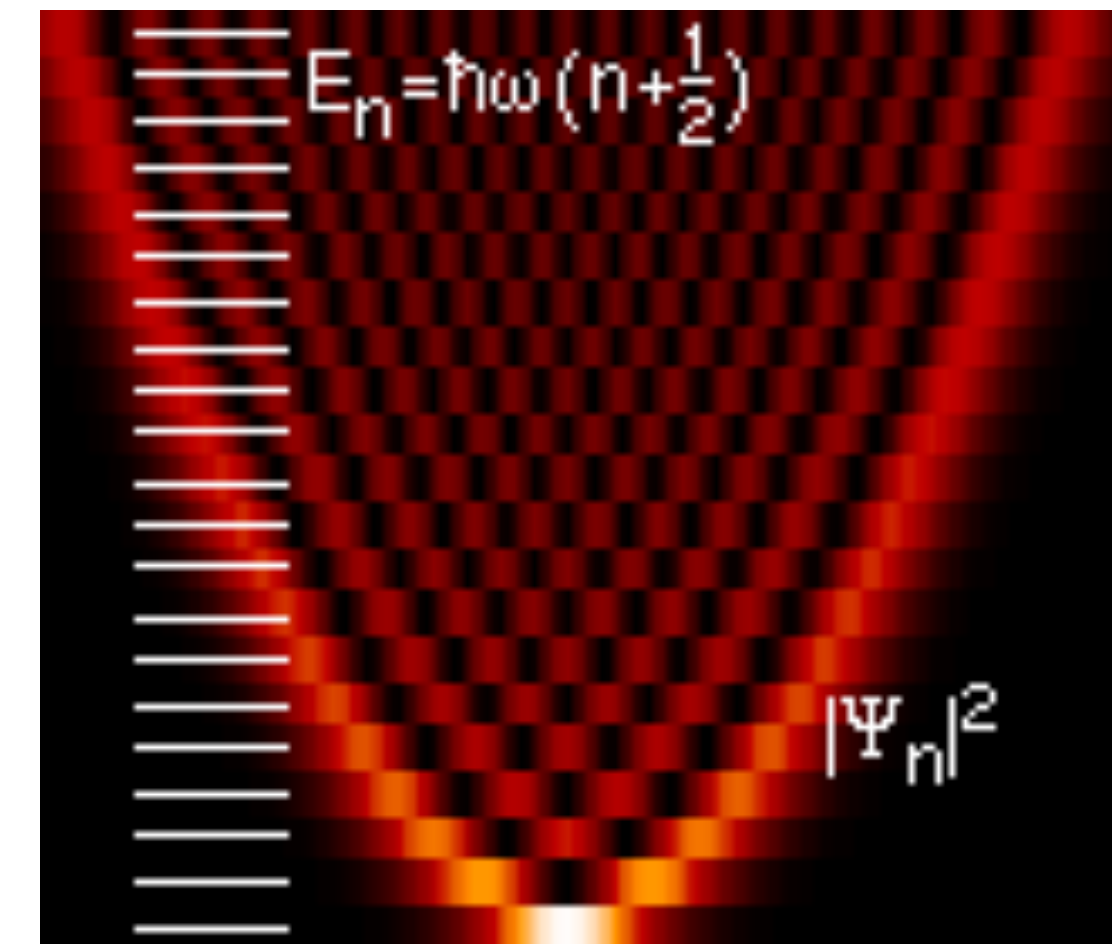
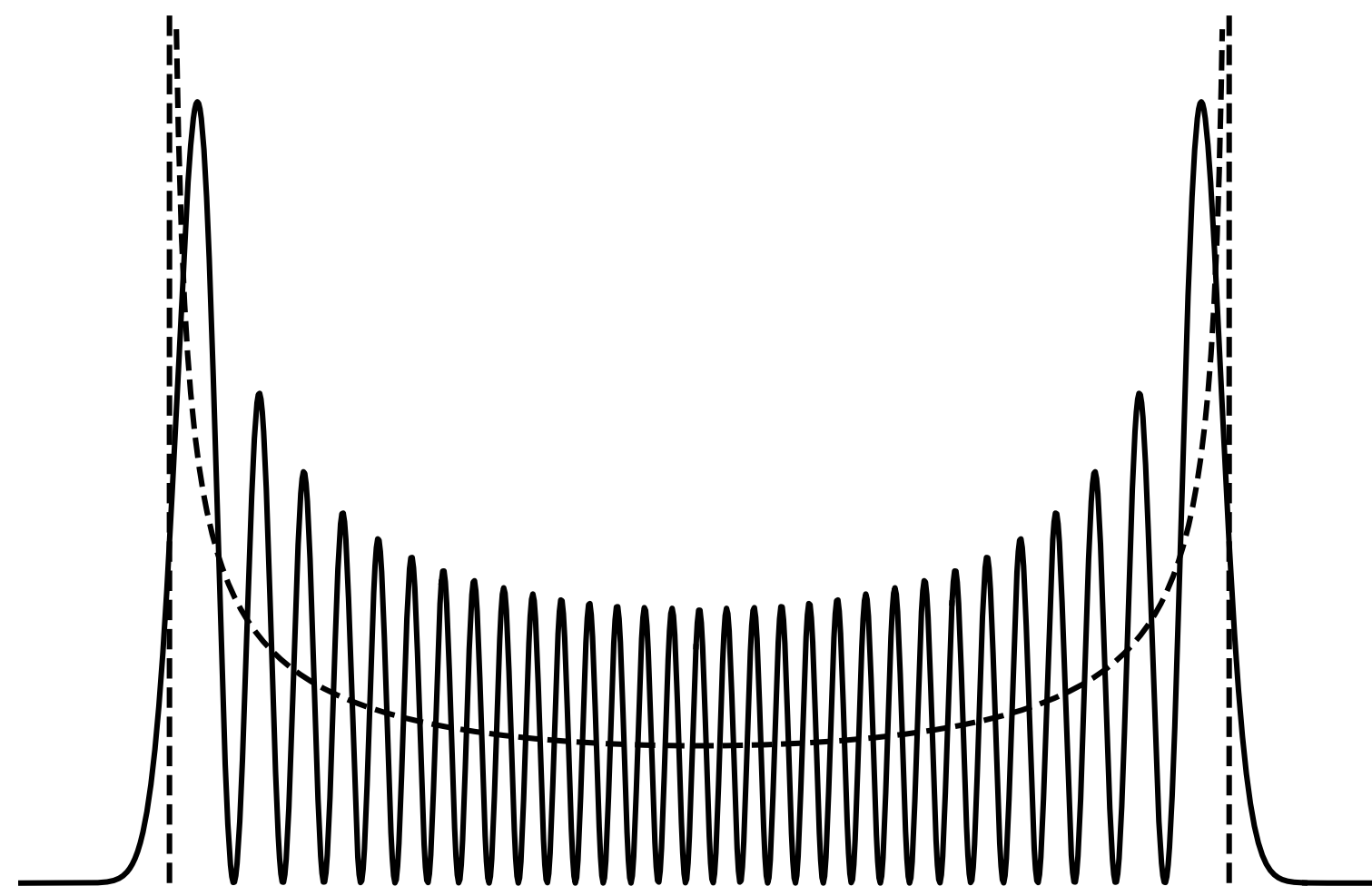


## Quantum-classical correspondence

“classical mechanics emerges not directly, but only after averaging over phase-scrambling effects that can be ascribed to the environment [...] — in modern parlance, decoherence effects.”

*Berry, Quantum Mechanics: Scientific perspectives on divine action, 41 (2001)*

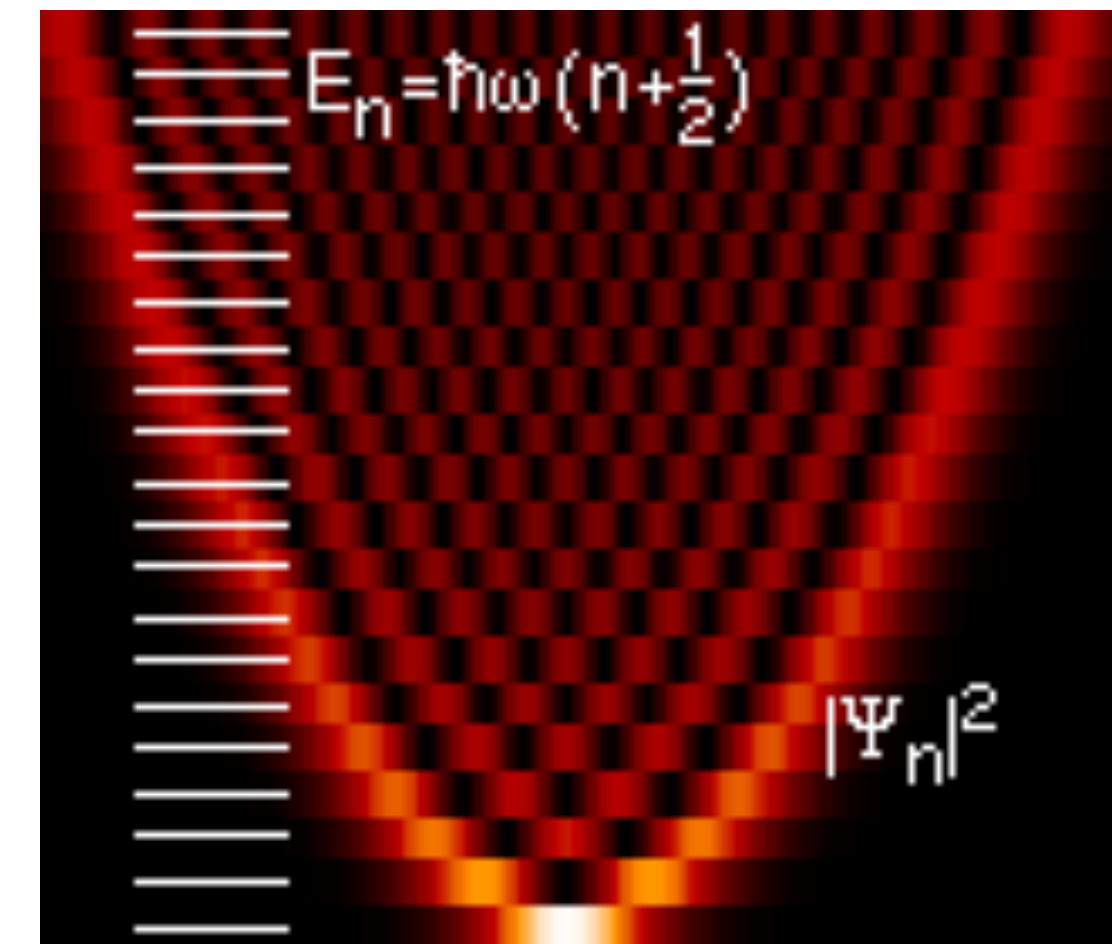
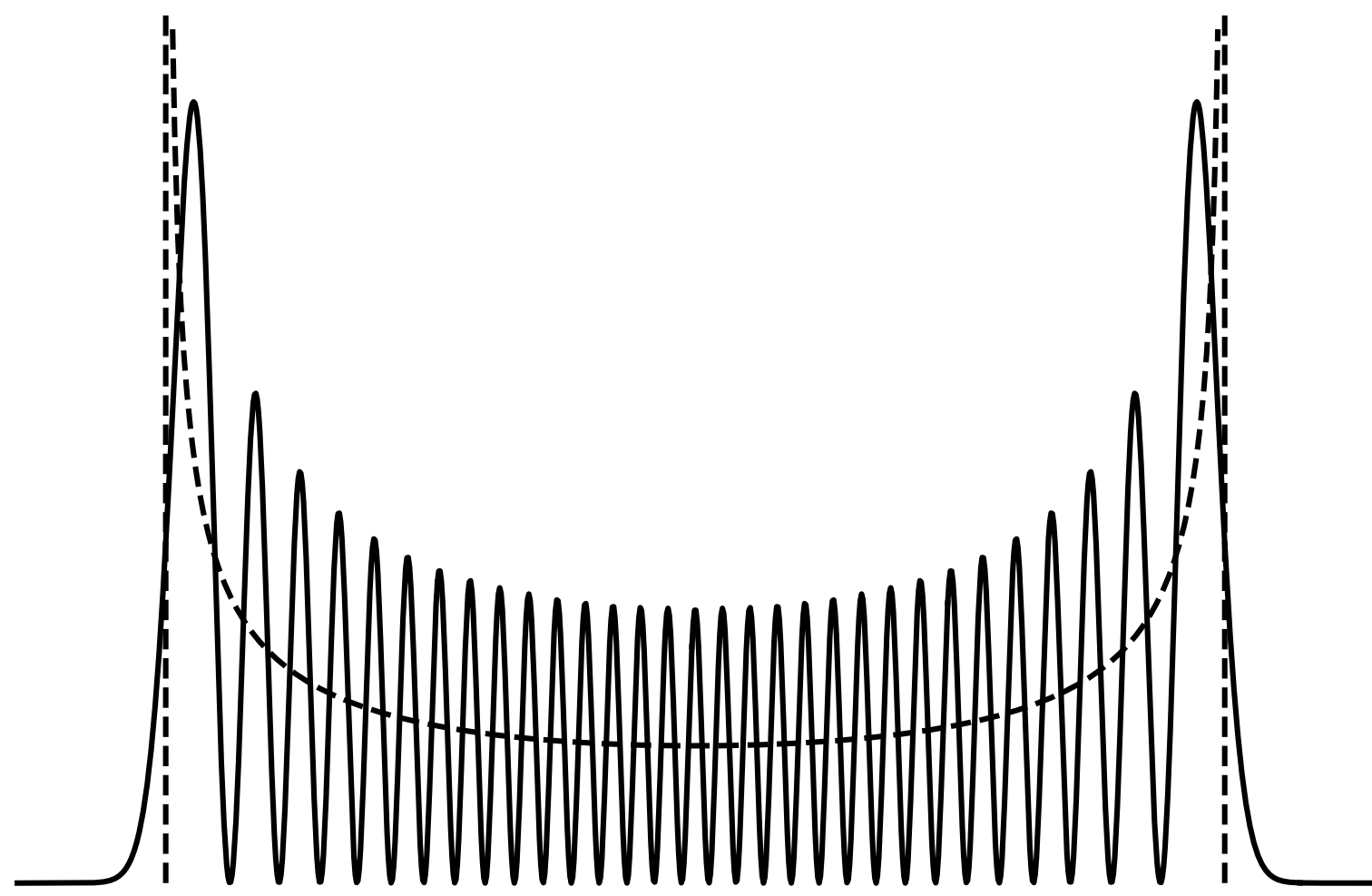




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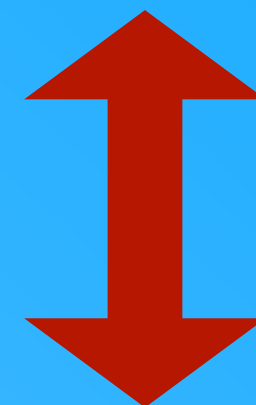
“classical mechanics emerges not directly, but only after averaging over phase-scrambling effects that can be ascribed to the environment [...] — in modern parlance, decoherence effects.”

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**Quantum dynamics:**

linear in  $|\psi_h\rangle$

$$i\hbar\partial_t|\psi_h\rangle = \sqrt{\hat{H}_h}|\psi_h\rangle$$



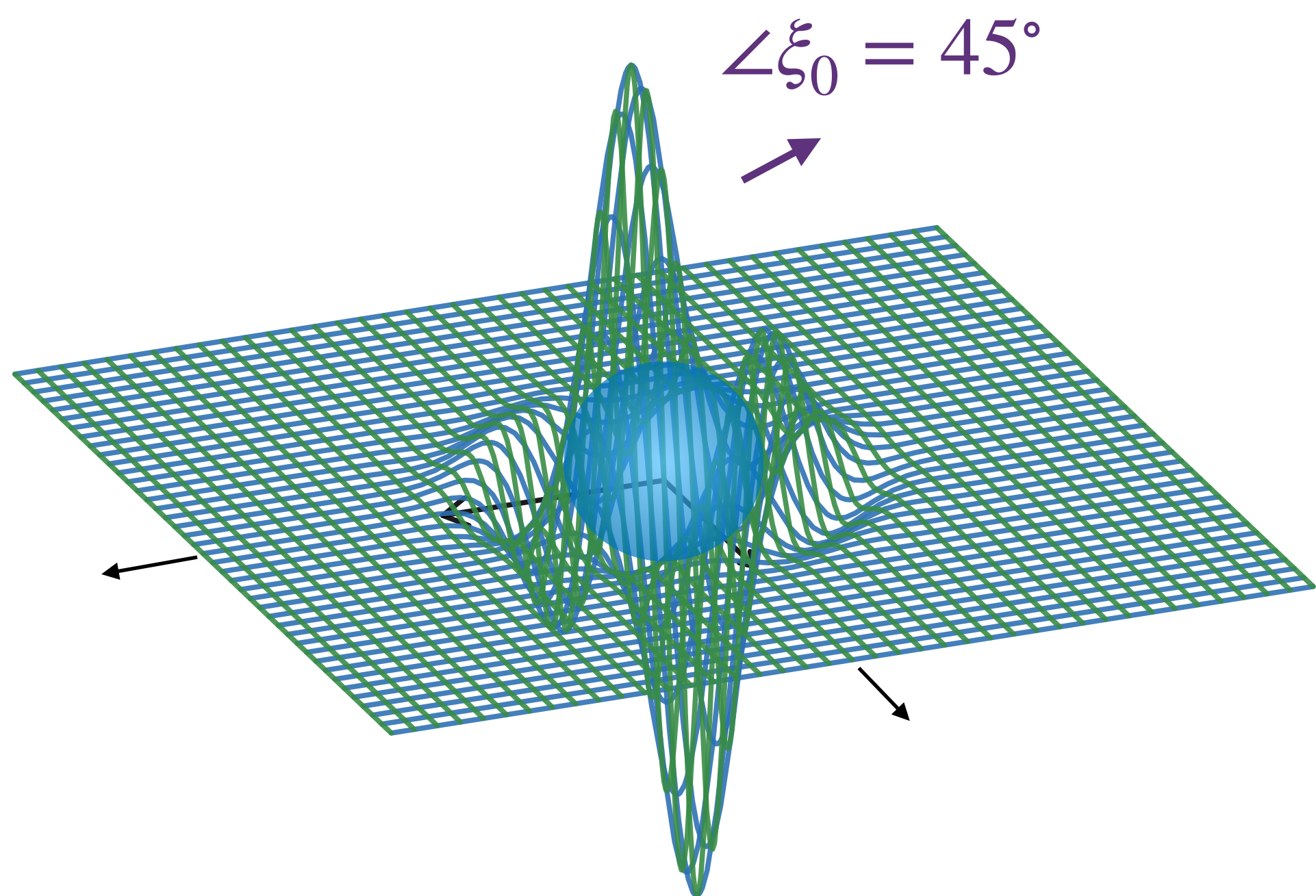
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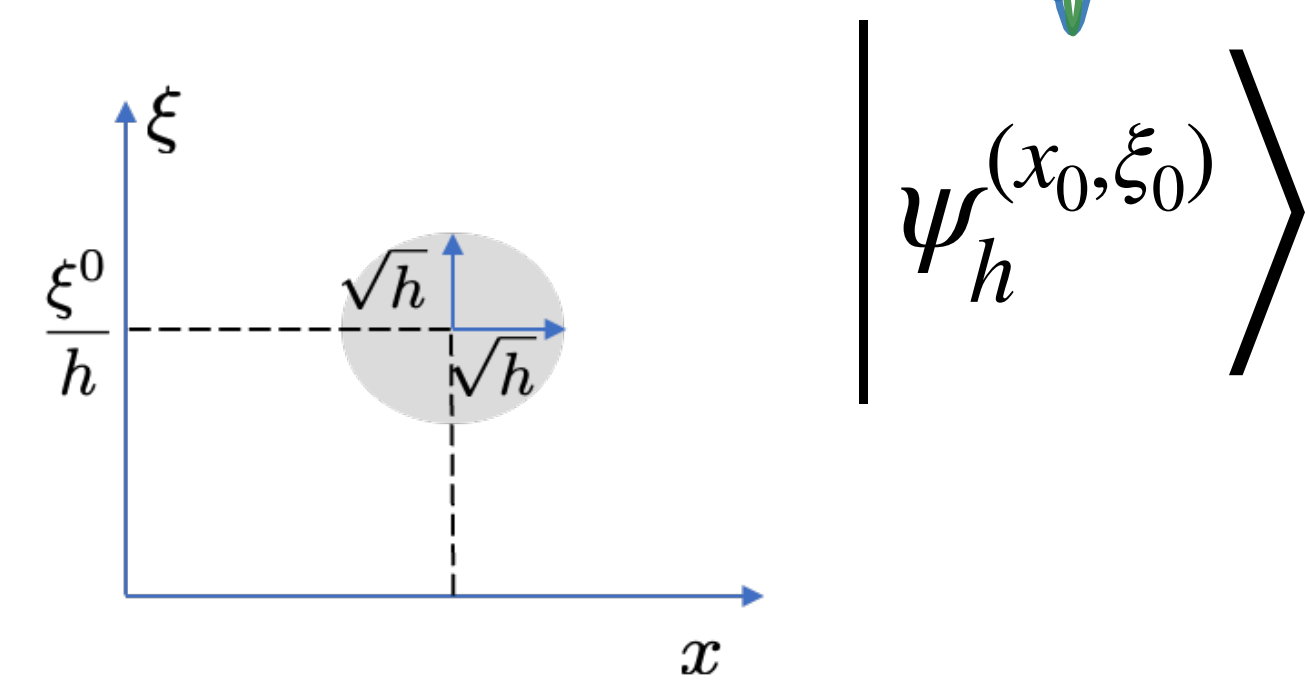
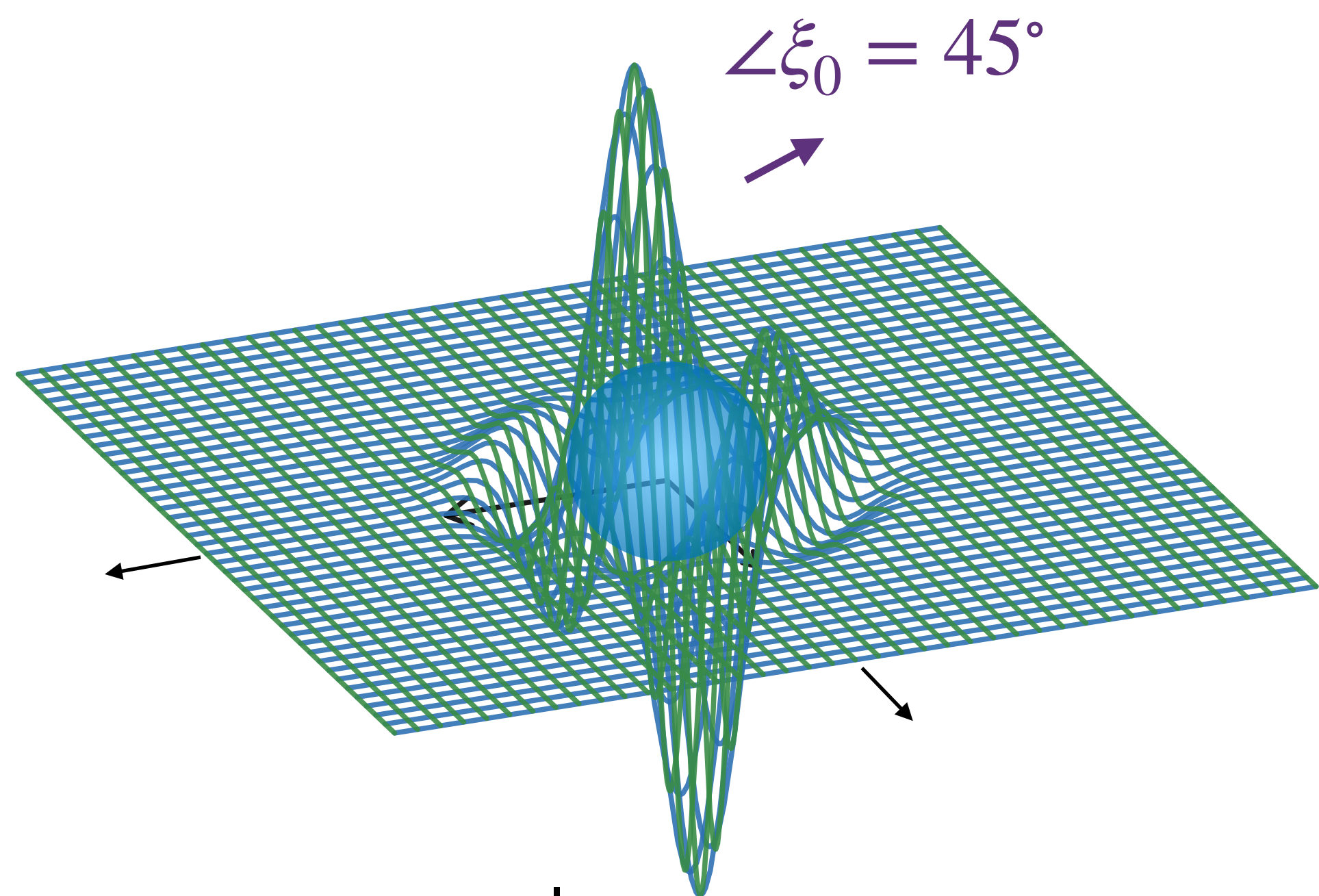
nonlinear in  $x, \xi$



# Quantizing particles



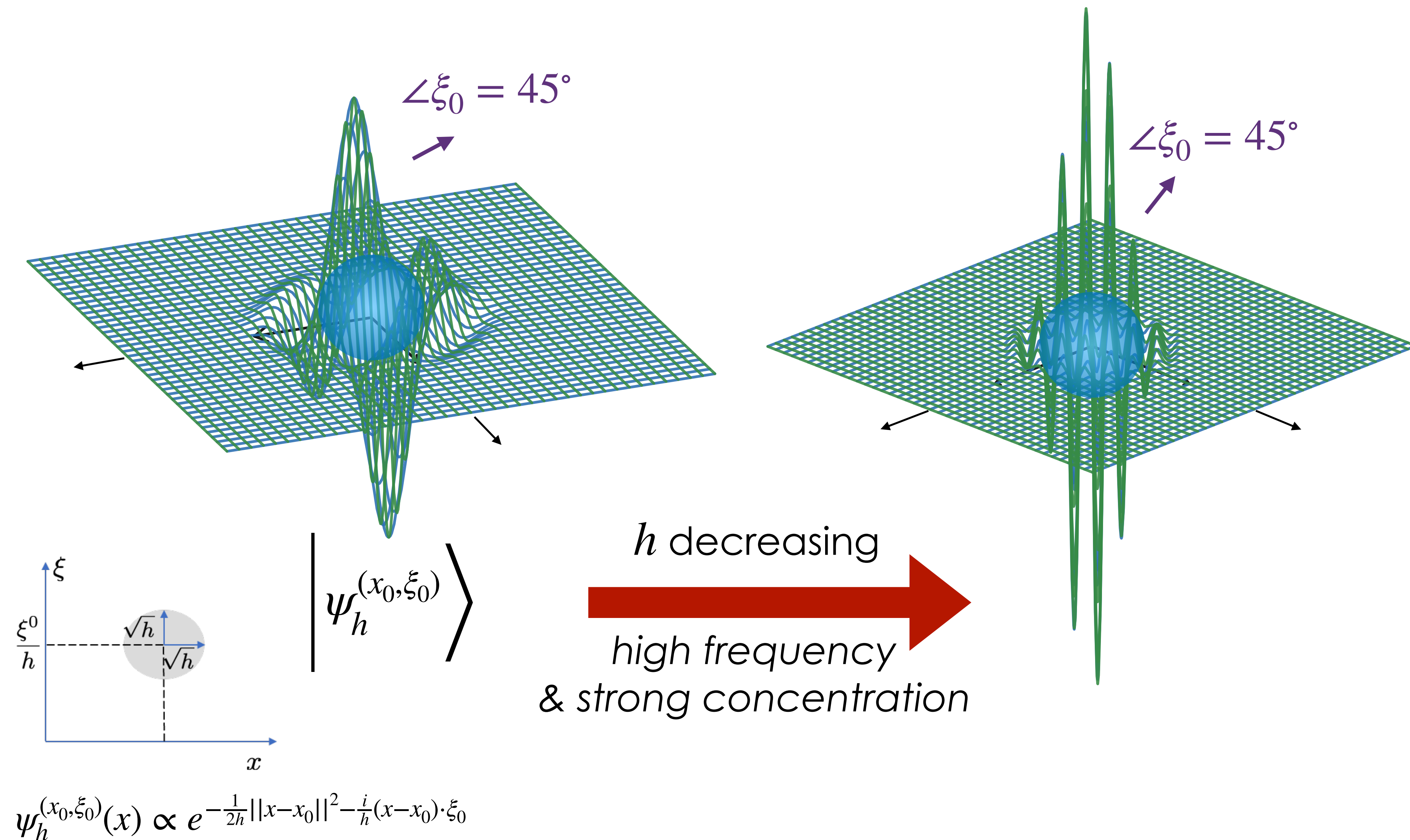
# Quantizing particles



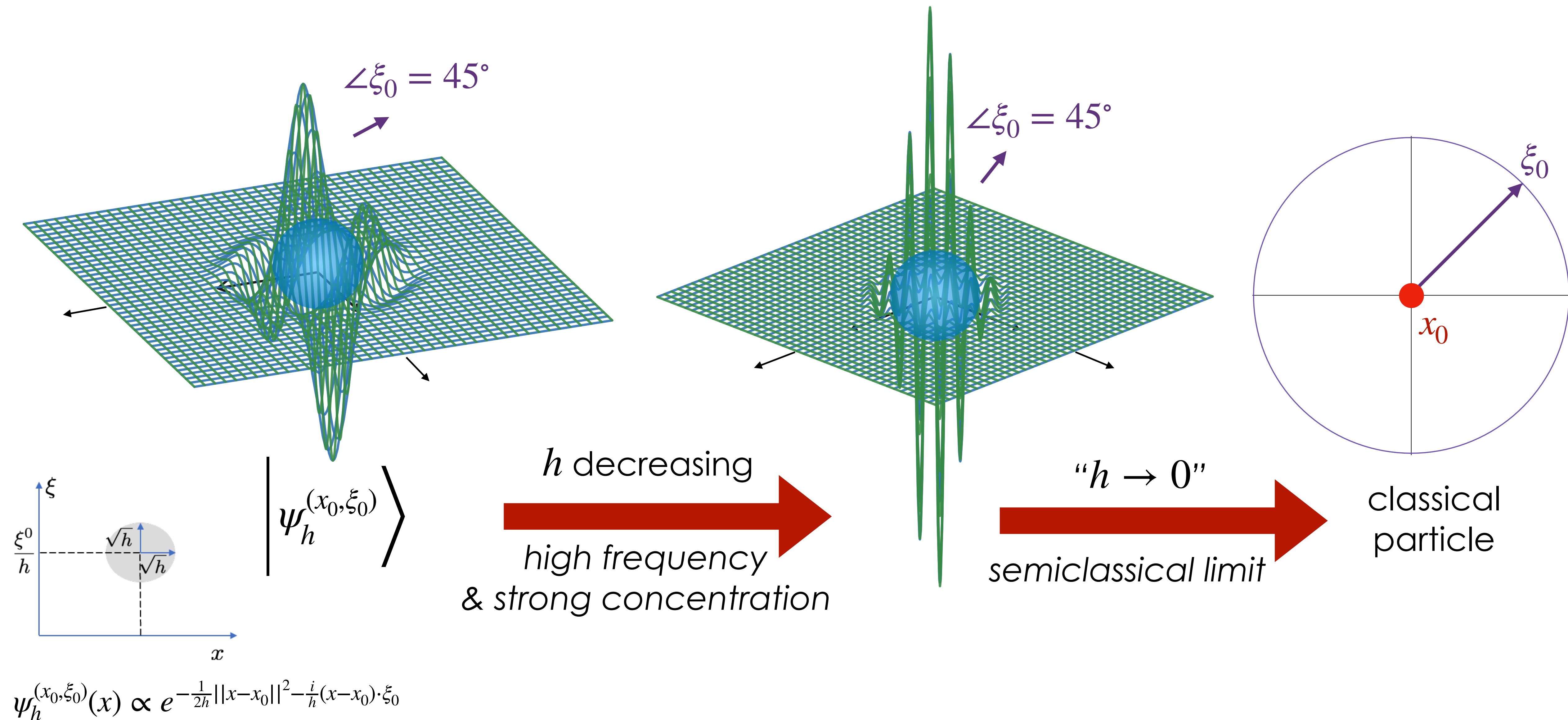
$$\psi_h^{(x_0, \xi_0)}(x) \propto e^{-\frac{1}{2h} \|x-x_0\|^2 - \frac{i}{h} (x-x_0) \cdot \xi_0}$$



# Quantizing particles



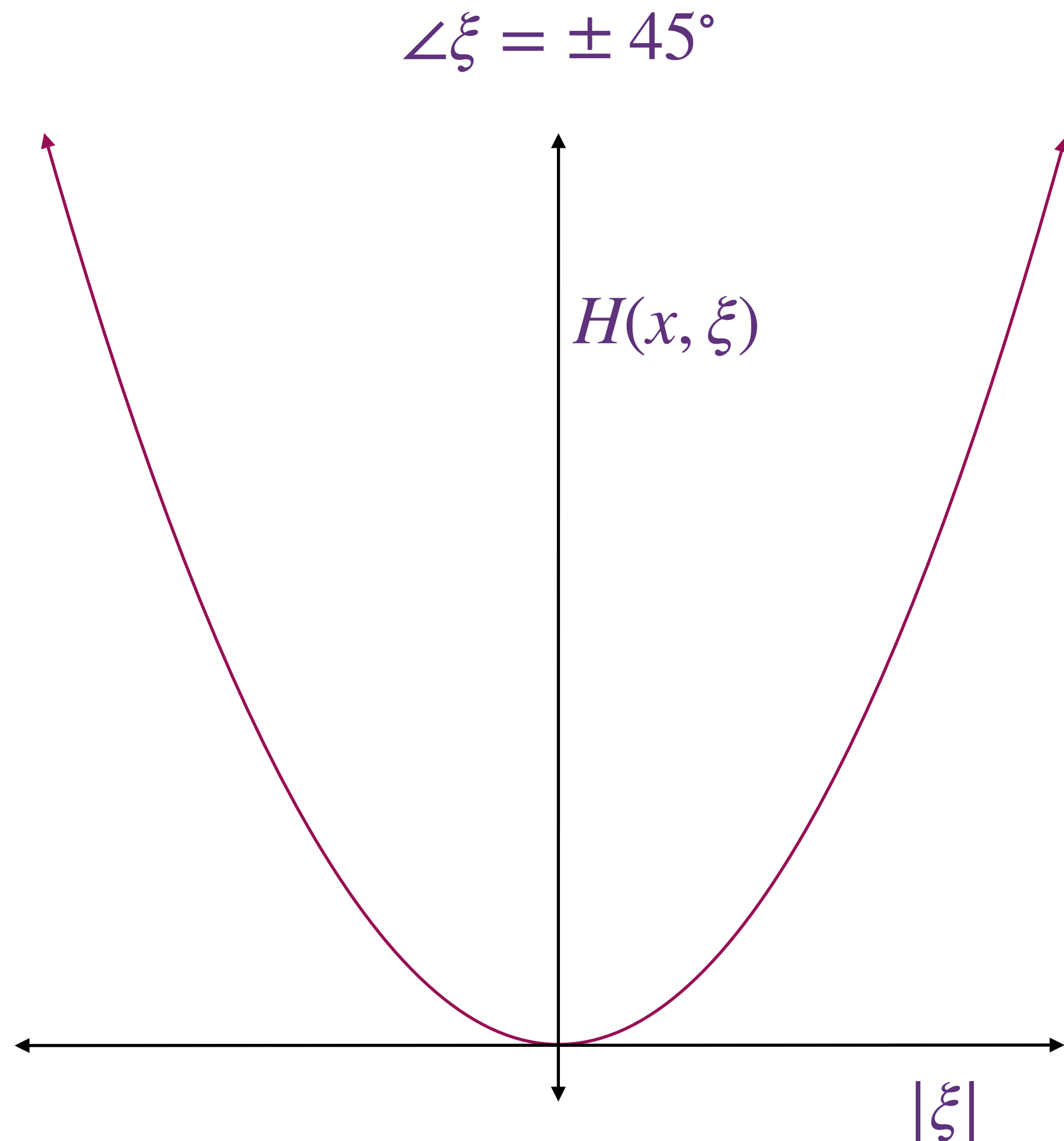
# Quantizing particles





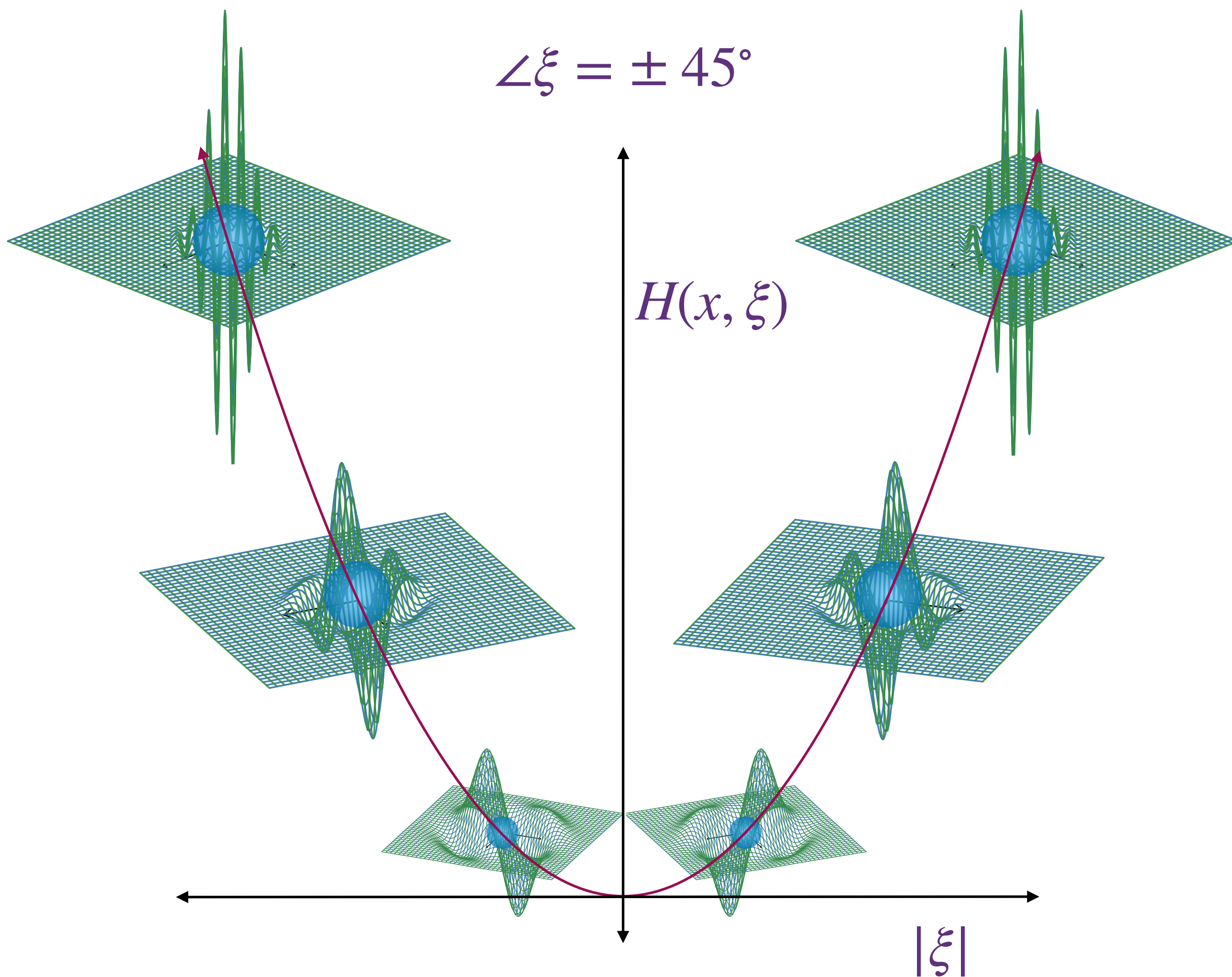
## Quantizing the geodesic flow

Hamiltonian flow governed by  $H(x, \xi) := |\xi|_{g(x)}^2$



# Quantizing the geodesic flow

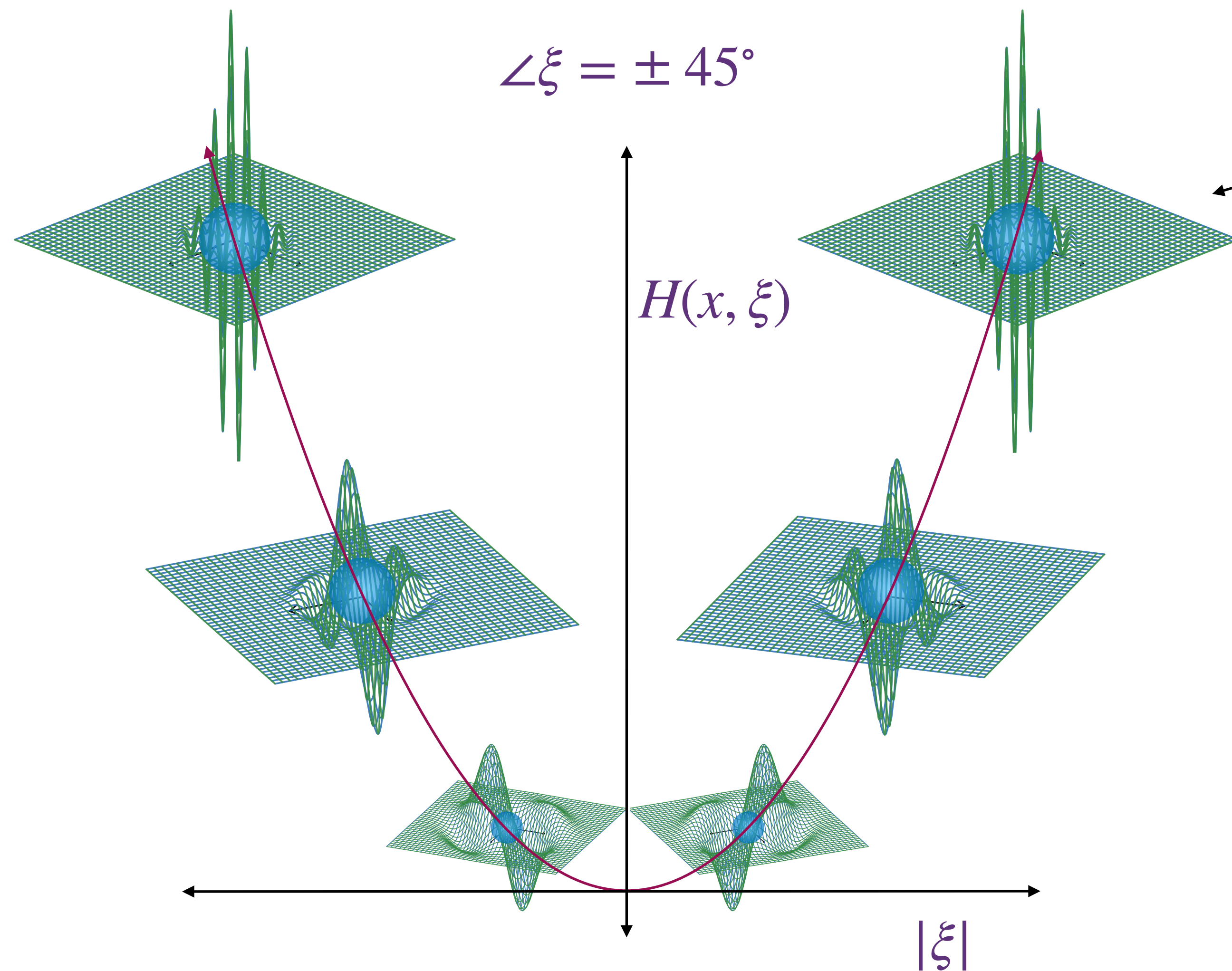
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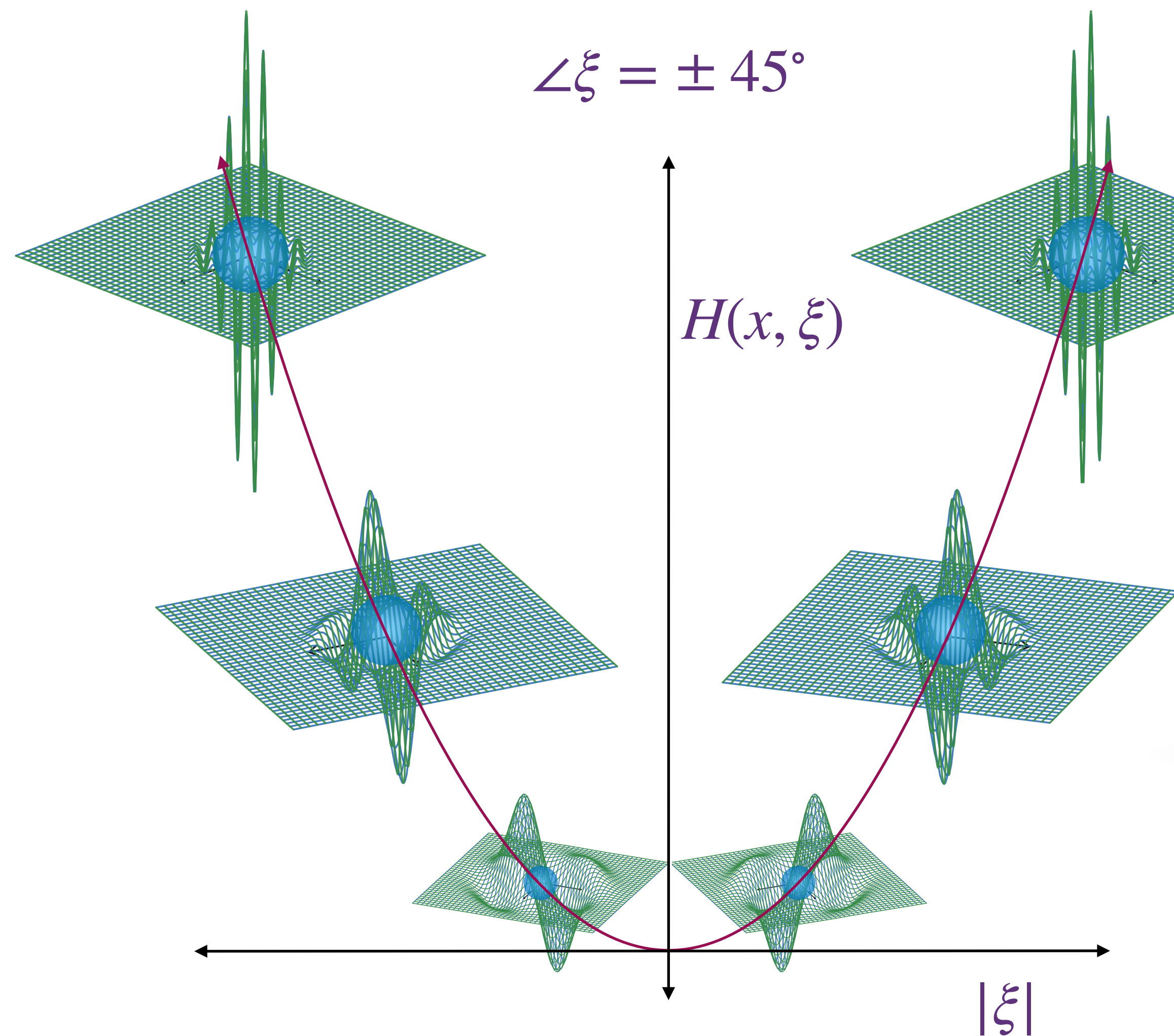
$$\hat{H}_h = \sum_{x, \xi} H(x, \xi) \left| \psi_h^{(x, \xi)} \right\rangle \left\langle \psi_h^{(x, \xi)} \right|$$

$$\langle \psi_h^{(x, \xi)} | \psi_h^{(x, \xi)} \rangle = 1 + O(h^\infty)$$

$$\implies \langle \psi_h^{(x, \xi)} | \hat{H}_h | \psi_h^{(x, \xi)} \rangle = H(x, \xi) + O(h)$$

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Hamiltonian flow governed by  $H(x, \xi) := |\xi|_{g(x)}^2$



$$\hat{H}_h = \sum_{x, \xi} H(x, \xi) |\psi_h^{(x, \xi)}\rangle \langle \psi_h^{(x, \xi)}|$$

**THEOREM.**

$$\hat{H}_h = h^2 \Delta_{\mathcal{M}} + \text{lower order terms}$$

$$\langle \psi_h^{(x, \xi)} | \psi_h^{(x, \xi)} \rangle = 1 + O(h^\infty)$$

$$\implies \langle \psi_h^{(x, \xi)} | \hat{H}_h | \psi_h^{(x, \xi)} \rangle = H(x, \xi) + O(h)$$

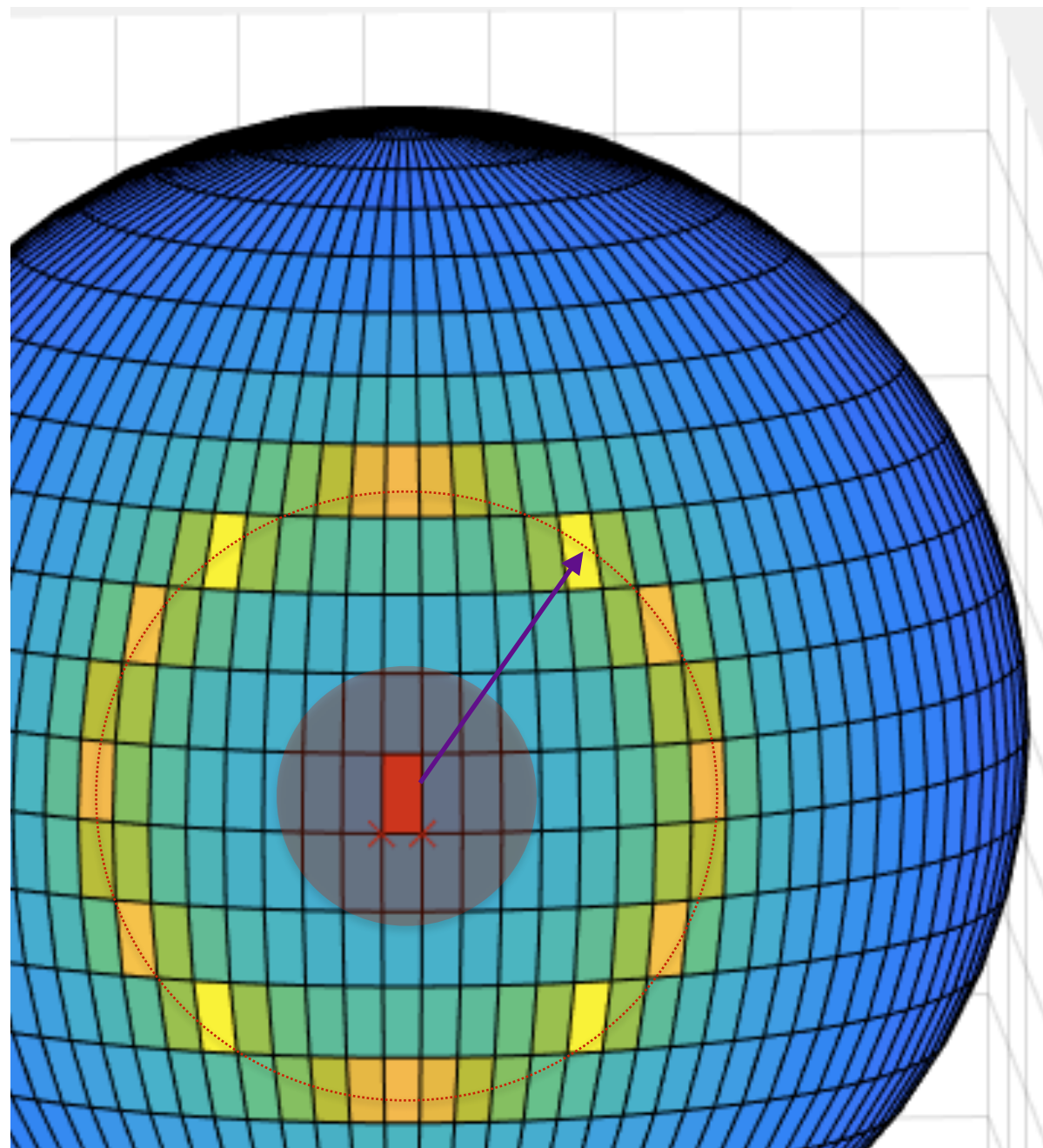


## Quantizing the geodesic flow

Schrödinger equation  $ih\partial_t |\psi_h\rangle = \sqrt{\hat{H}_h} |\psi_h\rangle$

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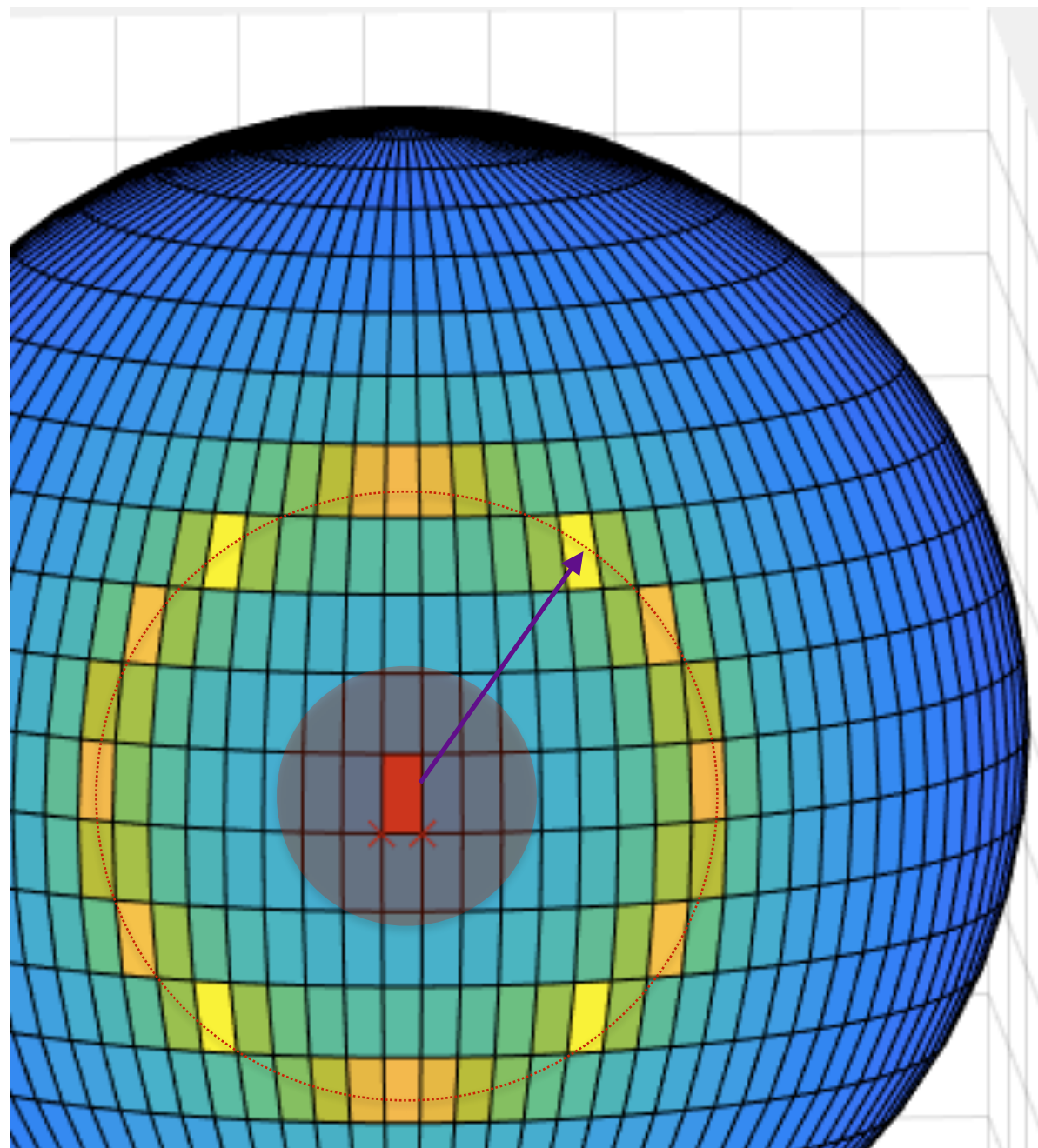
**Initial state**

$$|\psi_h^{(x_0, \xi_0)}\rangle$$



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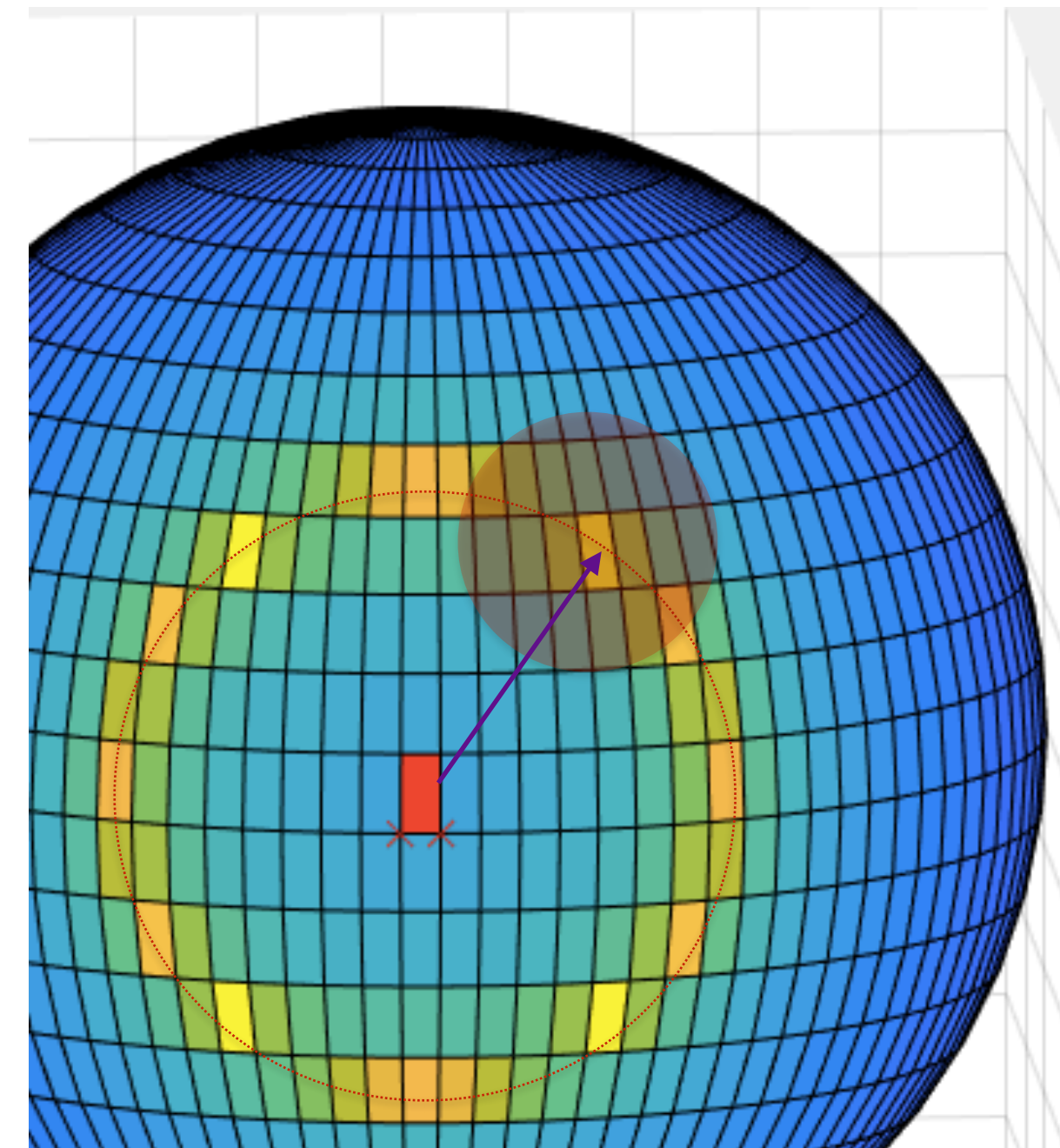
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Propagated state

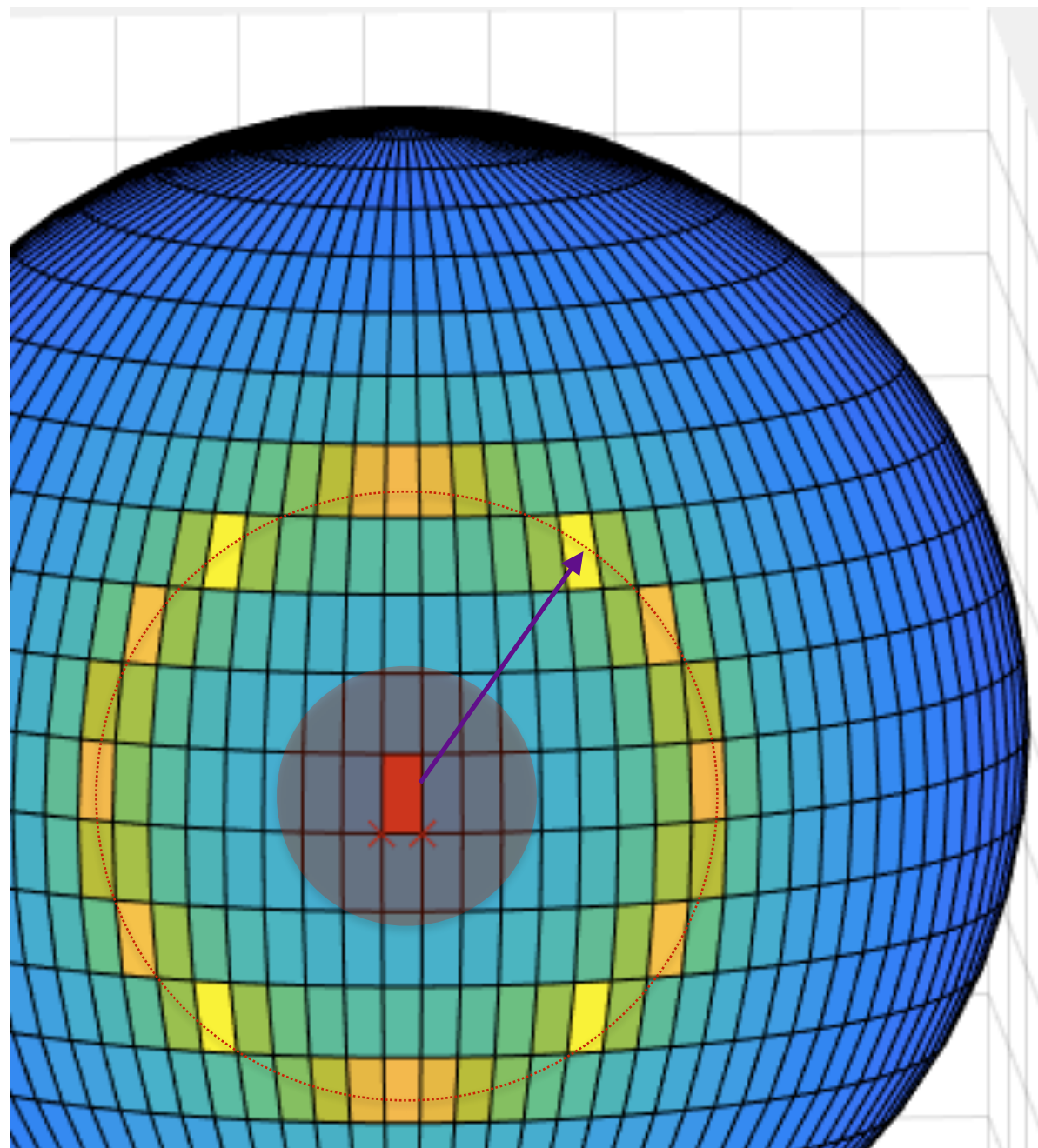
$$|\psi_h(t)\rangle := e^{\frac{i}{\hbar}t\sqrt{\hat{H}_h}} |\psi_h^{(x_0, \xi_0)}\rangle$$





## Quantizing the geodesic flow

$$\text{Schrödinger equation } ih\partial_t |\psi_h\rangle = \sqrt{\hat{H}_h} |\psi_h\rangle$$



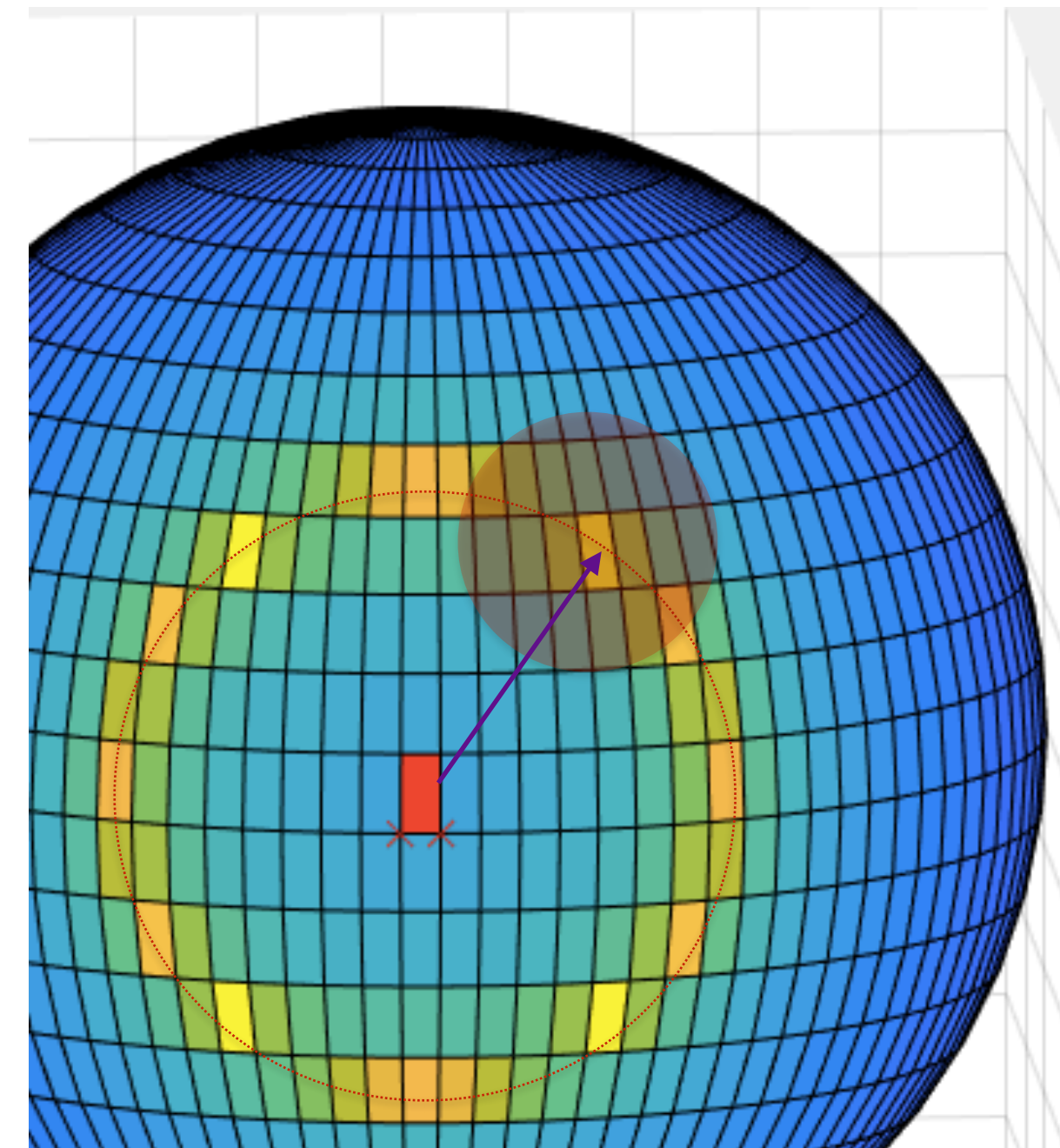
Initial state

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Propagated state

$$|\psi_h(t)\rangle := e^{\frac{i}{h}t\sqrt{\hat{H}_h}} |\psi_h^{(x_0, \xi_0)}\rangle$$



**THEOREM.**

The density  $|\psi_h(t)|^2$  is concentrated in an  $O(h)$  nbd. of  $x(t) := \pi_{\mathcal{M}}\Gamma^t(x_0, \xi_0)$ .



## ***Discrete quantum-classical correspondence***

“If you want to see something, you send waves in its general direction,  
you don’t throw heat at it.”

*Attributed to Peter Lax (Cloninger & Steinerberger, Applied & Computational Harmonic Analysis (2017))*

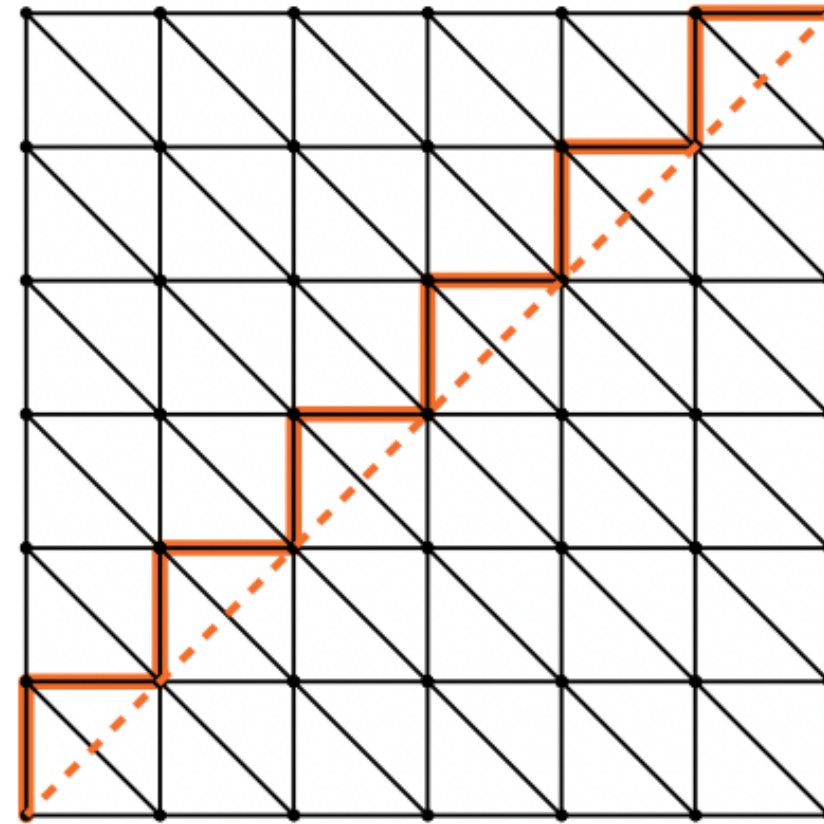
# Random walks on data lead to diffusion

## Random walk:

### 1. Nbd. graph:

$$[\mathcal{A}_{\epsilon, N}]_{i,j} := \begin{cases} \approx 1 & \text{if } |v_j - v_i| \ll \sqrt{\epsilon} \\ \approx 0 & \text{if } |v_j - v_i| \gg \sqrt{\epsilon} \end{cases}$$

### 2. Markov chain: $A_{\epsilon, N} := \frac{1}{\mathcal{A}_{\epsilon, N}[1]} \mathcal{A}_{\epsilon, N}$



Crane et al., Comm. ACM (2017)



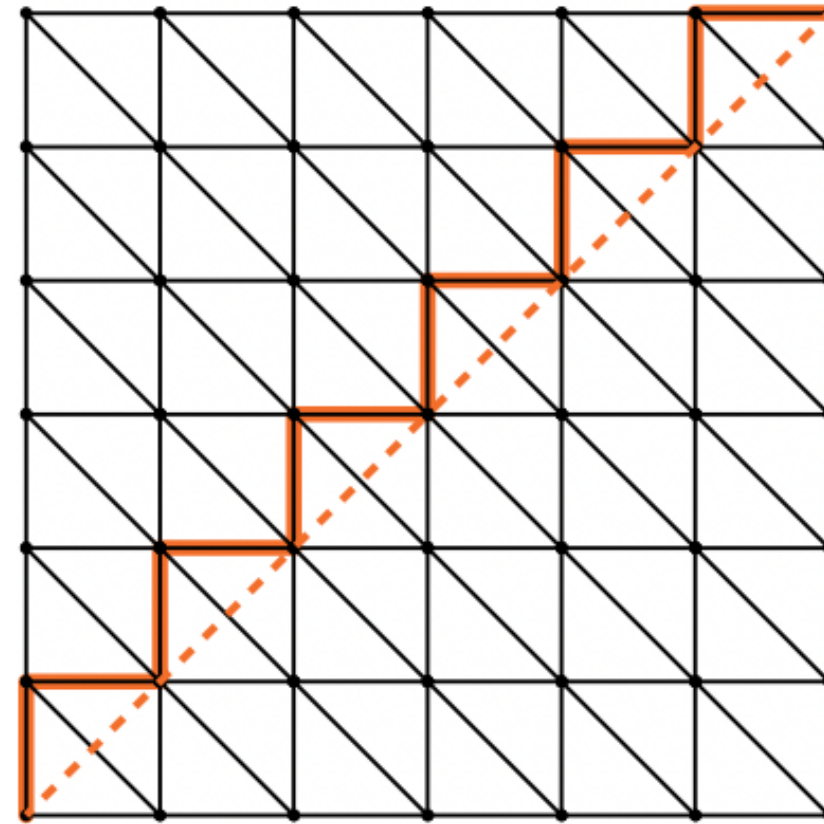
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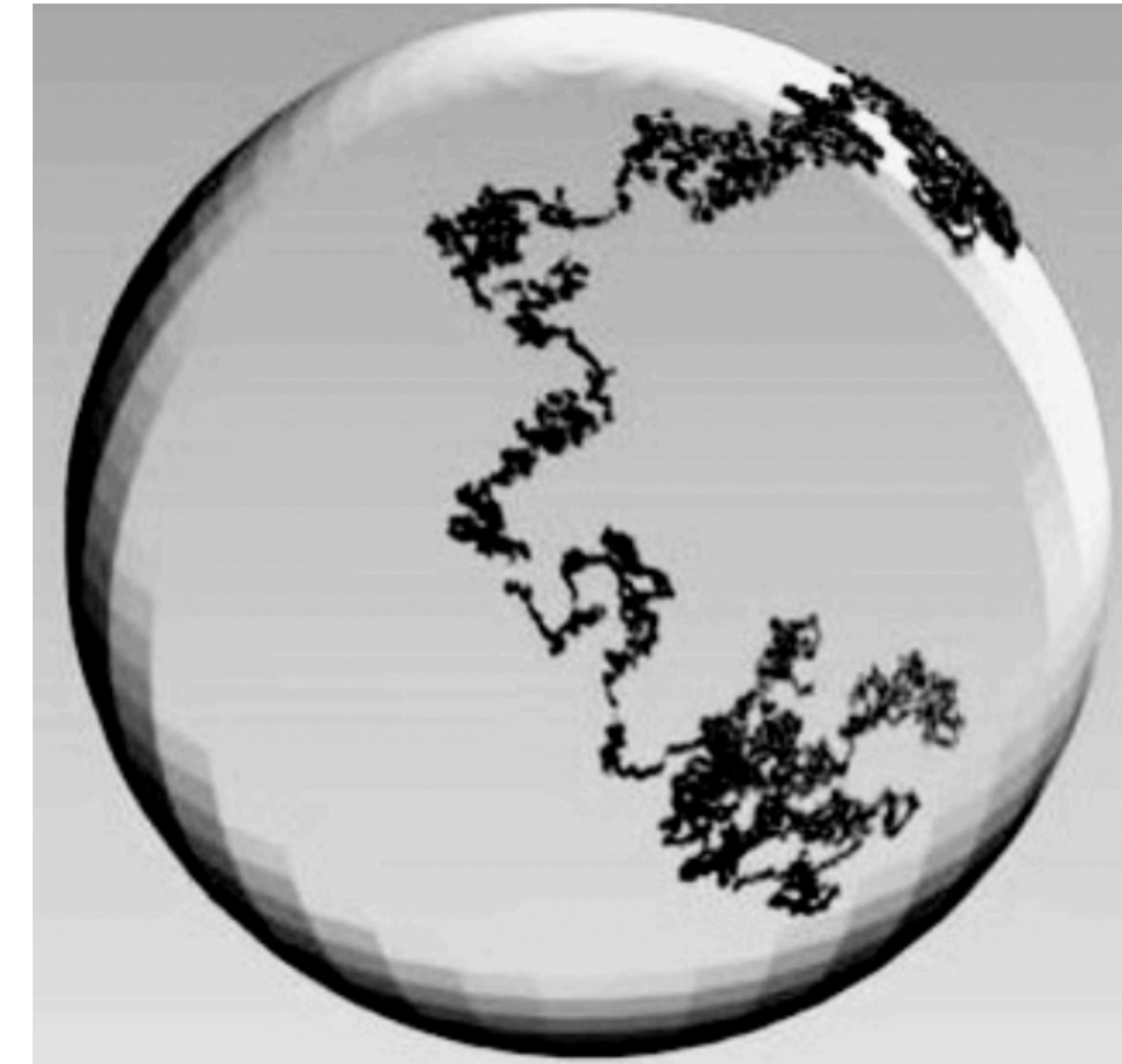
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Crane et al., Comm. ACM (2017)

large  $N$   
with high prob.,  
 $\sqrt{\epsilon} \ll 1$

## Geodesic random walk



Ginkel & Redig, Journal of Statistical Physics (2020).

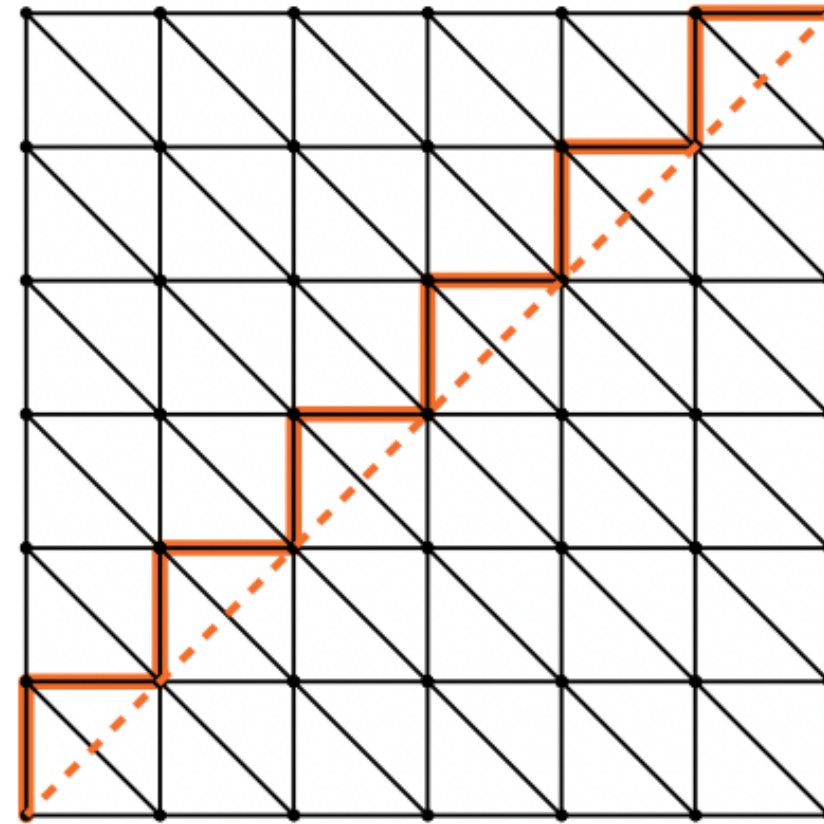
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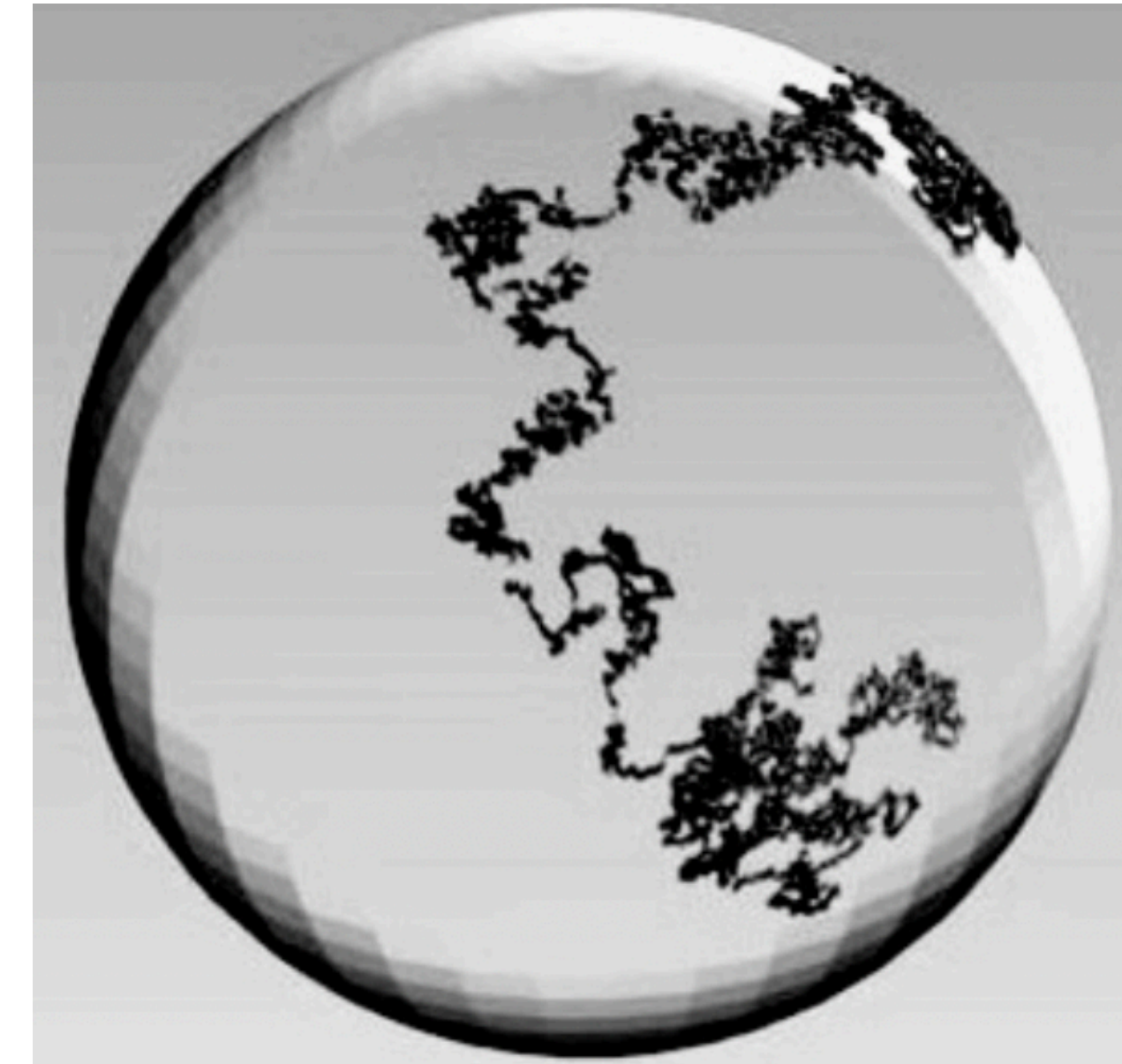
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Crane et al., Comm. ACM (2017)

large  $N$   
  
 with high prob.,  
 $\sqrt{\epsilon} \ll 1$

## Geodesic random walk



Ginkel & Redig, Journal of Statistical Physics (2020).

**DISCRETE GENERATOR:**  $\Delta_{\epsilon,N} := c(I - A_{\epsilon,N})/\epsilon$  IS THE RANDOM WALK GRAPH LAPLACIAN.

With high probability,

Hein, PhD thesis (2005).

$$\Delta_{\epsilon,N} |\psi\rangle = \underbrace{\Delta_{\mathcal{M}} |\psi\rangle}_{\text{sampling density}} + \underbrace{O(\partial^1) |\psi\rangle + O(\epsilon)}_{\text{diffusion terms}}$$

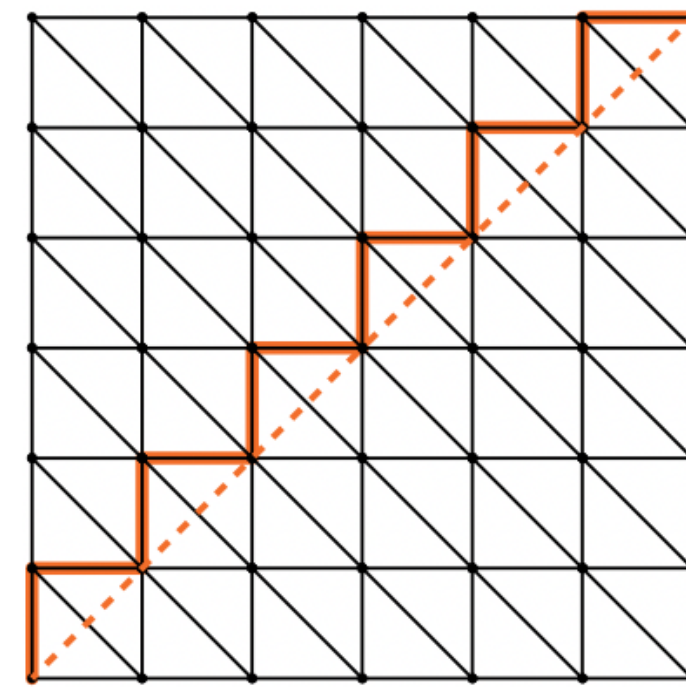


# From **random walks** to **quantum dynamics** on data

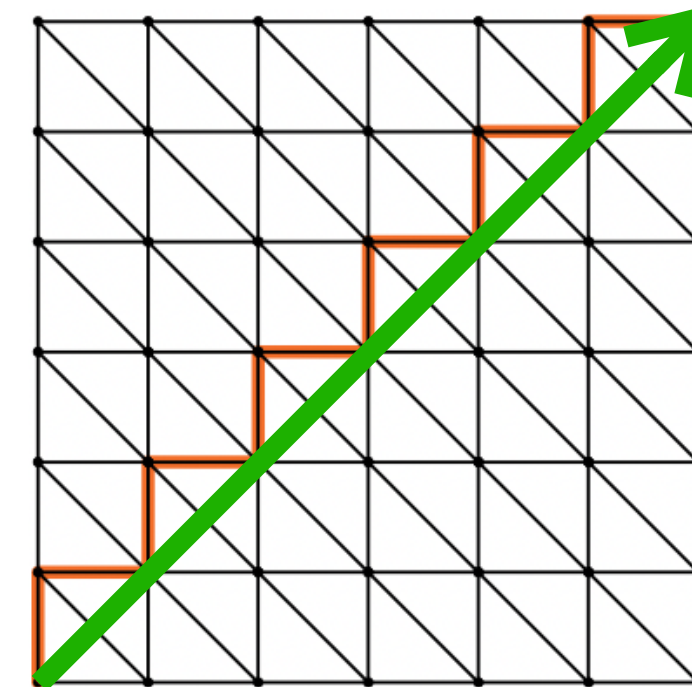
$$\text{Schrödinger equation } i\hbar\partial_t |\psi_h\rangle = \sqrt{h^2 \Delta_{\epsilon, N}} |\psi_h\rangle$$



Ginkel & Redig, *Journal of Statistical Physics* (2020).

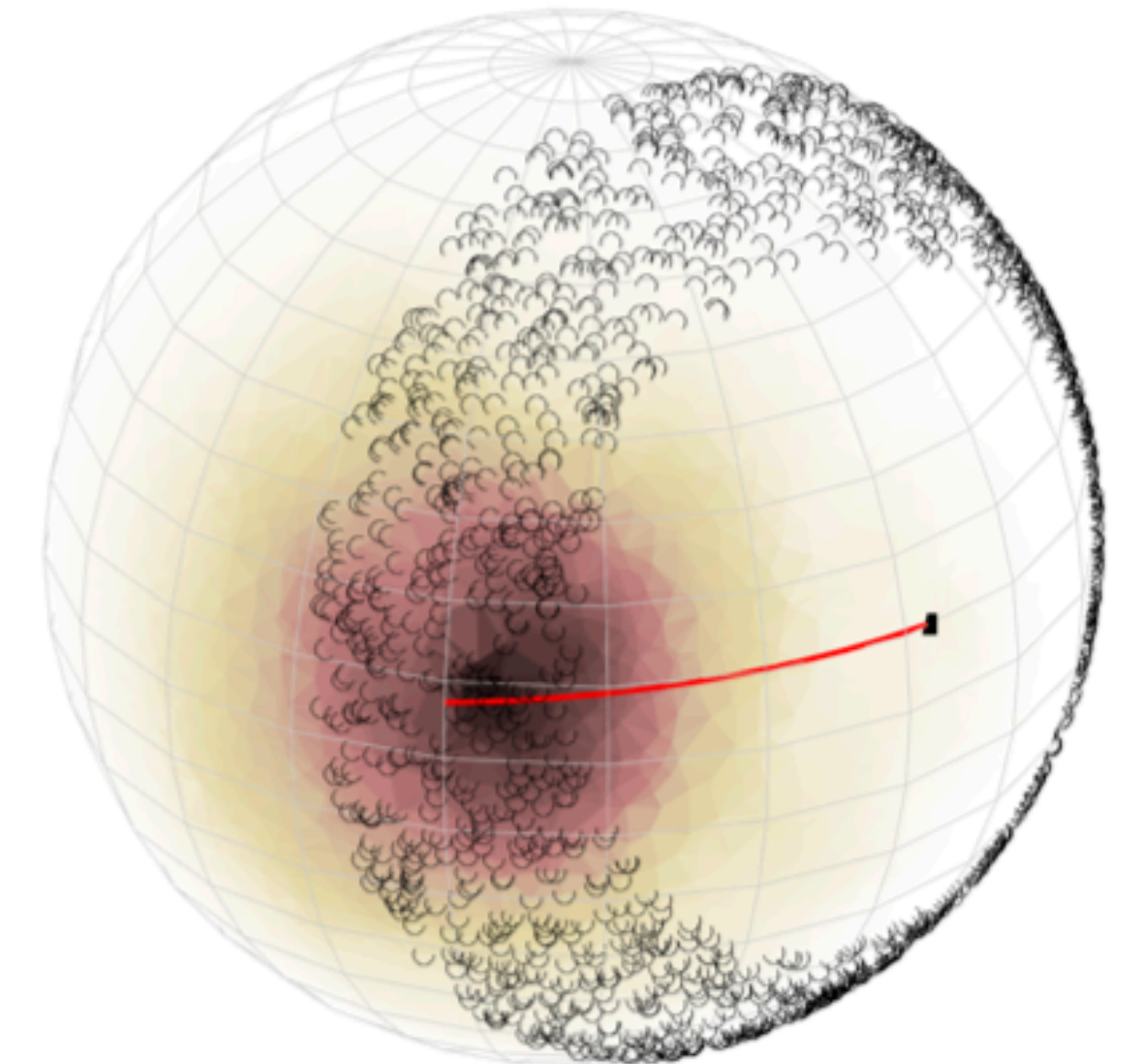


Crane et al., *Comm. ACM* (2017)



with high prob.,

$$h \gg \sqrt{\epsilon}$$



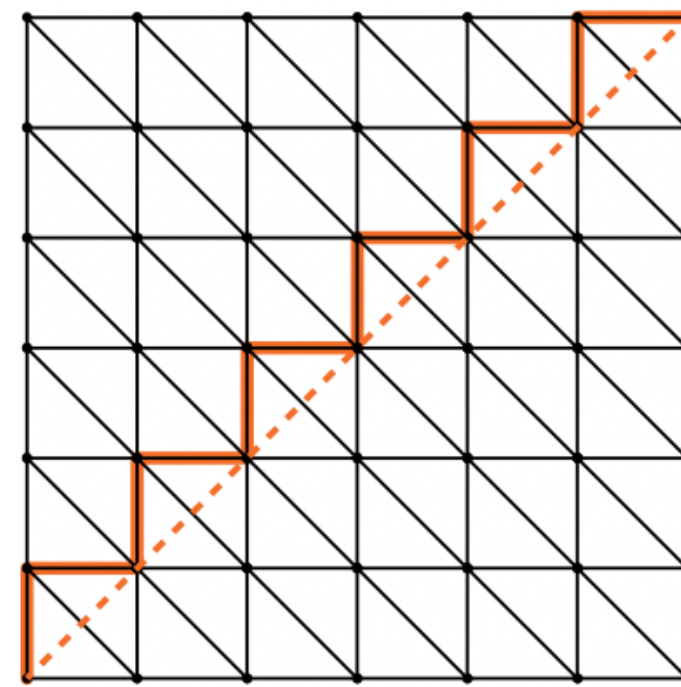


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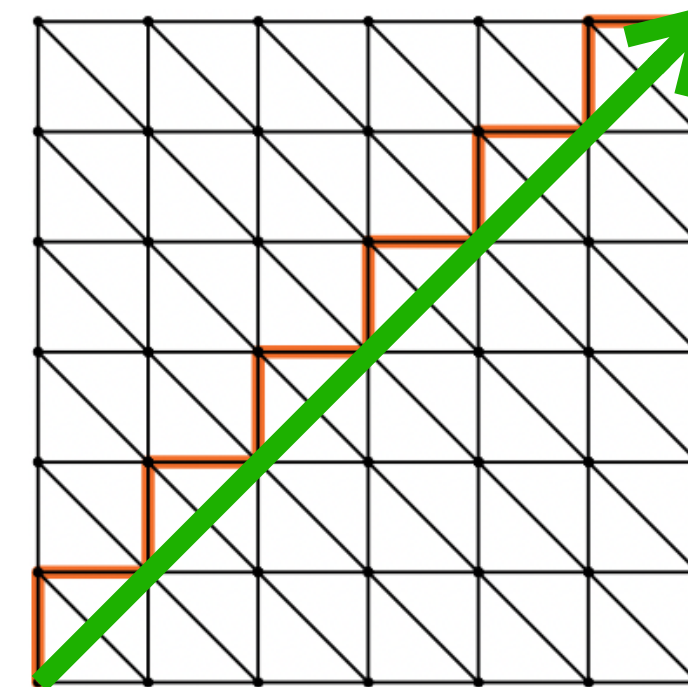
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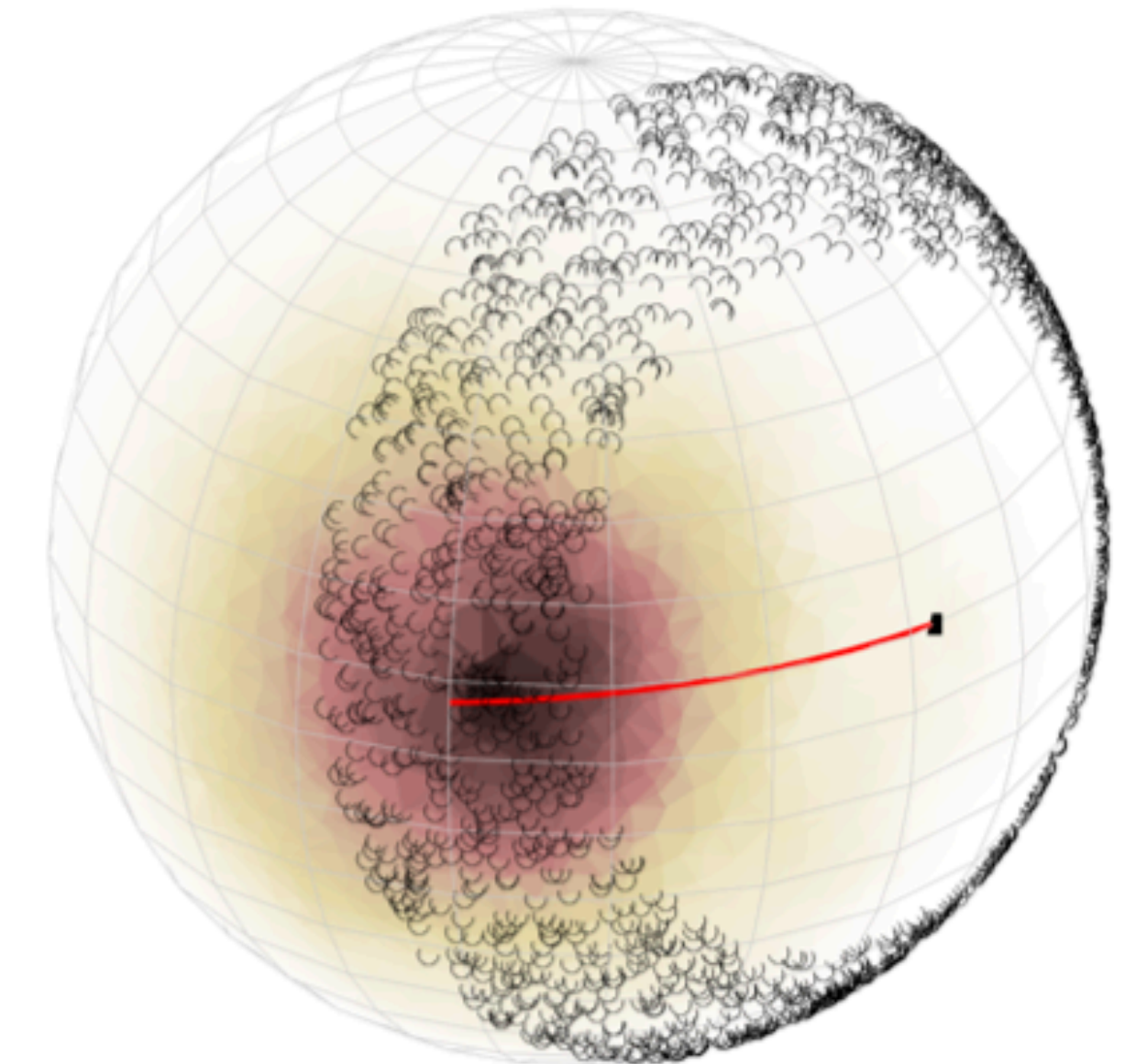


Crane et al., *Comm. ACM* (2017)



with high prob.,

$$h \gg \sqrt{\epsilon}$$



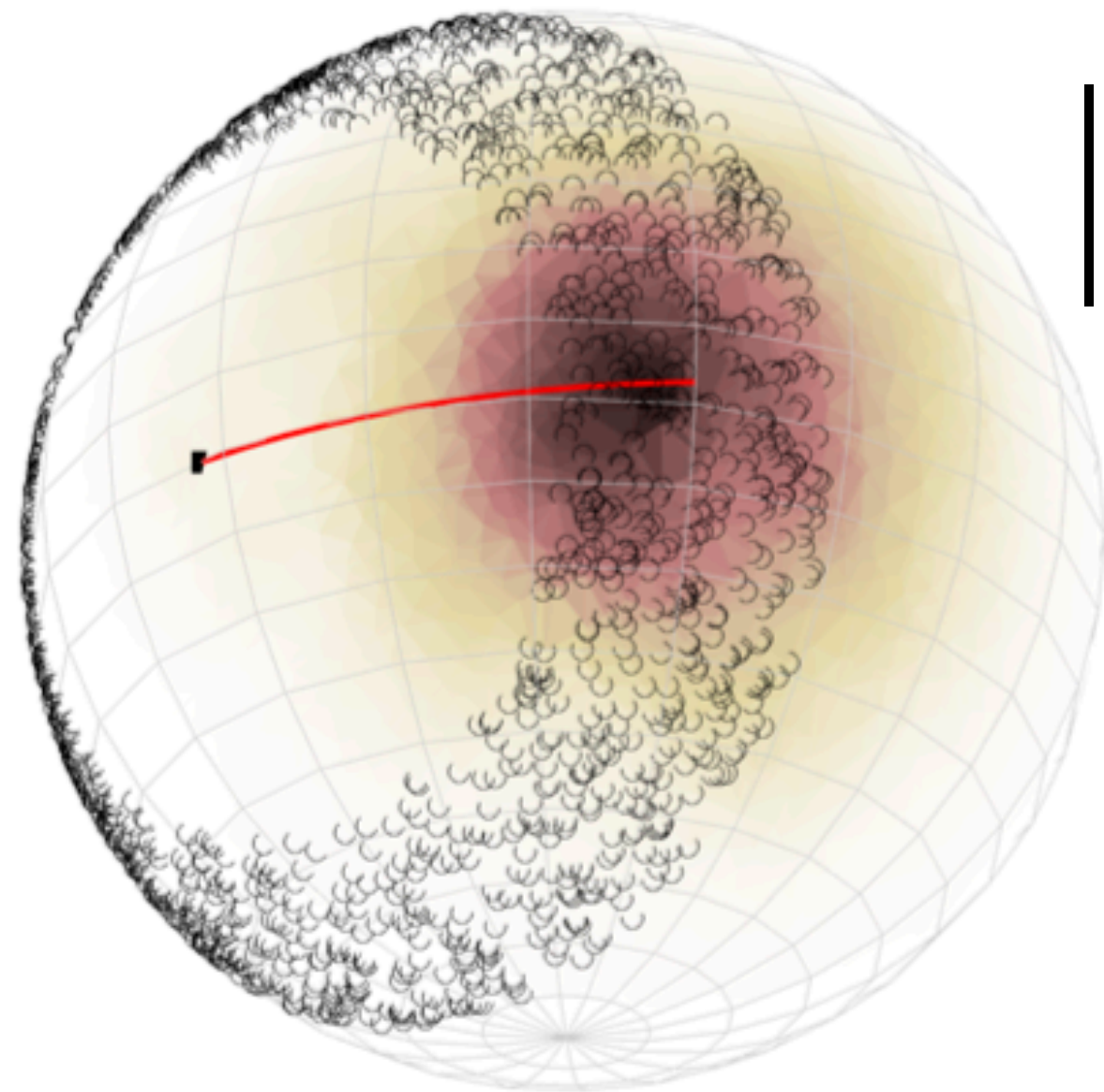
**THEOREM.** IF  $h \gg \sqrt{\epsilon}$ , THEN  $\left| e^{it\sqrt{\Delta_{\epsilon,N}}} |\psi_h^{(x_0, \xi_0)}\rangle \right|^2 = \left| e^{\frac{i}{h}t\sqrt{\hat{H}_h}} |\psi_h^{(x_0, \xi_0)}\rangle \right|^2 + O(h)$

with probability at least  $1 - e^{-\Omega(Nh^\beta)}$  ( $\beta > 0$  a constant). Kumar, arXiv:2112.10748 (2022)



# From **random walks** to quantum dynamics of observables on data

Heisenberg equation  $i\partial_t \text{diag}(a |_{X_N}) = \left[ \sqrt{\Delta}_{\epsilon, N}, \text{diag}(a |_{X_N}) \right]$



$|\psi_h(t)\rangle$

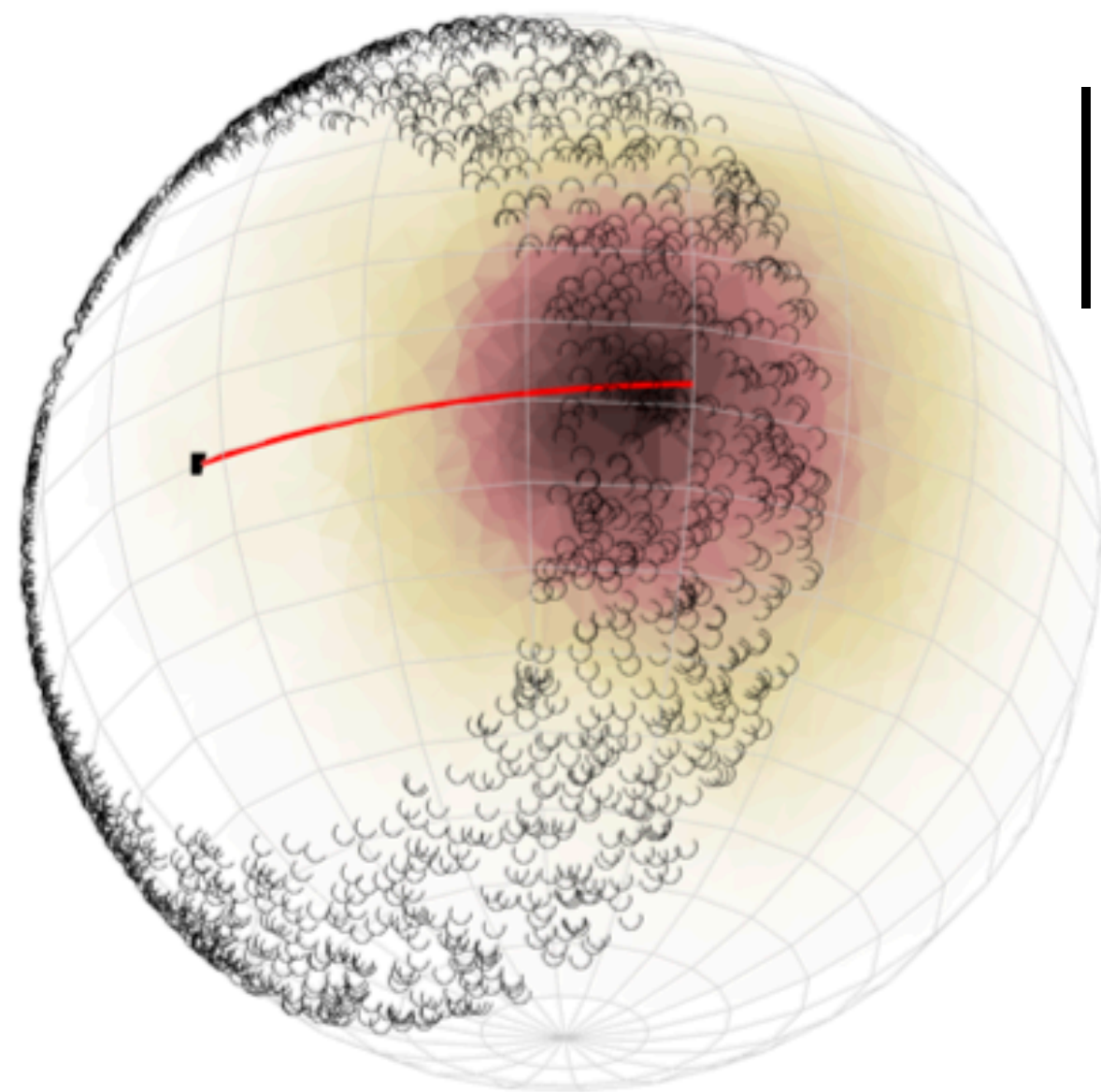
with high prob.,  
 $h \gg \sqrt{\epsilon}$

$a \in C^\infty(\mathcal{M})$

$$\langle \psi_h(t) | \text{diag}(a |_{X_N}) | \psi_h(t) \rangle = a(x(t)) + O(h)$$

# From **random walks** to **quantum dynamics of observables on data**

$$\text{Heisenberg equation } i\partial_t \text{diag}(a |_{X_N}) = \left[ \sqrt{\Delta}_{\epsilon, N}, \text{diag}(a |_{X_N}) \right]$$


 $|\psi_h(t)\rangle$ 

with high prob.,  
 $h \gg \sqrt{\epsilon}$

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$$\langle \psi_h(t) | \text{diag}(a |_{X_N}) | \psi_h(t) \rangle = a(x(t)) + O(h)$$

**THEOREM.** IF  $a \in C^\infty(\mathcal{M})$  AND  $h \gg \sqrt{\epsilon}$ , THEN  $\langle \psi_h(t) | \text{diag}(a |_{X_N}) | \psi_h(t) \rangle = a(x(t)) + O(h)$

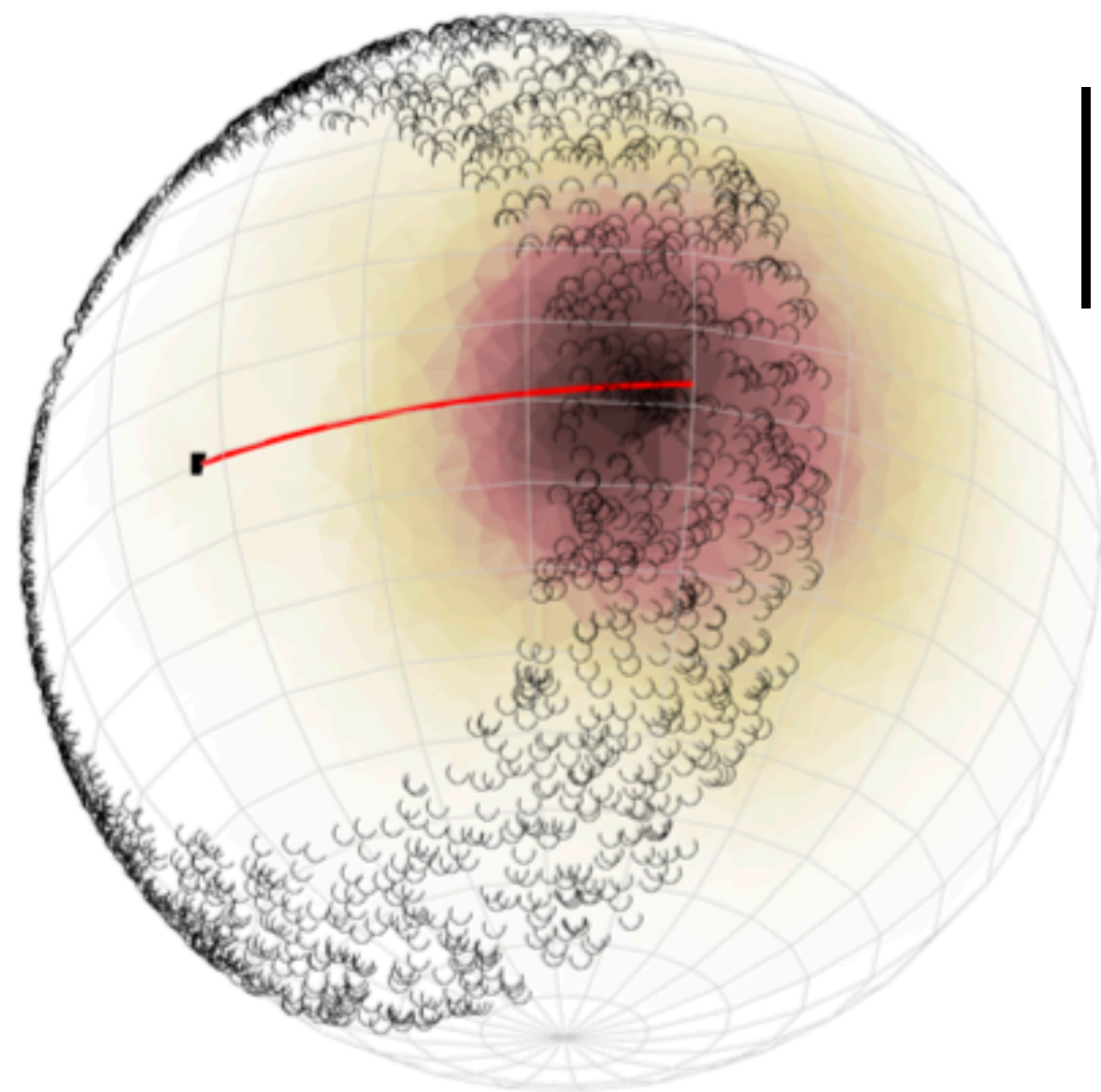
with probability at least  $1 - e^{-\Omega(Nh^\beta)}$  ( $\beta > 0$  a constant).

Kumar, arXiv:2112.10748 (2022)



# From **random walks** to **quantum dynamics of observables on data**

Heisenberg equation  $i\partial_t \text{diag}(a |_{X_N}) = \left[ \sqrt{\Delta}_{\epsilon, N}, \text{diag}(a |_{X_N}) \right]$



$|\psi_h(t)\rangle$

with high prob.,  
 $h \gg \sqrt{\epsilon}$

$a \in C^\infty(\mathcal{M})$

$$\langle \psi_h(t) | \text{diag}(a |_{X_N}) | \psi_h(t) \rangle = a(x(t)) + O(h)$$

Microlocal analysis  $\cap$  geometry  $\cap$  markov processes  
 $\cap$  probability/statistics  $\cap$  quantum dynamics

**THEOREM.** IF  $a \in C^\infty(\mathcal{M})$  AND  $h \gg \sqrt{\epsilon}$ , THEN  $\langle \psi_h(t) | \text{diag}(a |_{X_N}) | \psi_h(t) \rangle = a(x(t)) + O(h)$

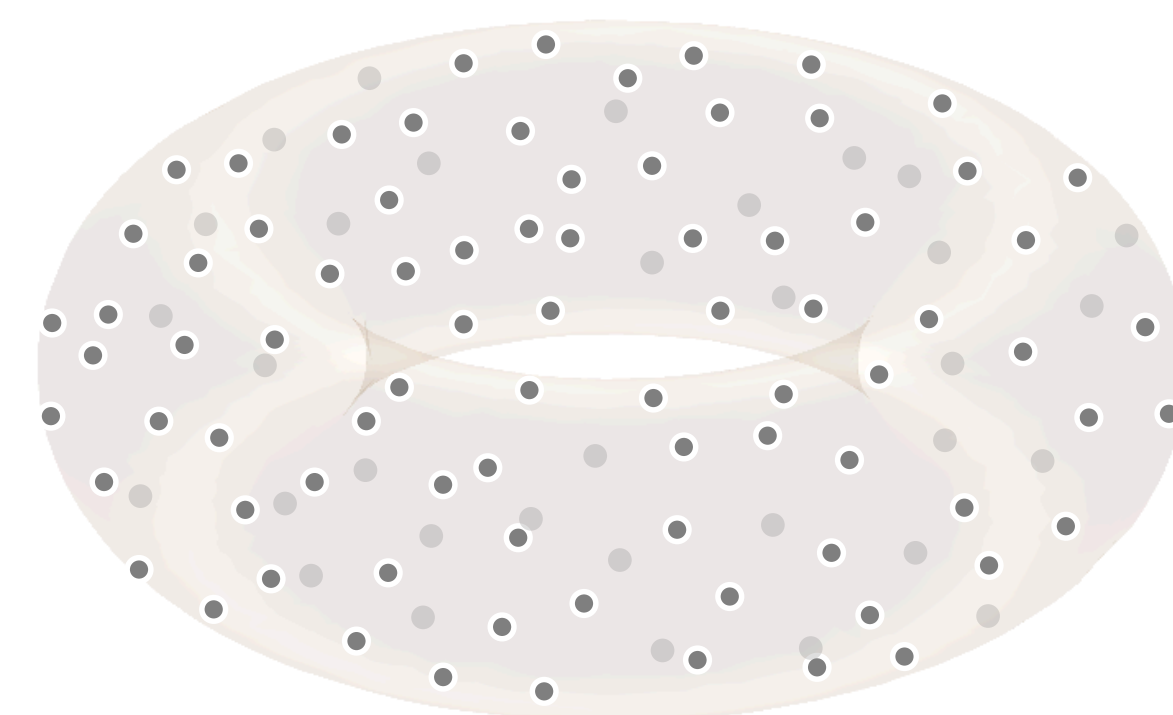
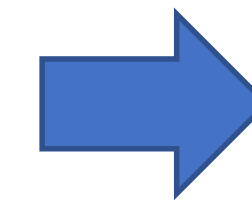
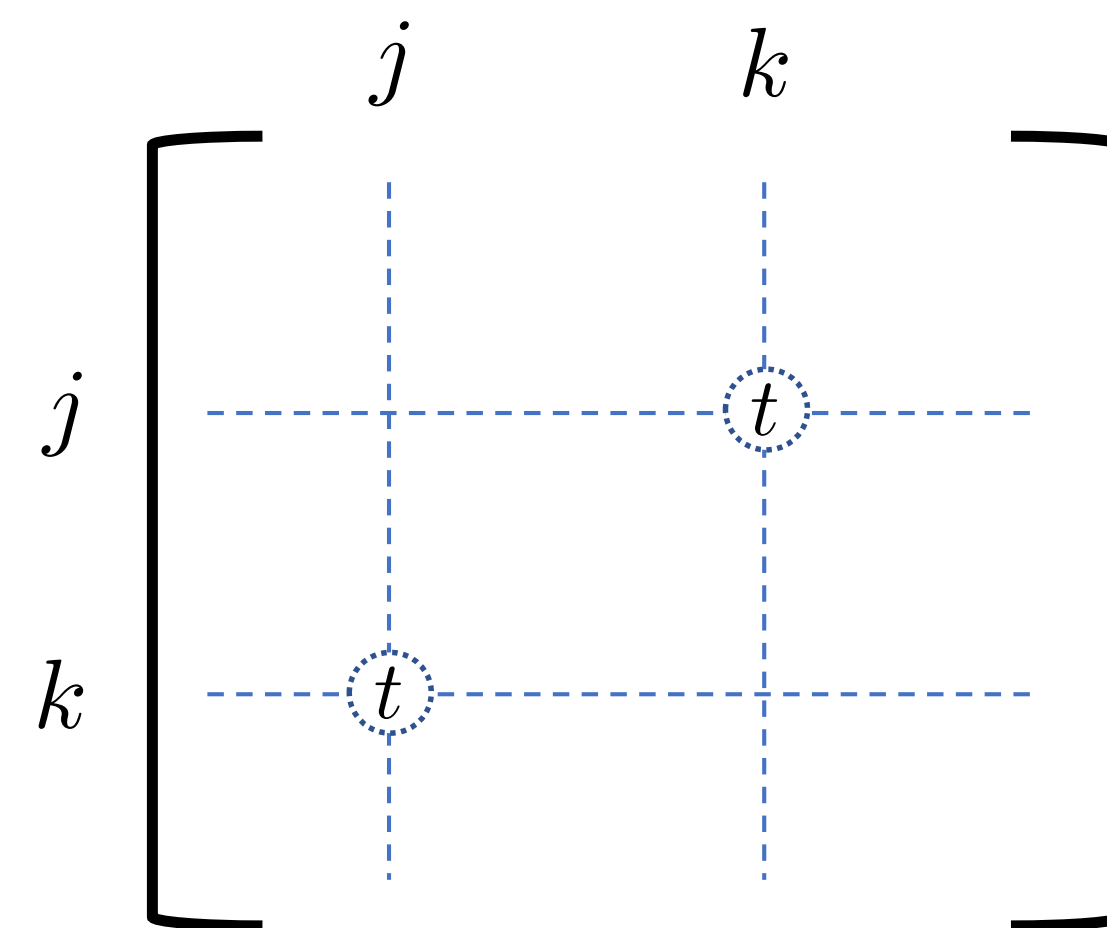
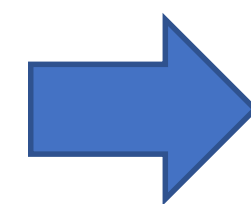
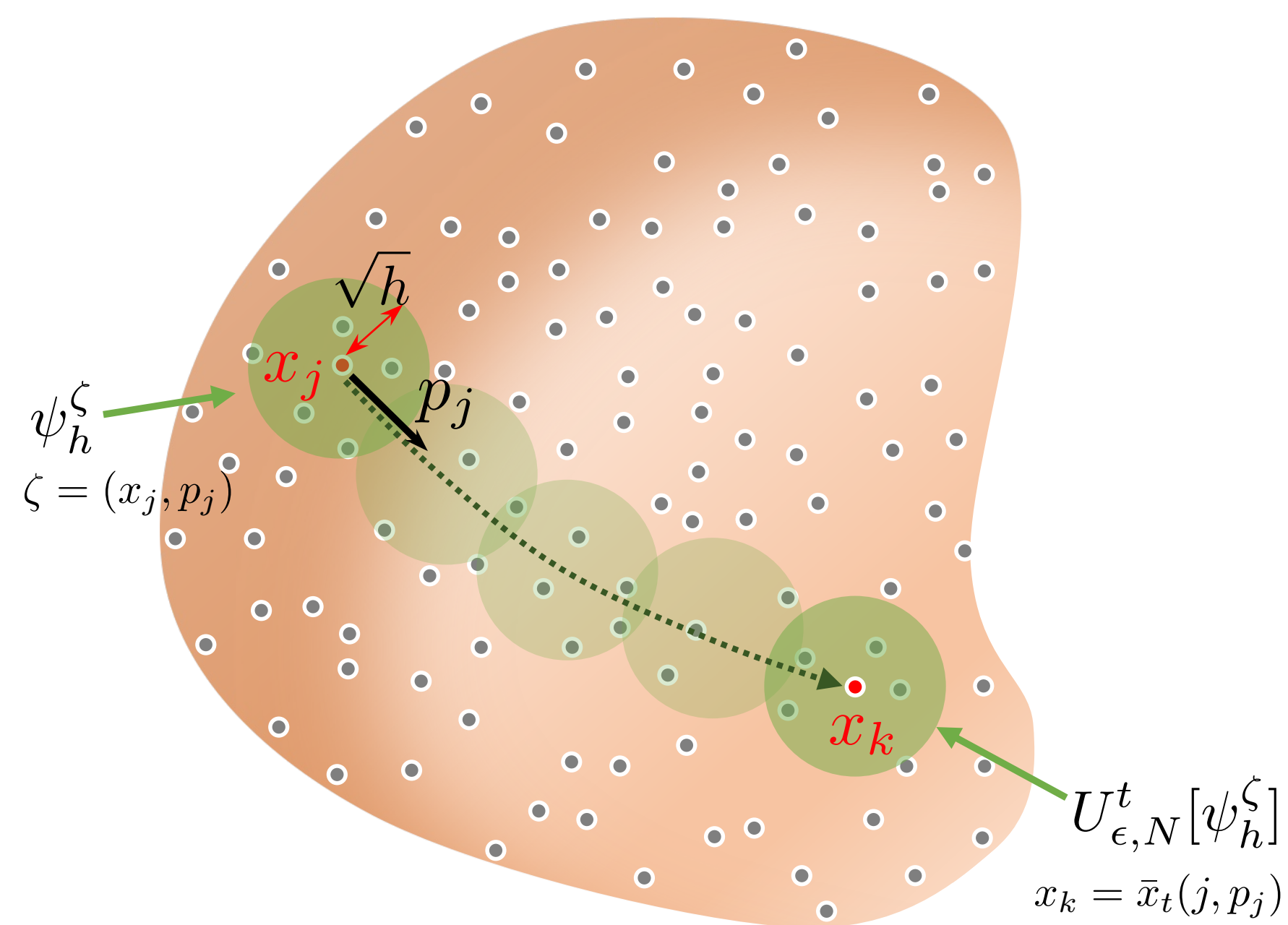
with probability at least  $1 - e^{-\Omega(Nh^\beta)}$  ( $\beta > 0$  a constant).

Kumar, arXiv:2112.10748 (2022)

# Applications



# Quantum dynamical *reach-time* embedding of datasets



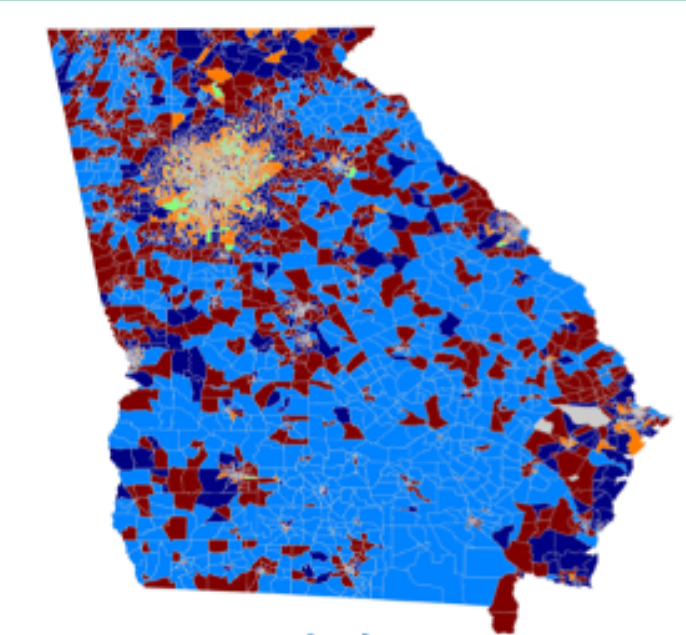
Cross-section of dataset of size  $N$  in  $\mathbb{R}^n$

$\mathcal{G}$  ( $N \times N$  matrix)

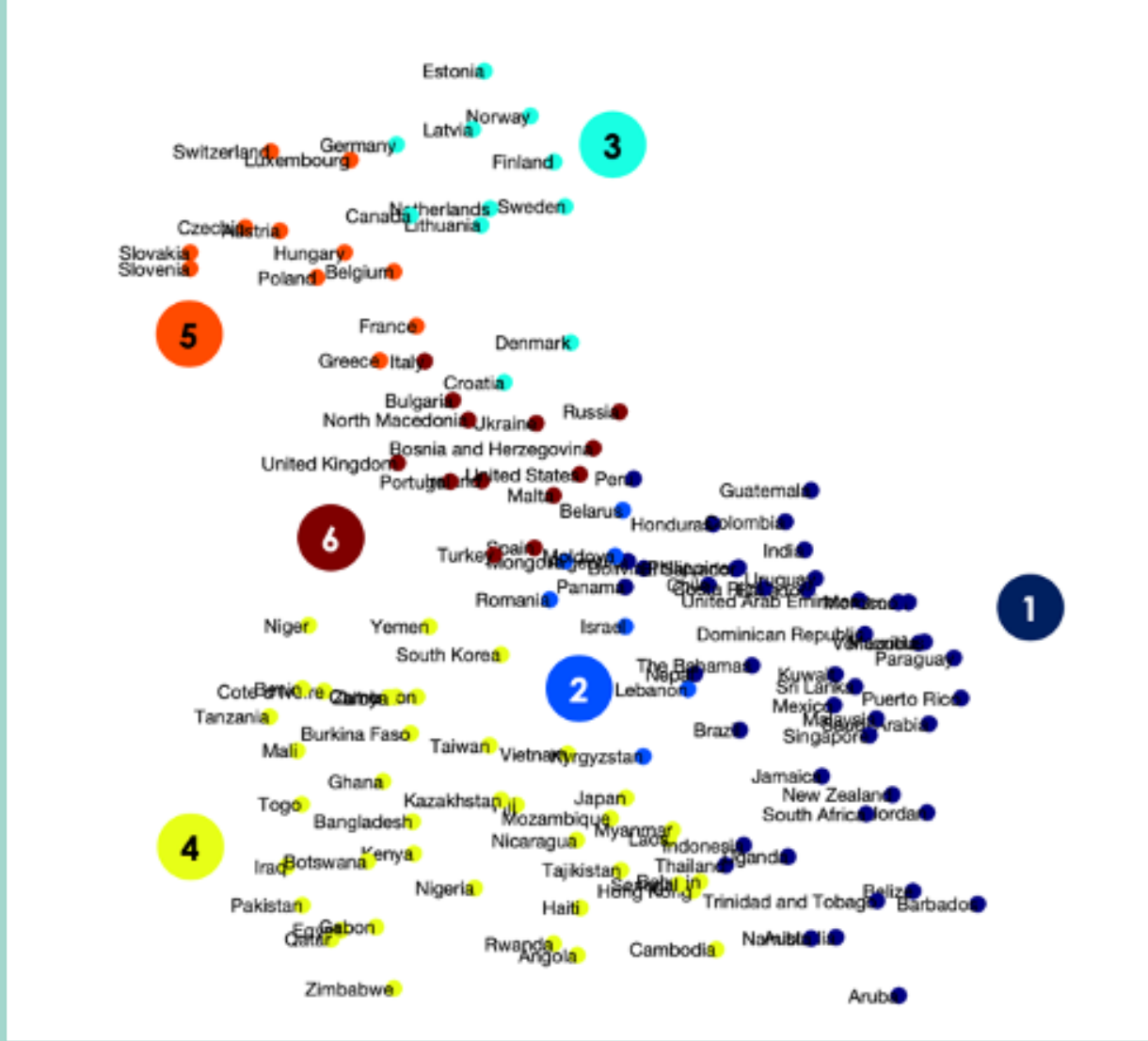
Graph embedding of dataset  
in  $\mathbb{R}^3$  based on weighted  
adjacency matrix  $\mathcal{G}$

# Example applications

Clustering of geographic regions according to COVID-19 social distancing behavior

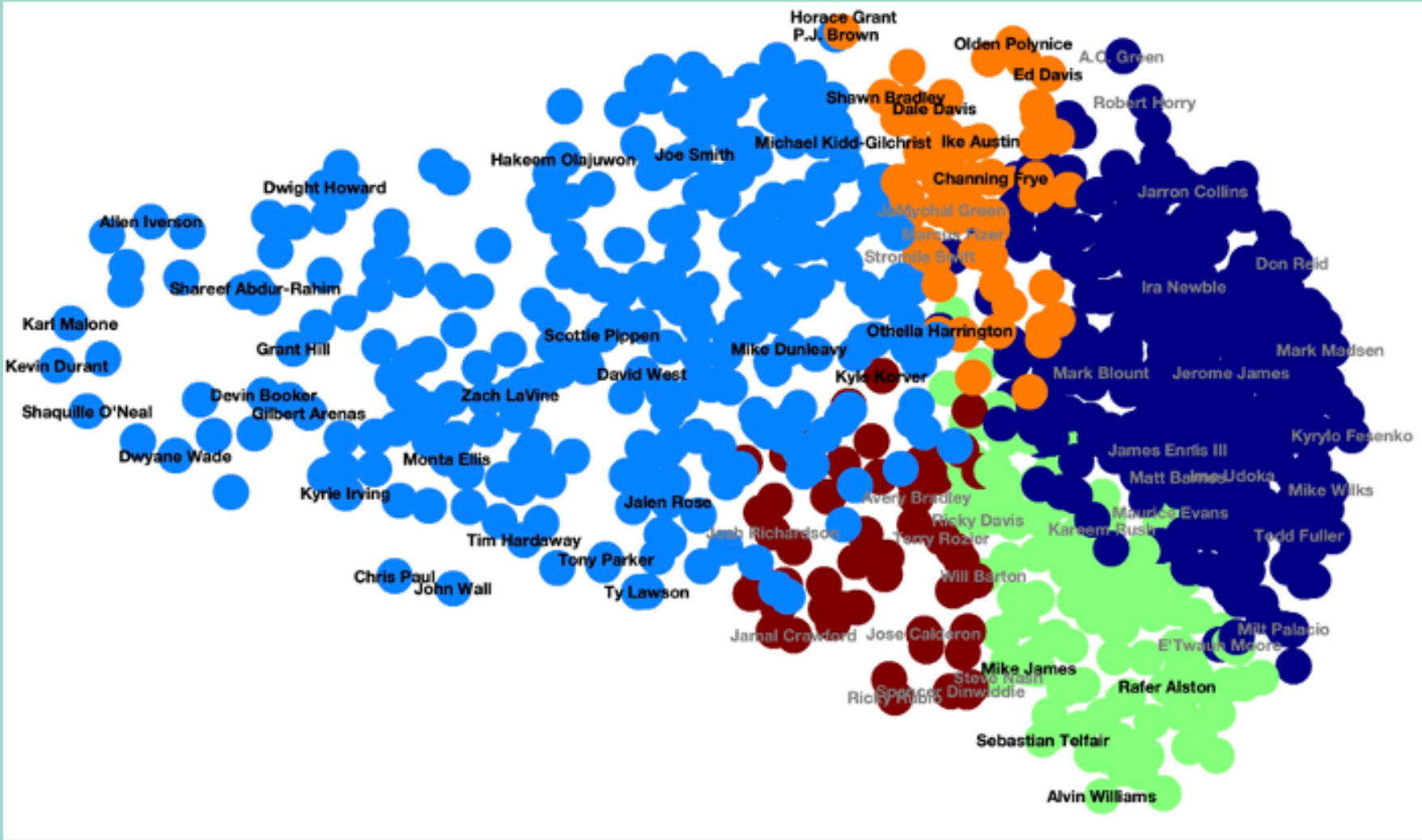


SafeGraph dataset for state of GA



Google dataset for worldwide mobility patterns

Clustering of NBA players based on performance



- NOTES:
- 1. Manifold hypothesis not necessary for utility
  - 2. Some of these datasets are small (e.g.,  $N = 126$ )

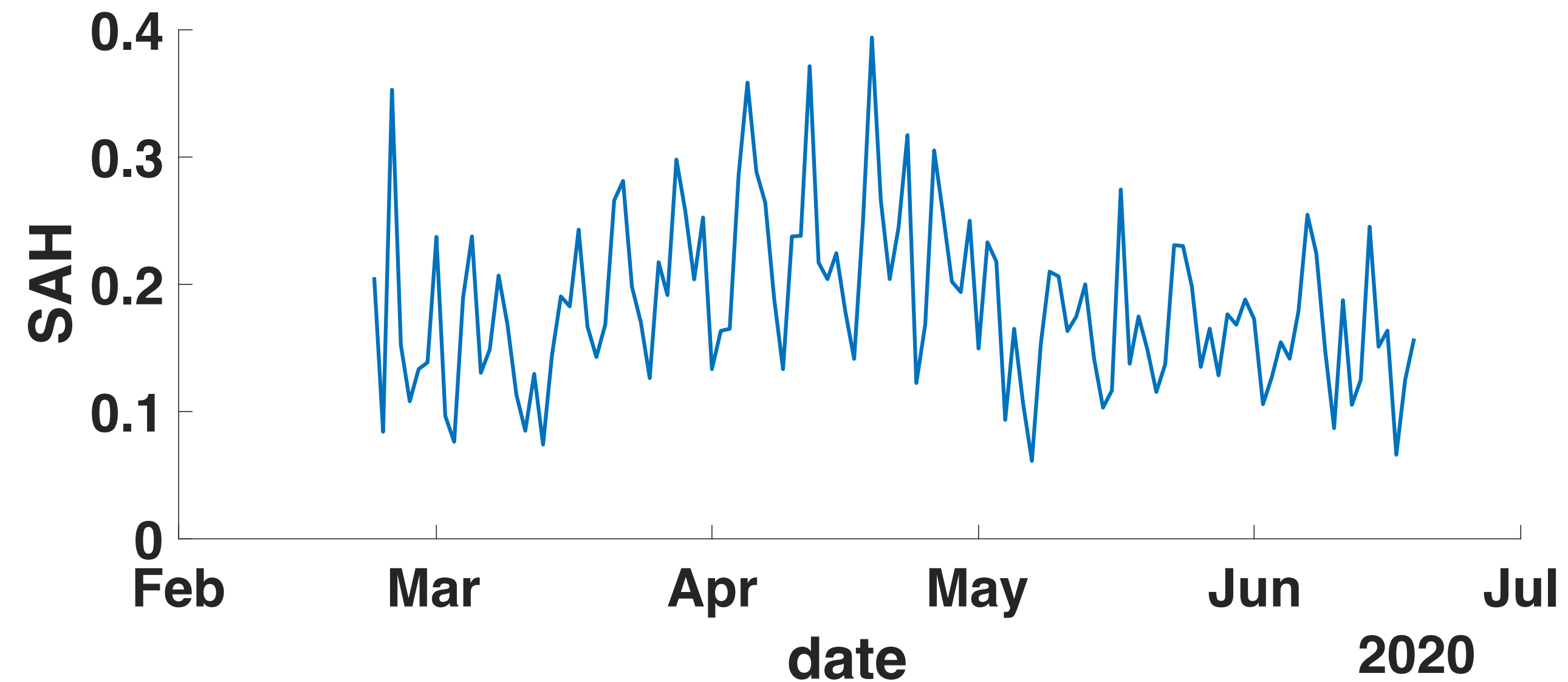
See "Manifold learning via quantum dynamics." A. Kumar & M. Sarovar. arXiv:2112.11161 (2021)



# Example: COVID-19 mobility data

Social Distancing Metric dataset from SafeGraph Inc.  
<https://docs.safegraph.com/docs/social-distancing-metrics>

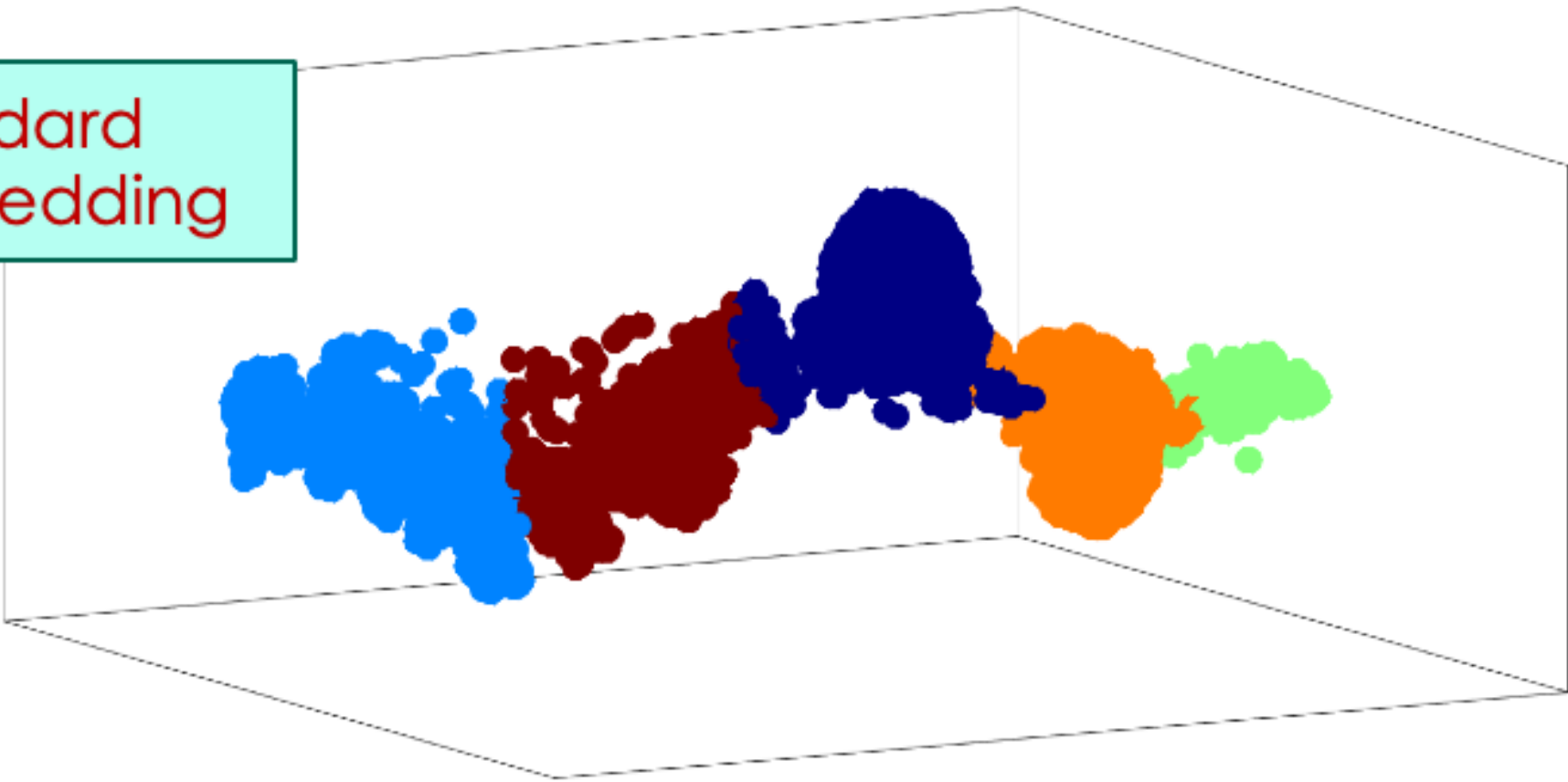
- Dataset collects user location information (from cellphone GPS data) over the course of the initial ~3 months of the COVID-19 pandemic (Feb 23, 2020 – June 19, 2020: 117 days).
- Data aggregated at the census block group (CBG) level.
- We compute a “stay-at-home” fraction for each CBG, which represents the fraction of devices that stayed at their home location on a day.
- We concentrate on the data for Georgia (GA), which has 5509 CBGs.
- Dataset: 5509 x 117



# Example: COVID-19 mobility data

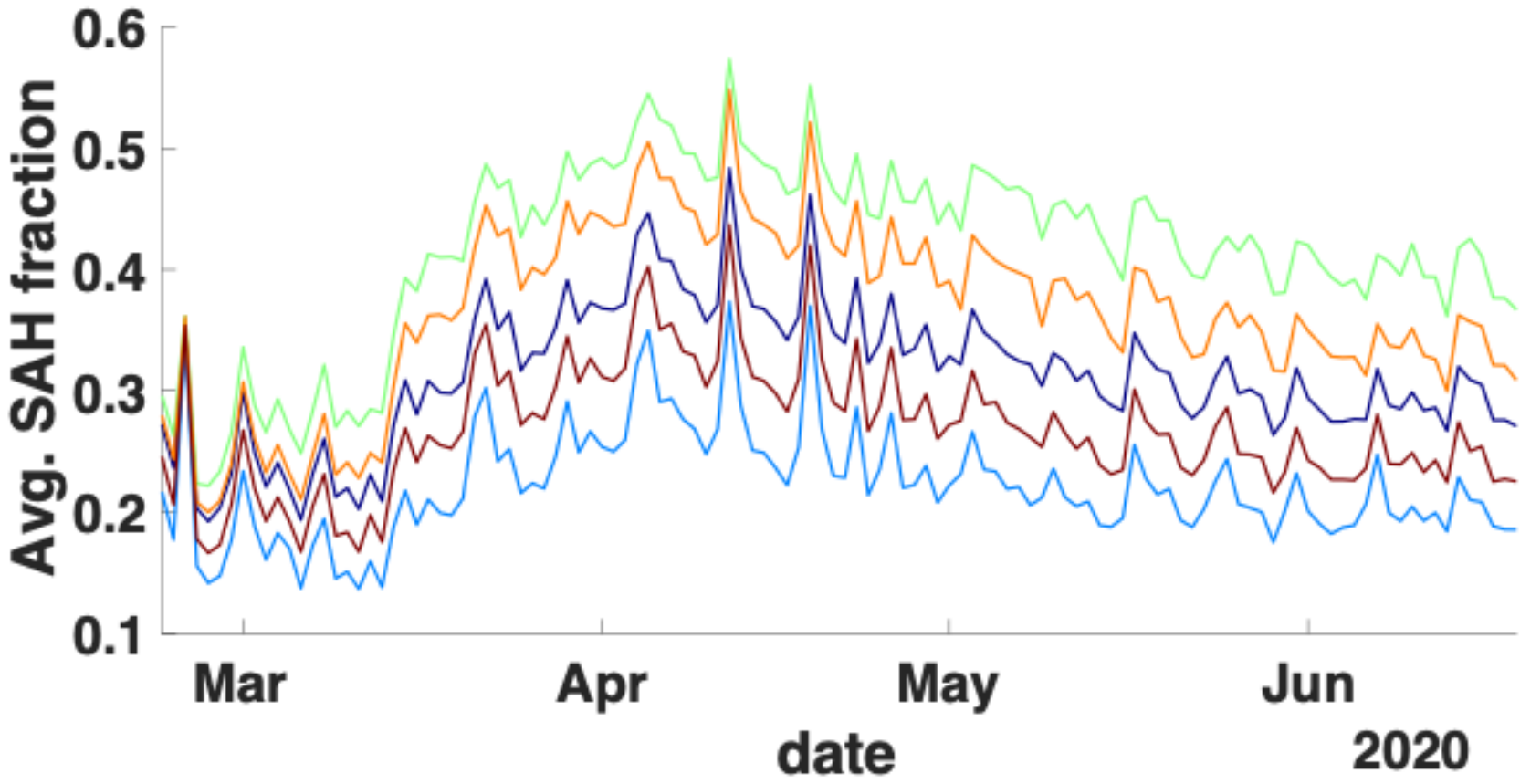
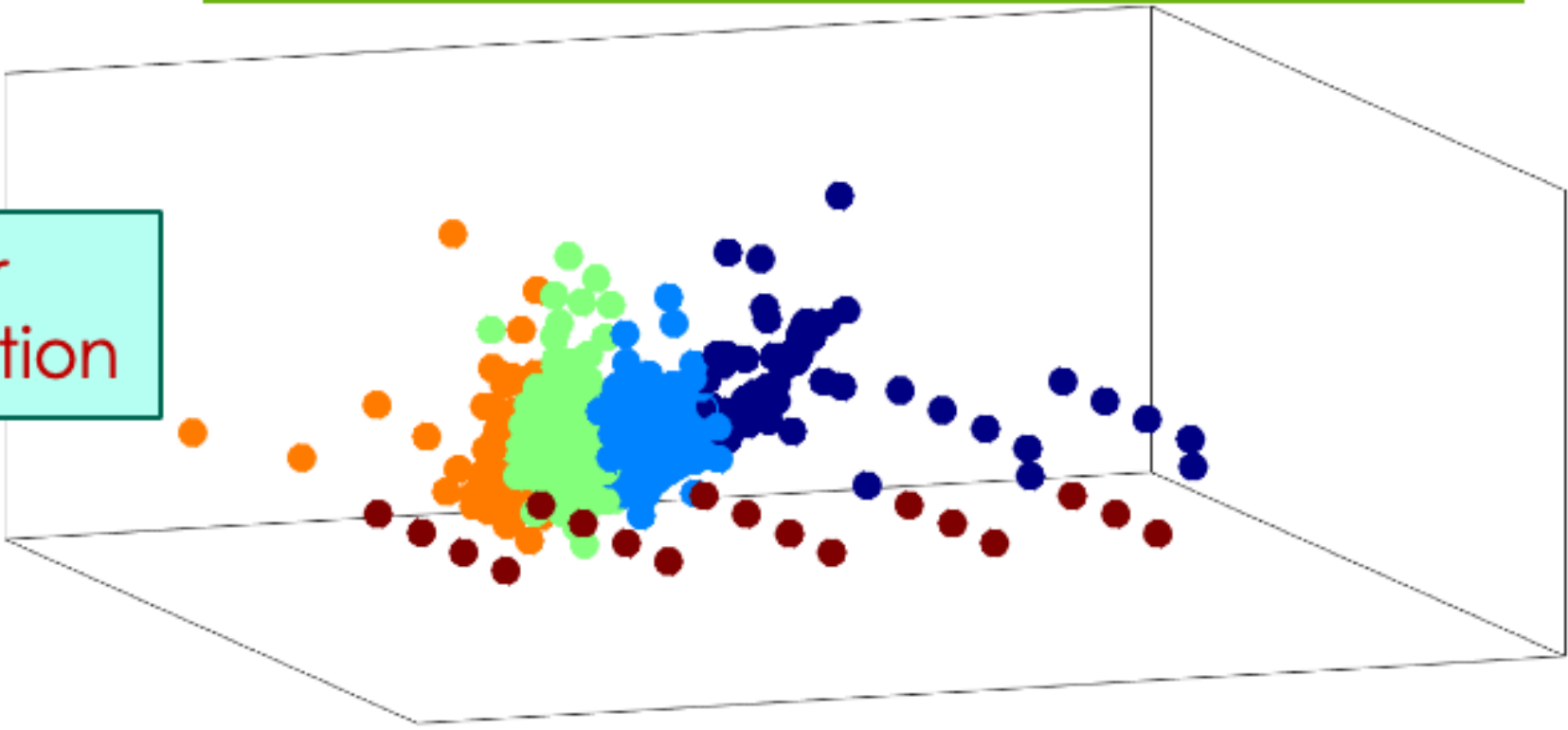
Social Distancing Metric dataset from SafeGraph Inc.  
<https://docs.safegraph.com/docs/social-distancing-metrics>

Standard embedding

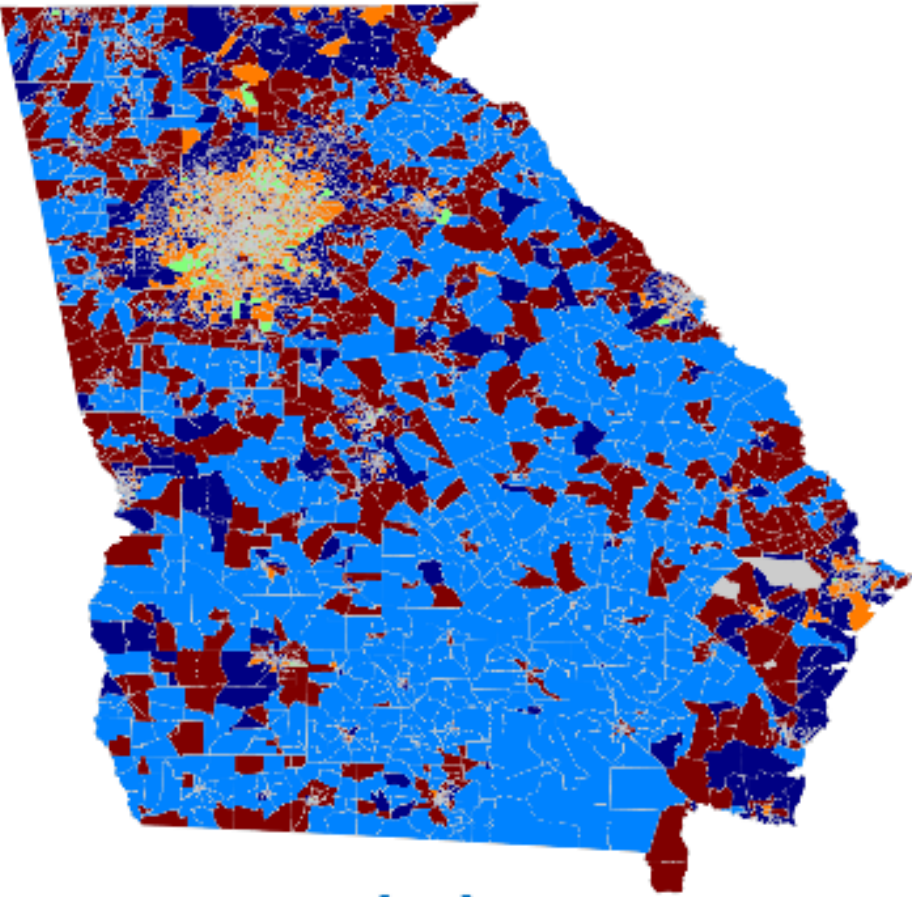
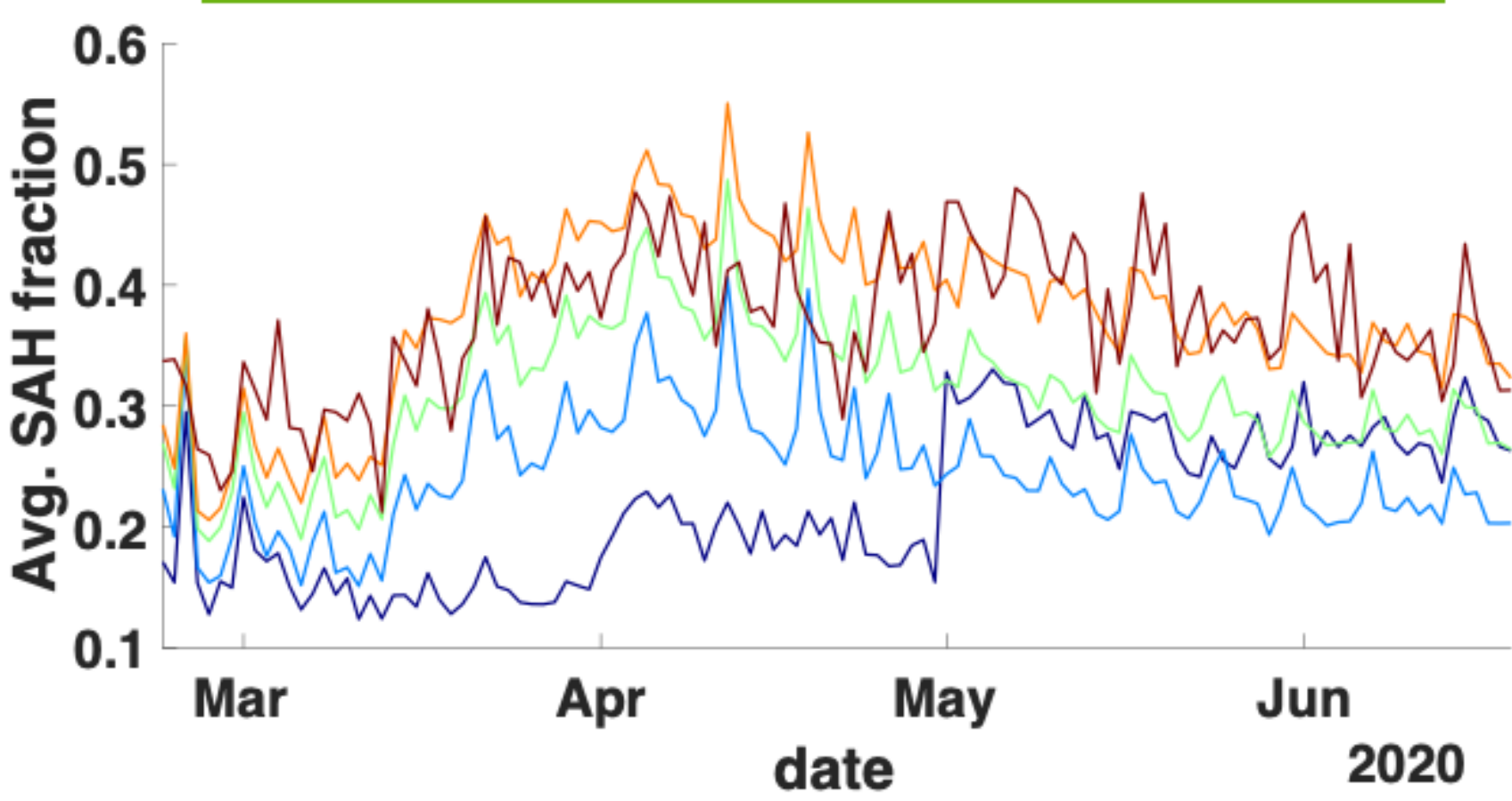


Embedding in 3D and k-means using these 3D coordinates

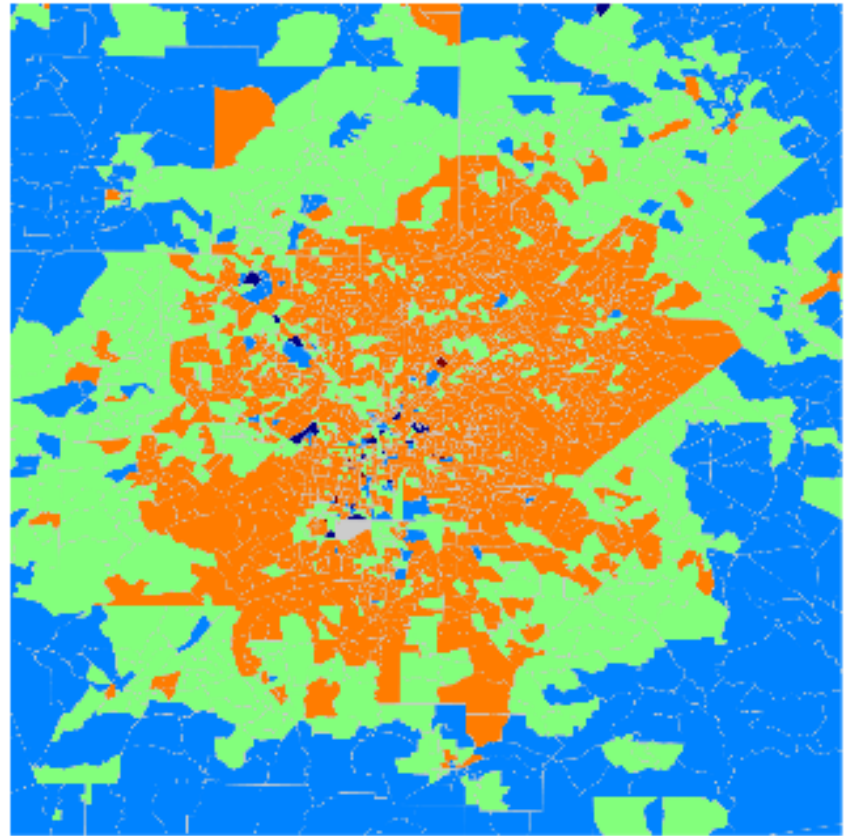
Outlier detection



Average SAH fraction time series for each cluster



(c)



(f)

(d)

(e)

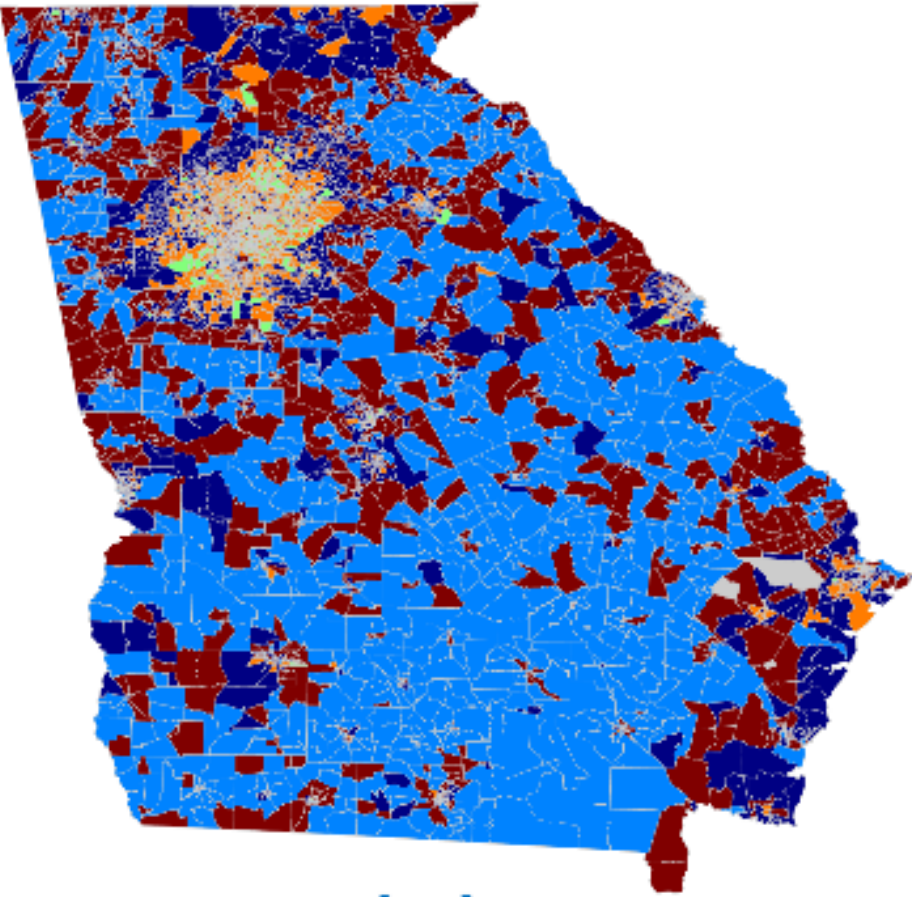
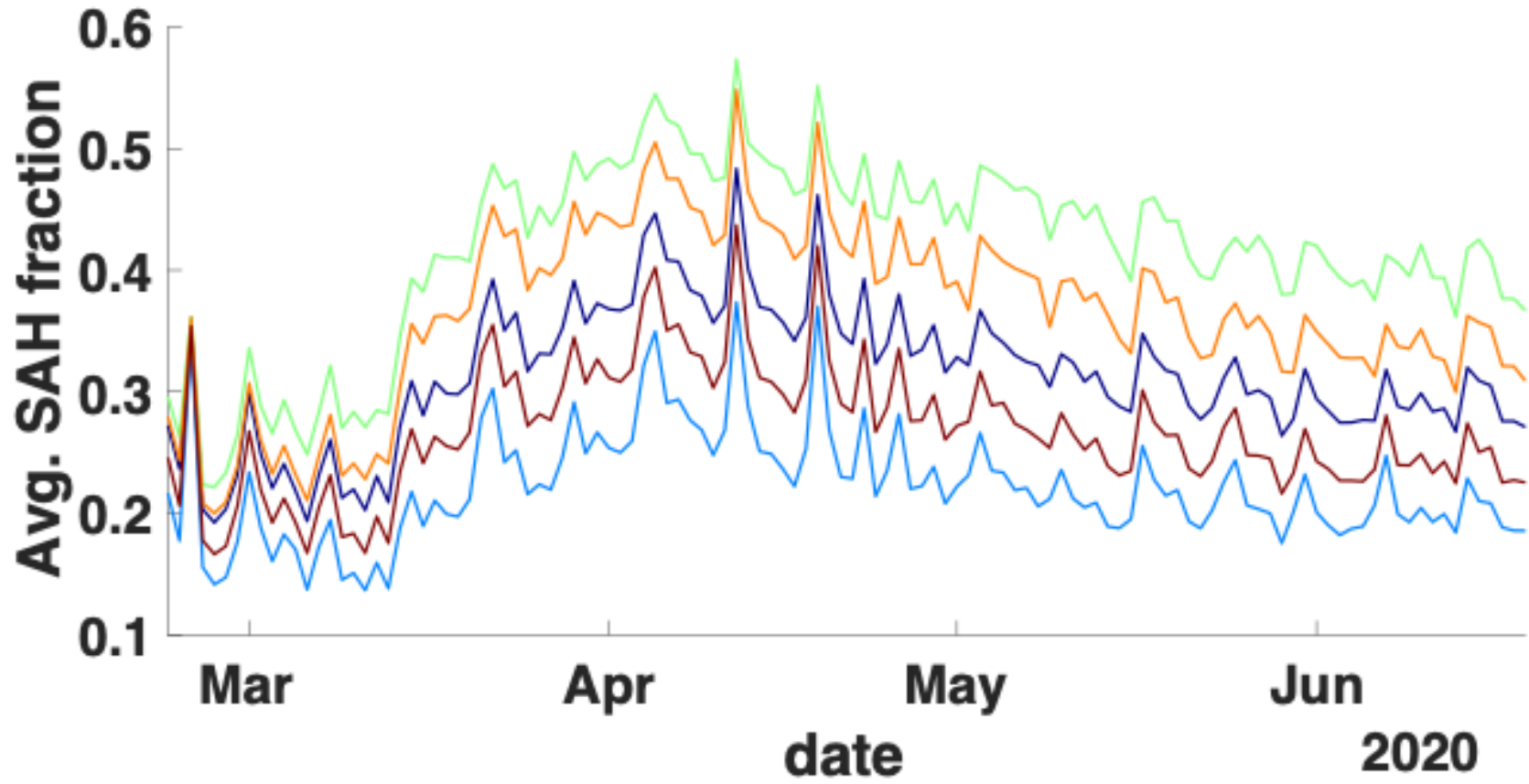
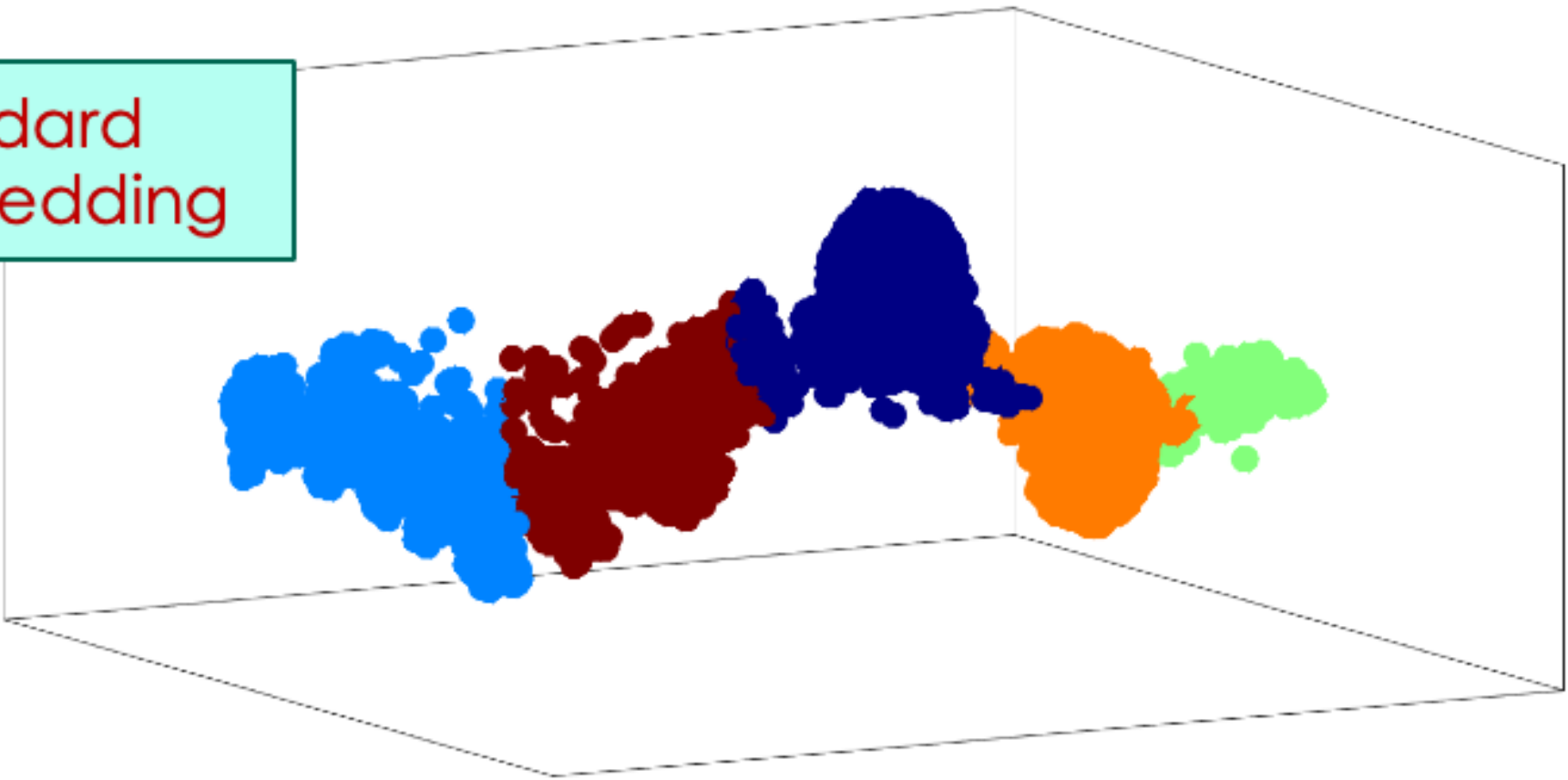
Outlier (1.2% of data)



# Example: COVID-19 mobility data

Social Distancing Metric dataset from SafeGraph Inc.  
<https://docs.safegraph.com/docs/social-distancing-metrics>

Standard embedding



Embedding in 2D and clustering using

Average SAH fraction time series for

(c)

c.f. Levin et al., "Cell Phone Mobility Data and Manifold Learning." <https://doi.org/10.1101/2020.10.31.20223776>

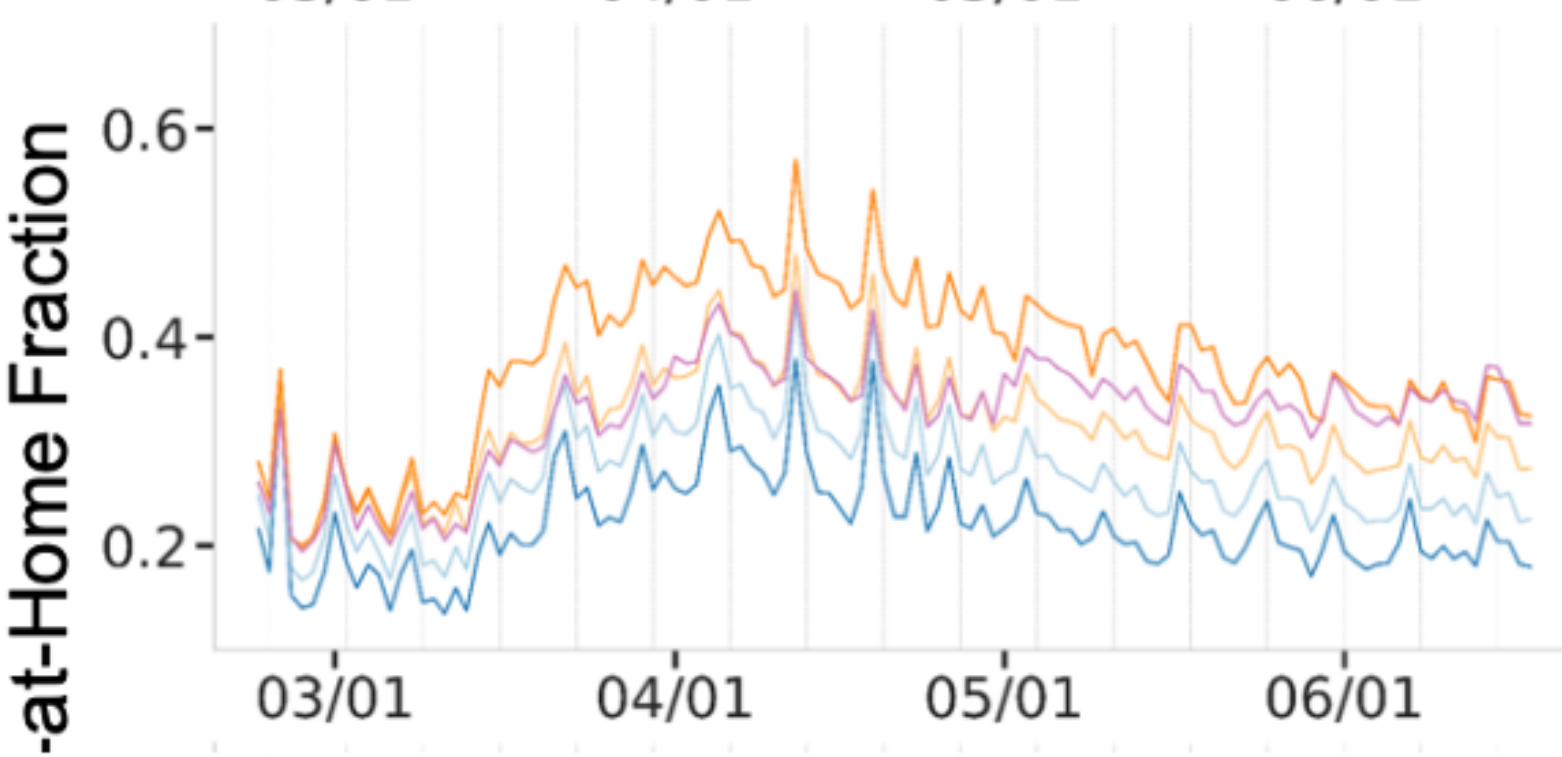
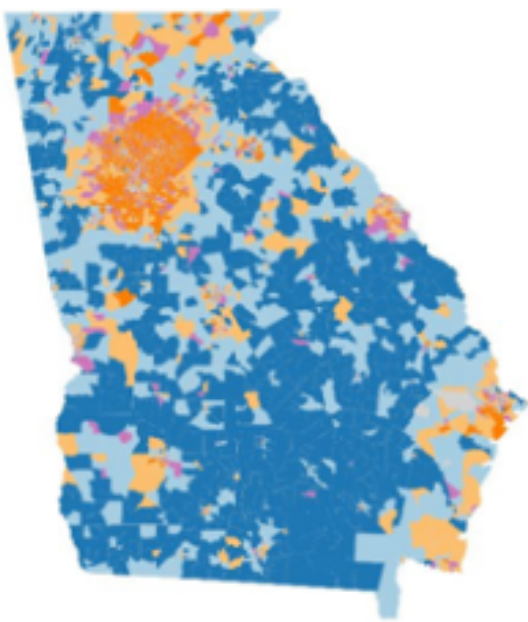


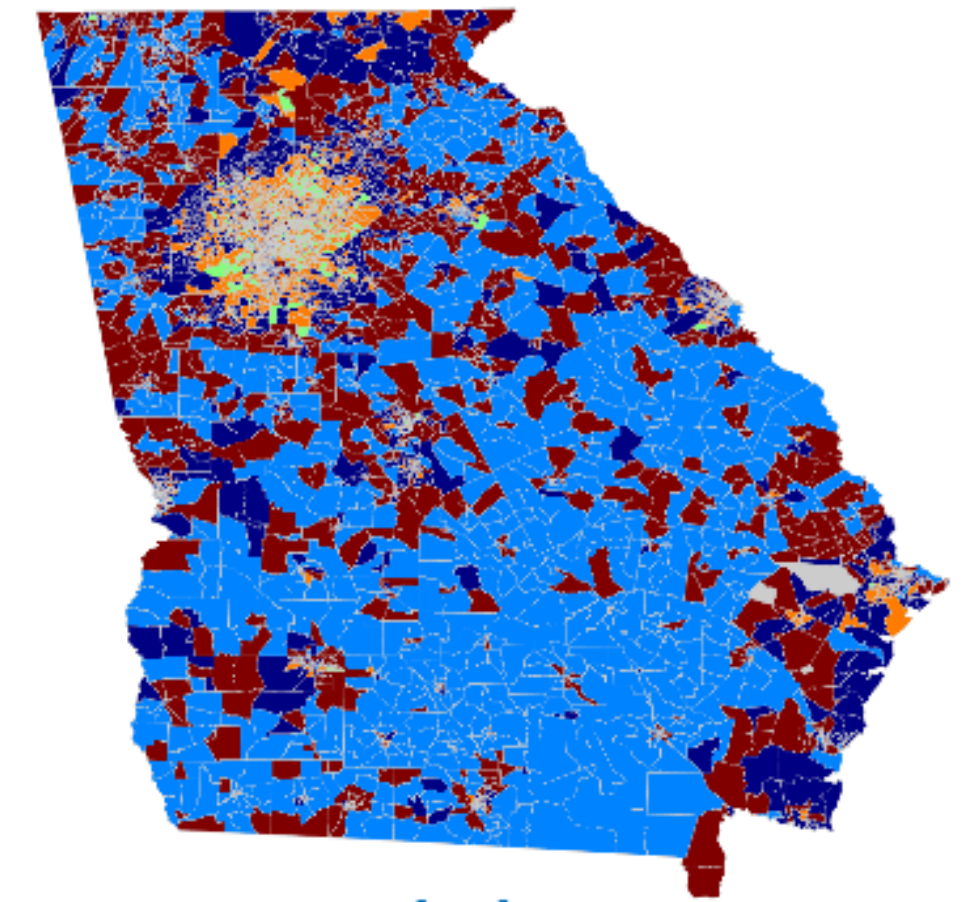
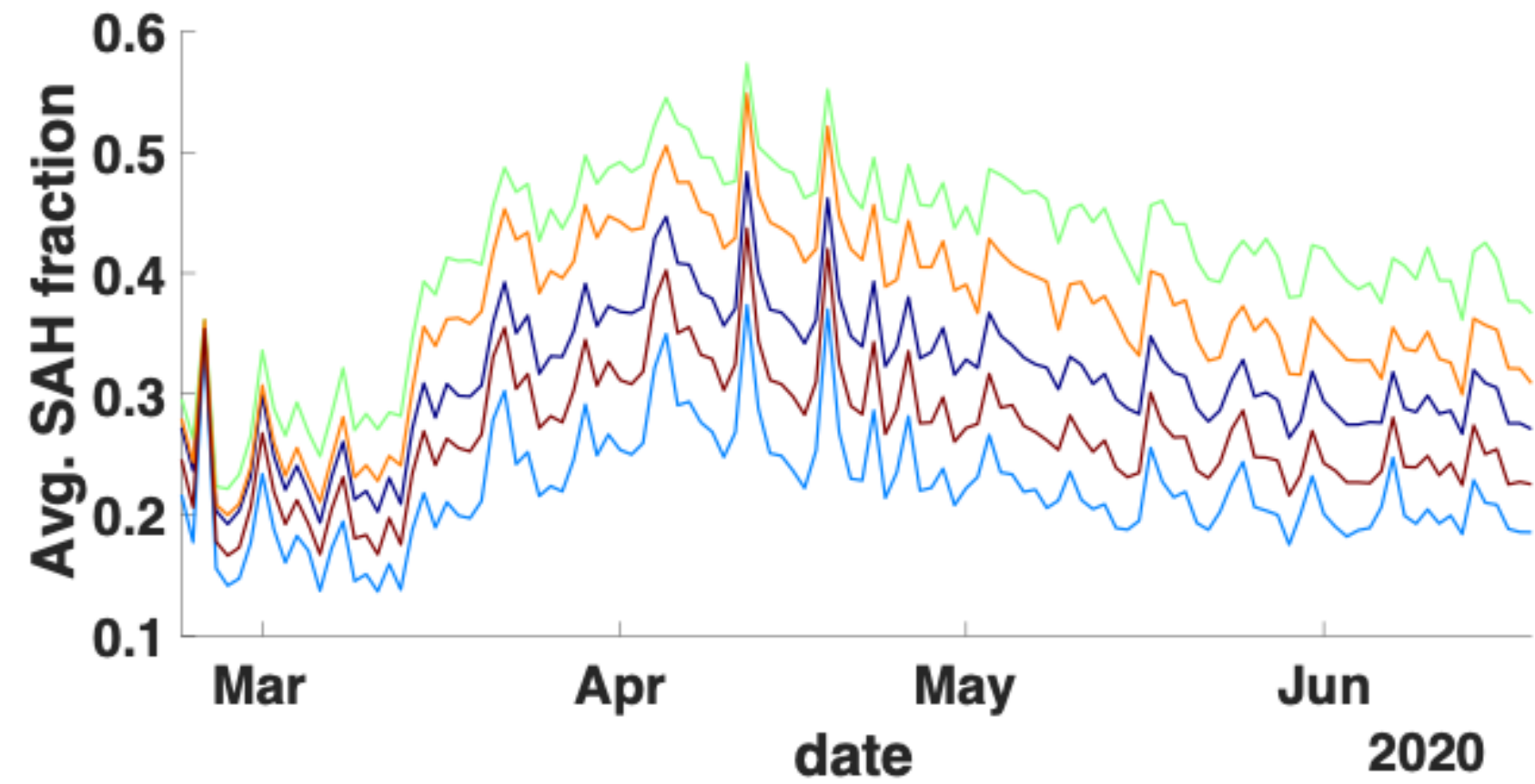
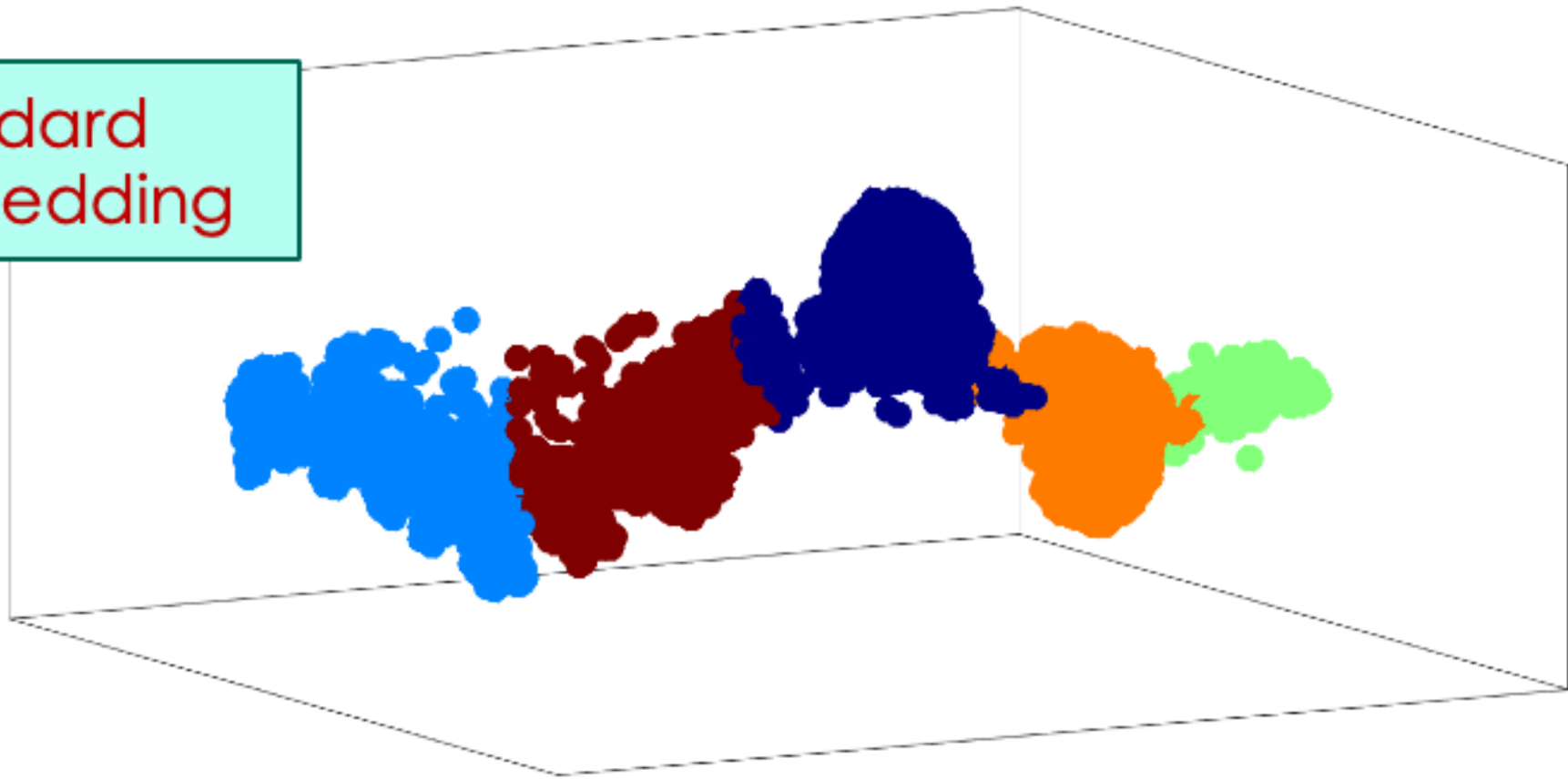
Figure 2: Laplacian eigenmaps, clustering done after embedding in **14 dimensions**



# Example: COVID-19 mobility data

Social Distancing Metric dataset from SafeGraph Inc.  
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Standard embedding

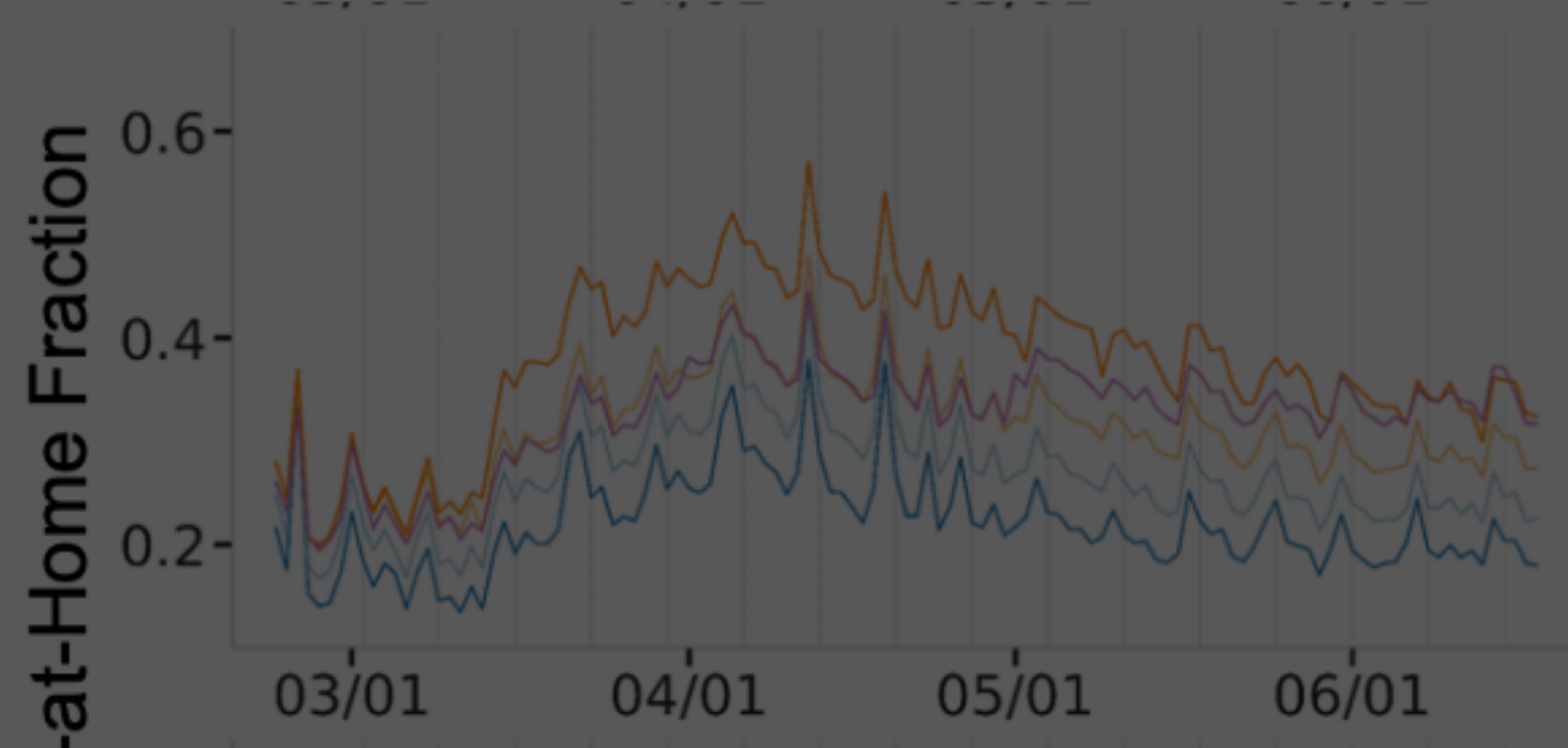
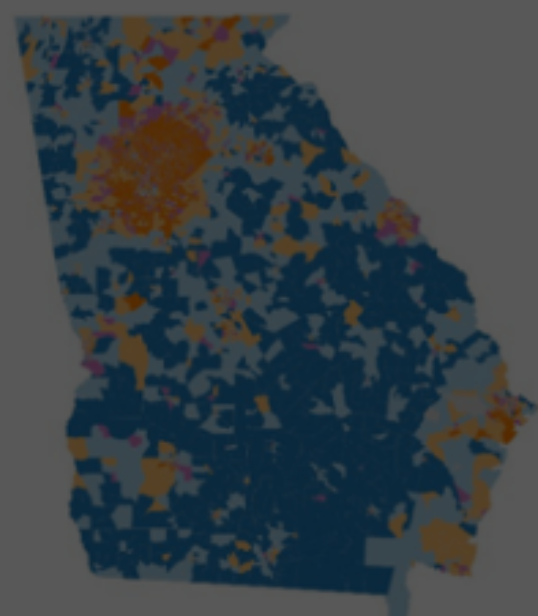


Embedding in 2D and 3D using

Average SAH fraction time series for

(c)

c.f. Levin et al., "Cell Phone Mobility Data and Manifold Learning." <https://doi.org/10.1101/2020.10.31.20223776>



We achieve better quality clustering and are able to identify outliers, even with an embedding into 3 dimensions (**reduction from 117 dimensions**)

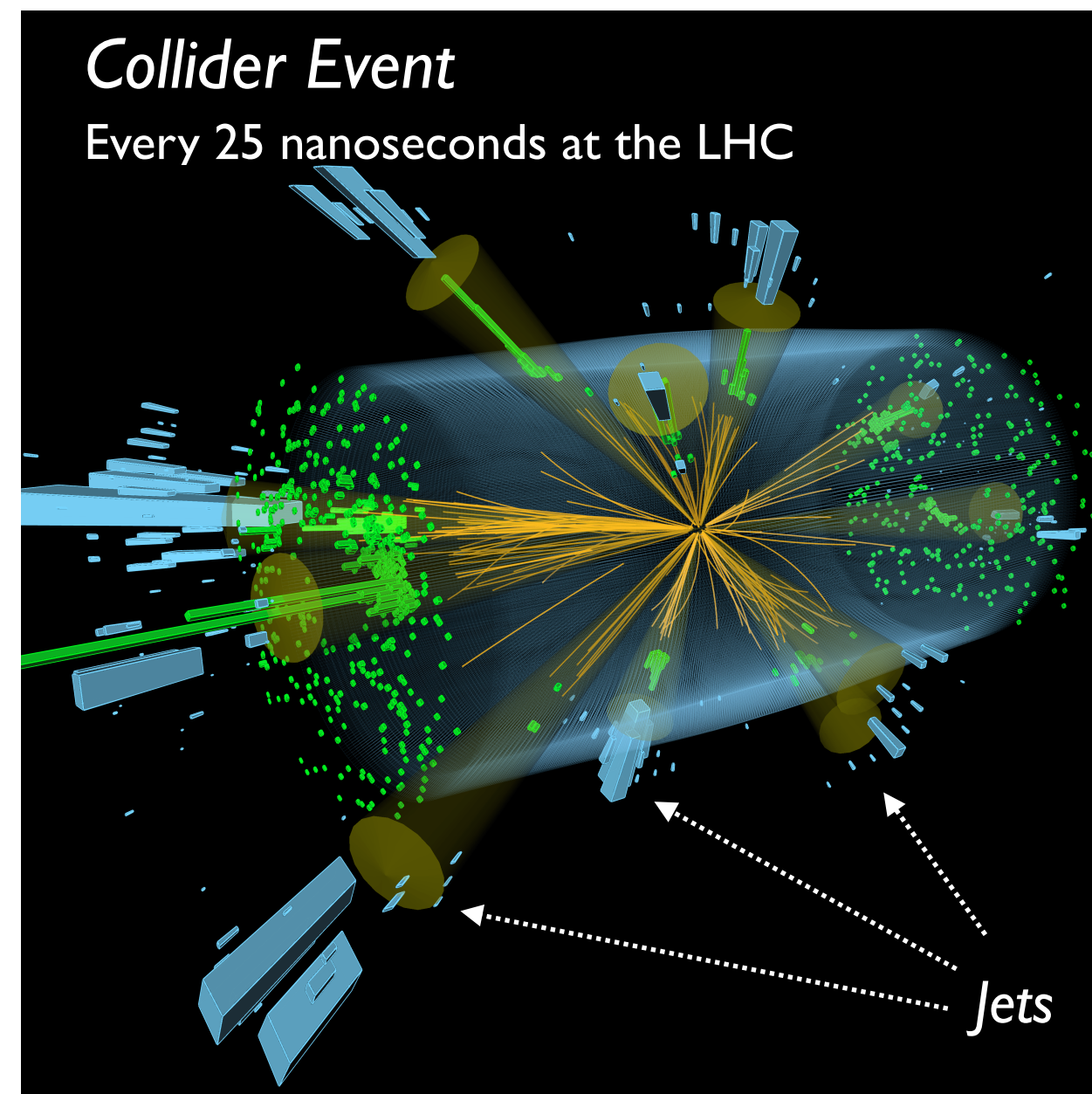
Figure 2: Laplacian eigenmaps, clustering done after embedding in **14 dimensions**



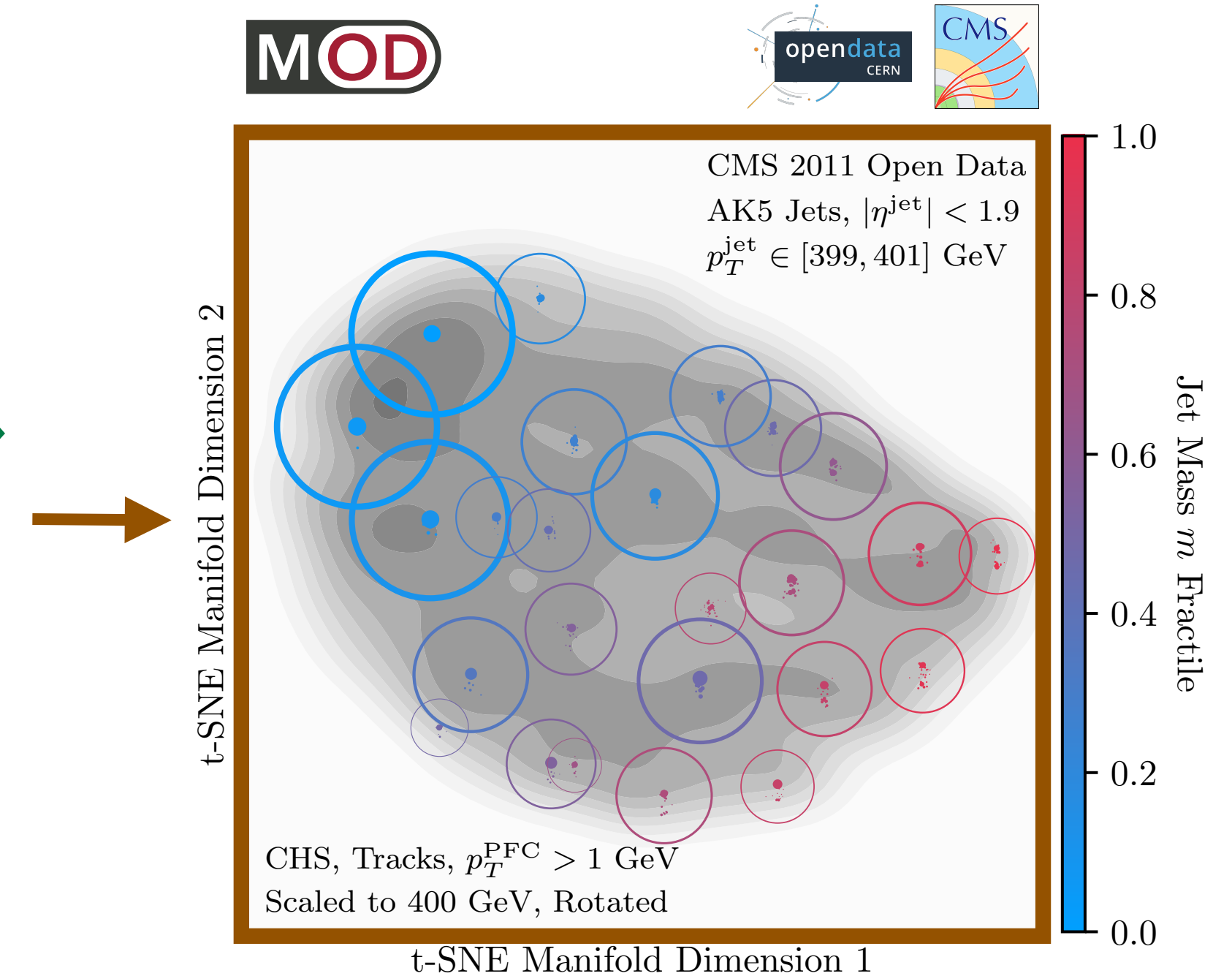
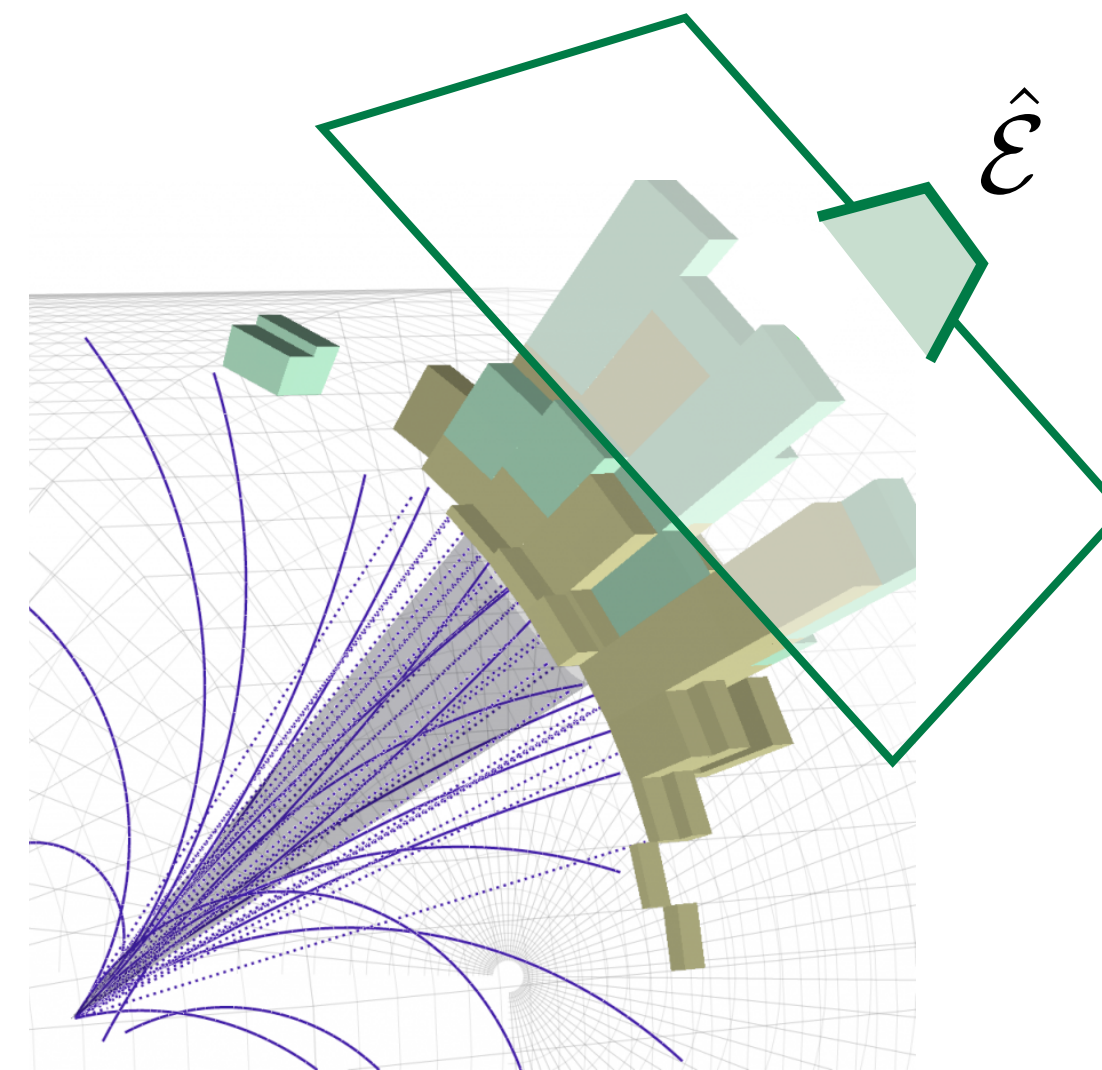
**Applications: HEP?**

# Future directions for HEP applications

**Recall:** Collider events have a geometry that can be used to organize, categorize and interpret collisions, e.g.,



Events summarized by  
"energy flow"



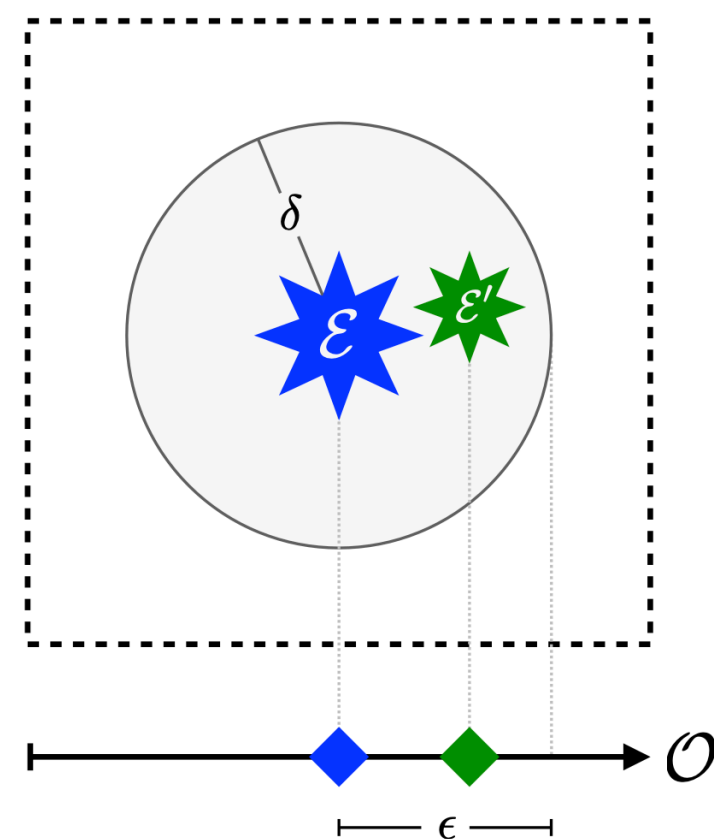
Komiske, Metodiev, Thaler,  
**The hidden geometry of particle collisions**  
J. HEP, 6 (2020)  
**The Metric Space of Collider Events**  
Phys. Rev. Lett. 123, 041801 (2019)



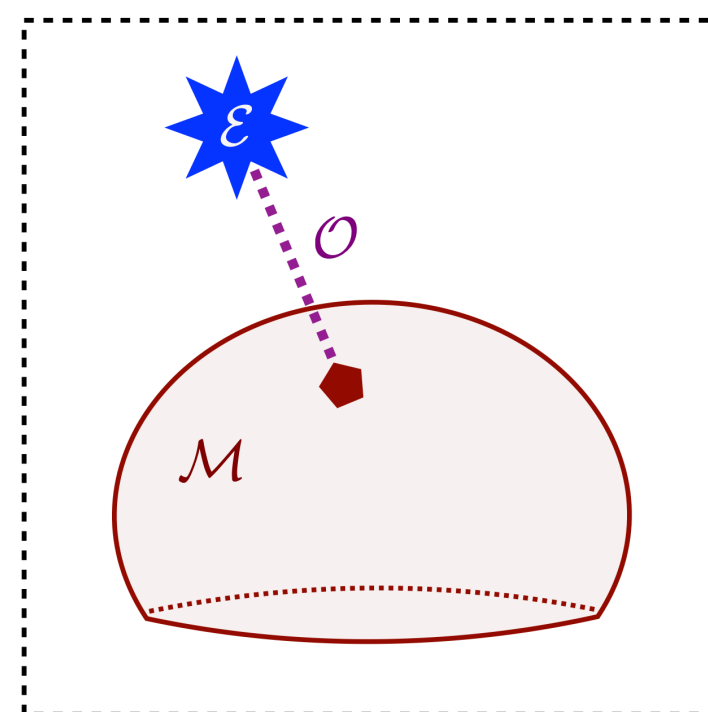
# Future directions for HEP applications

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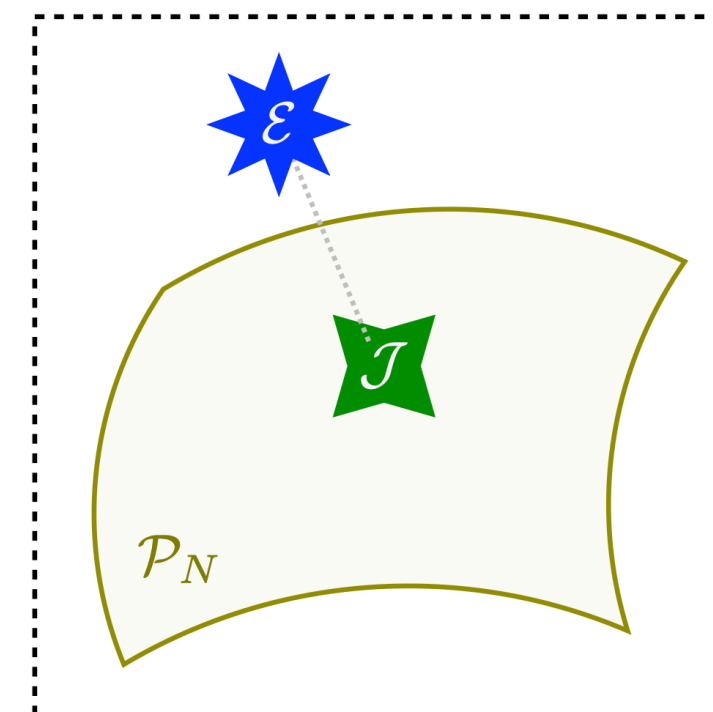
Infrared & Collinear Safety



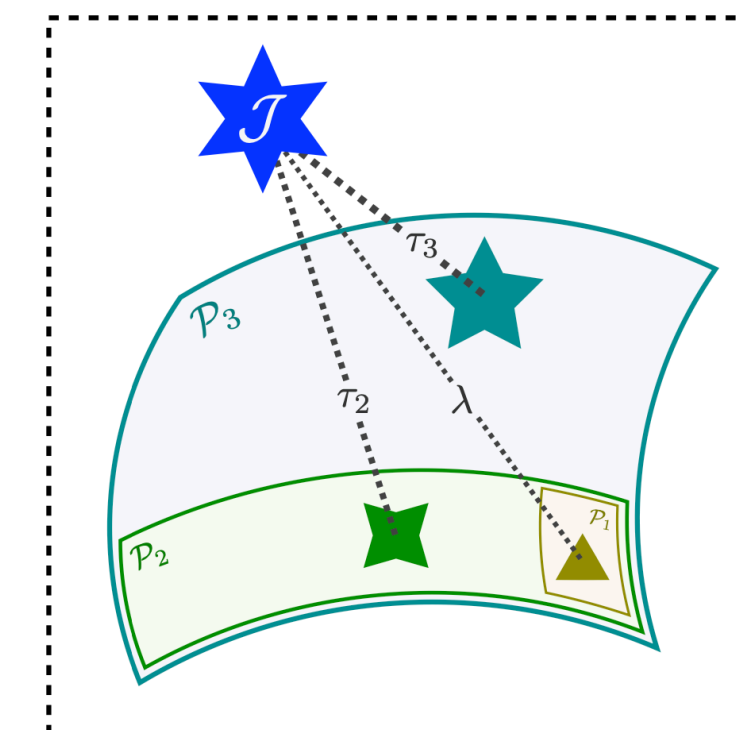
Observables



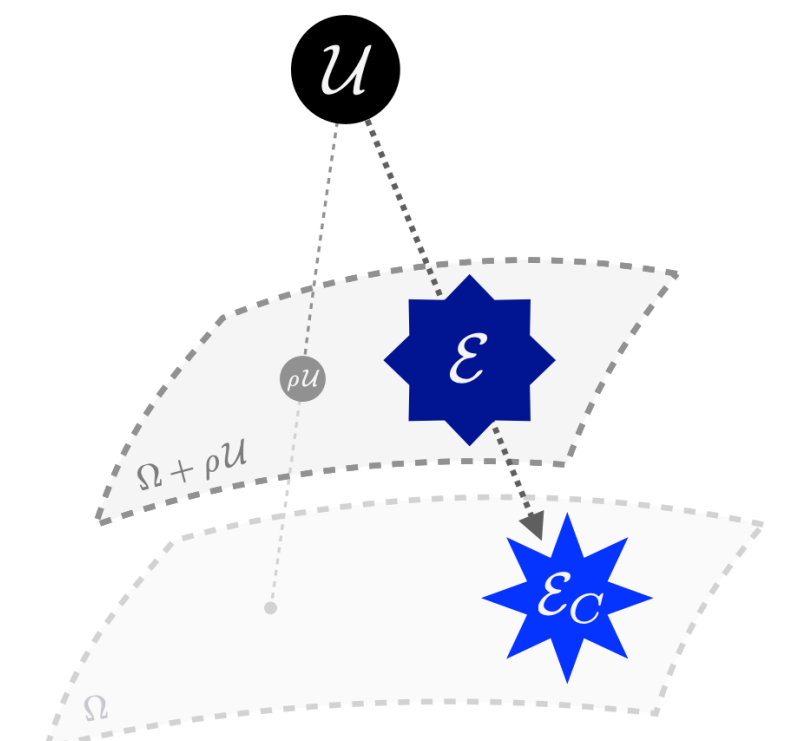
Jets



Jet substructure observables



Pileup subtraction



Komiske, Metodiev, Thaler,  
**The hidden geometry of particle collisions**  
J. HEP, 6 (2020)  
**The Metric Space of Collider Events**  
Phys. Rev. Lett. 123, 041801 (2019)

# Future directions for HEP applications

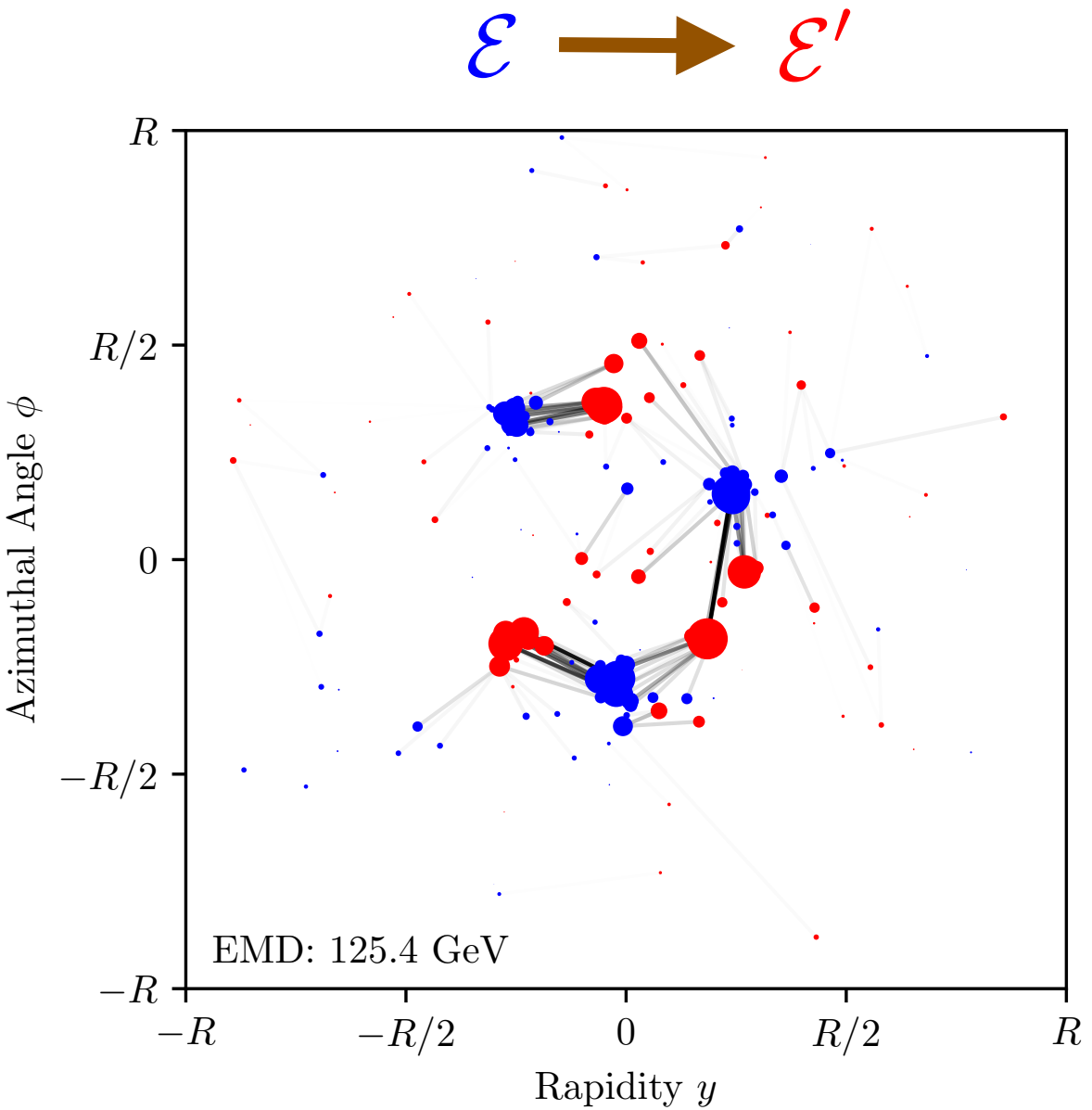
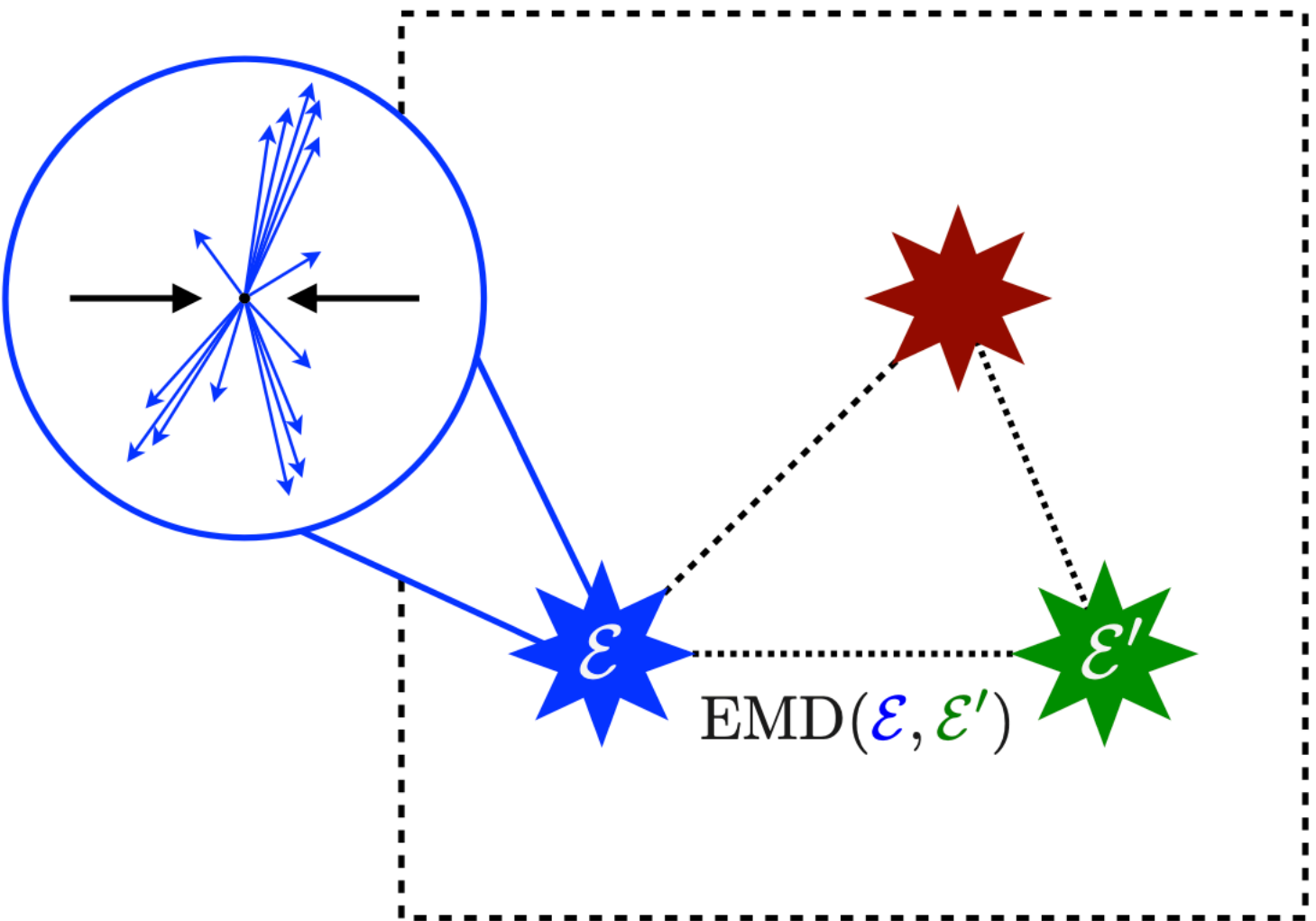
Does quantum dynamics make sense on this metric space?

energy (GeV)

$$\text{EMD}(\mathcal{E}, \mathcal{E}') := \min_{\{f_{i,j} \geq 0\}} \sum_{i=1}^N \sum_{j=1}^{N'} f_{i,j} \frac{\text{dist}(\hat{n}_i, \hat{n}_j)}{R} + \left| \sum_{i=1}^N E_i + \sum_{j=1}^{N'} E_j \right|$$

cost to move energy
cost to create energy

Metric\* space of possible events



\* for R sufficiently large  
i.e., R ≥ jet radius for conical jets



# Future directions for HEP applications

Does quantum dynamics make sense on this metric space?

- Not a Riemannian manifold!

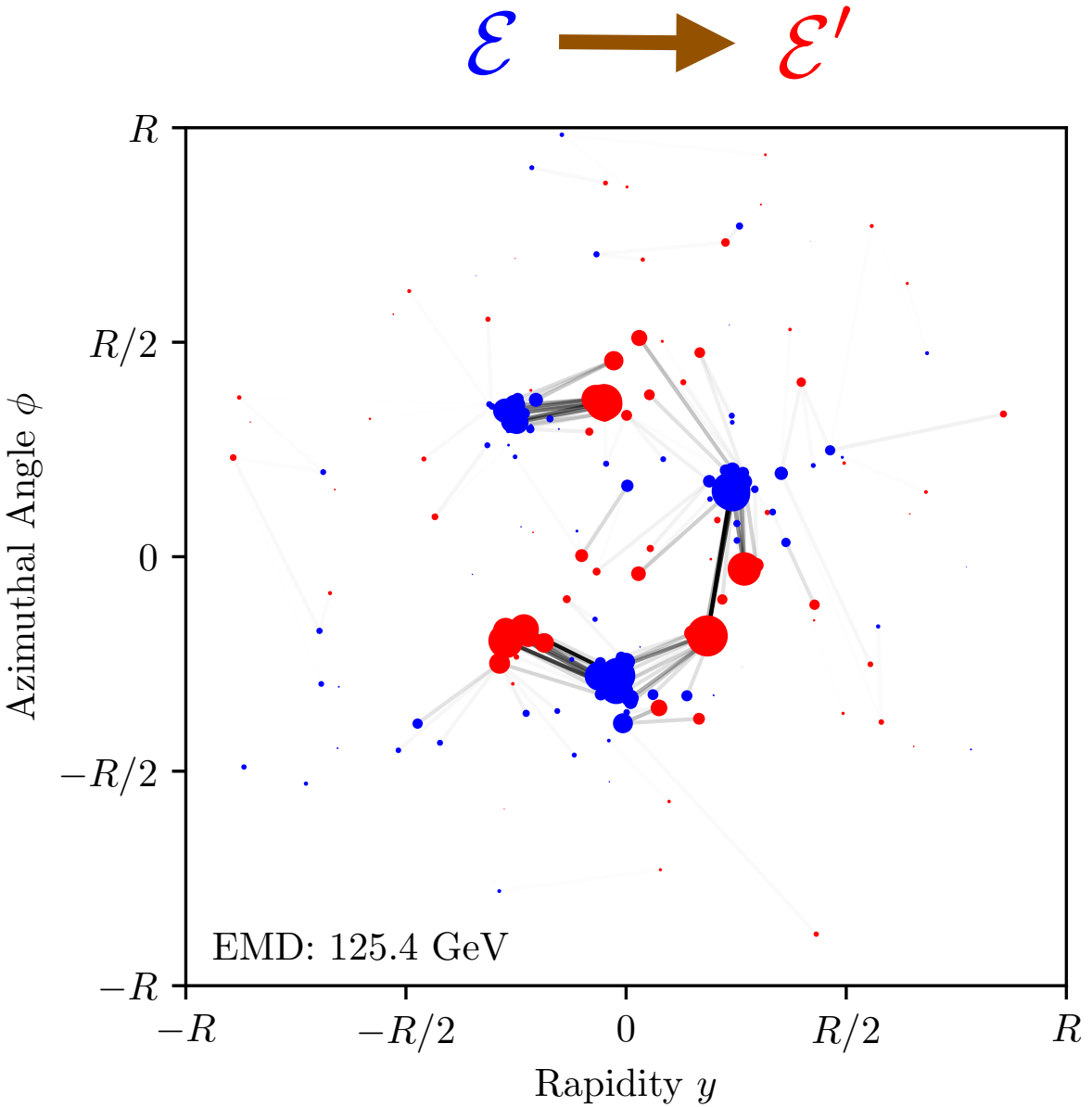
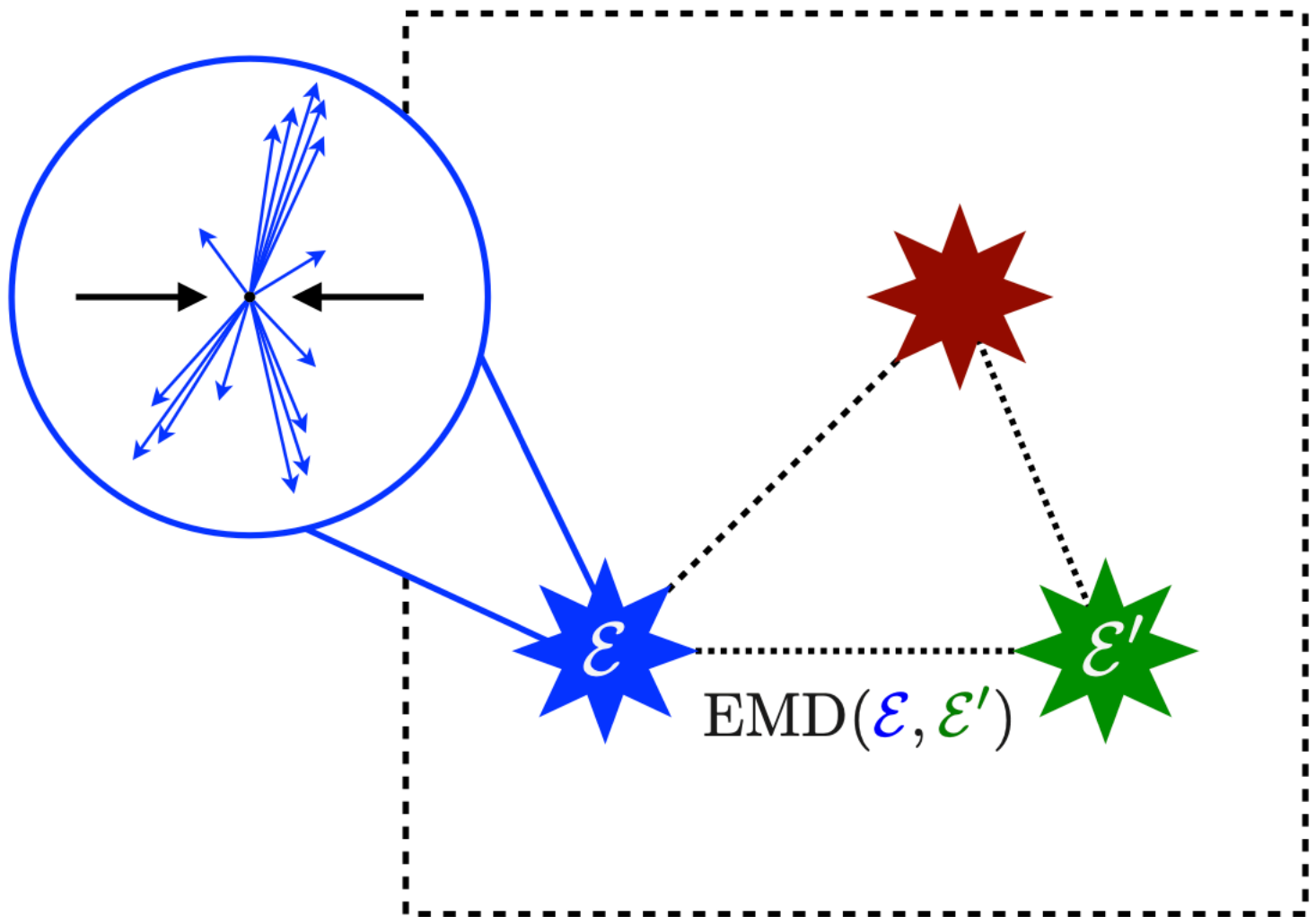
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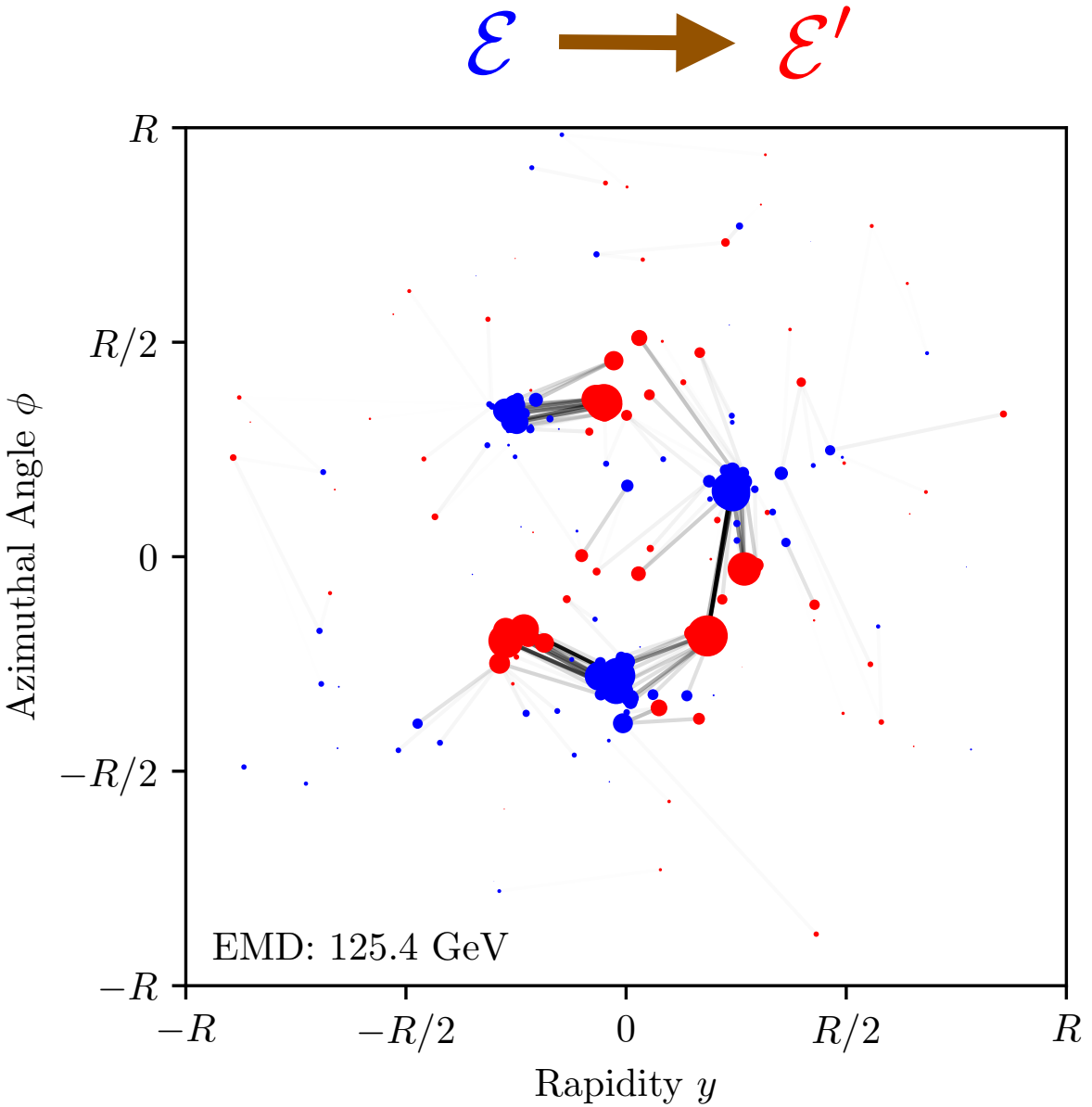
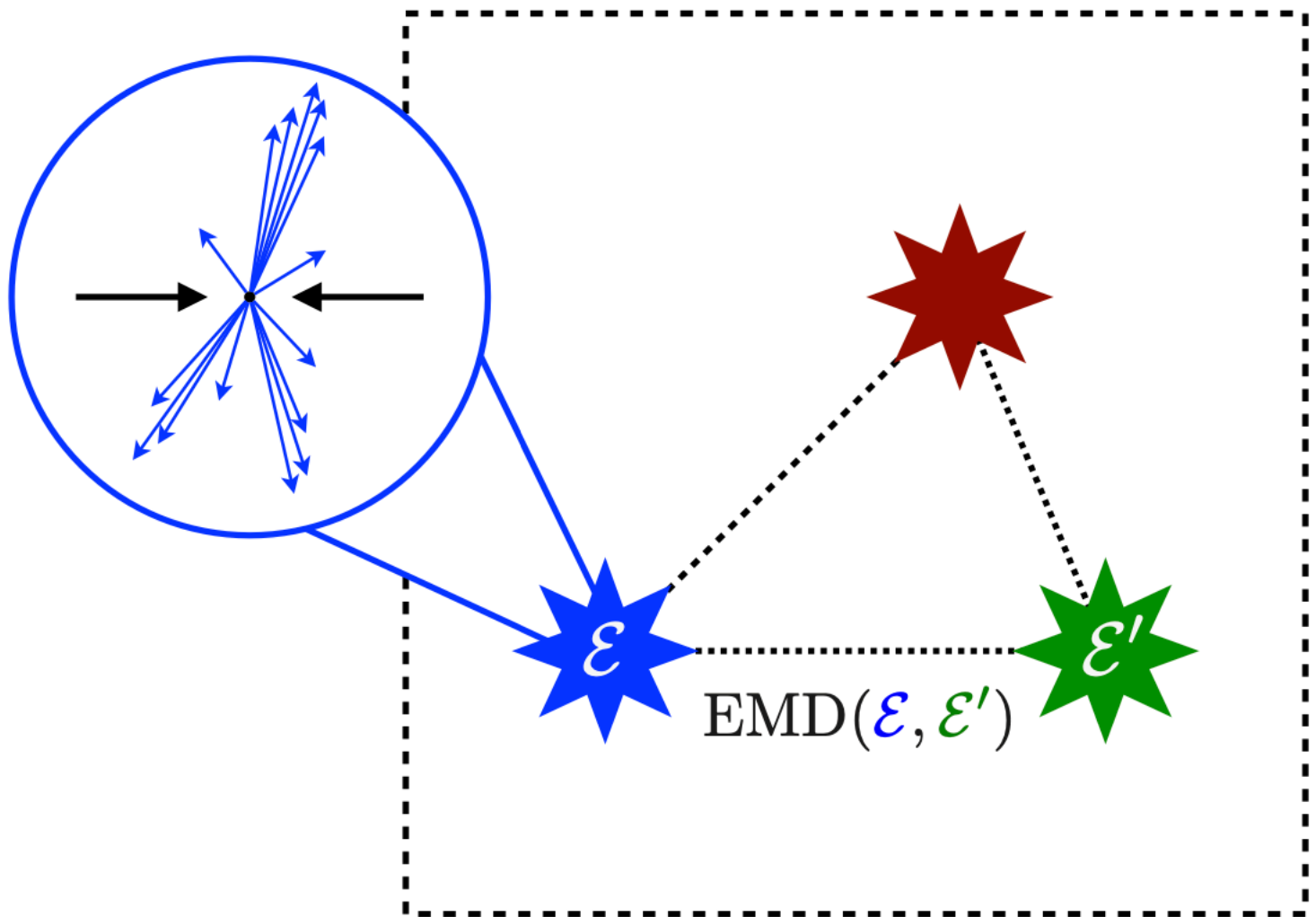


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# Future directions for HEP applications

## Does quantum dynamics make sense on this metric space?

- Not a Riemannian manifold!
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- What is the analogous quantum-classical correspondence principle?

energy (GeV)

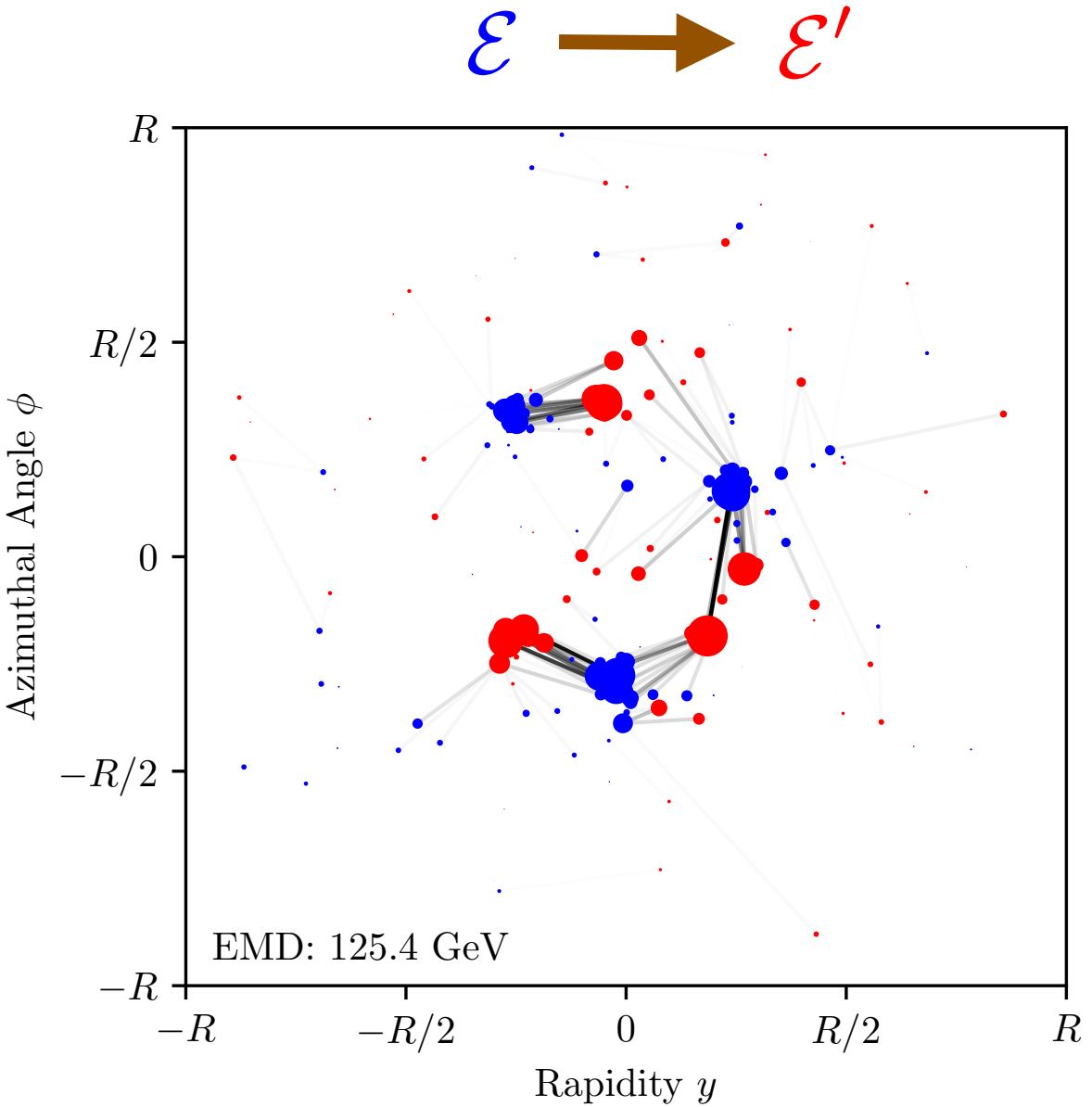
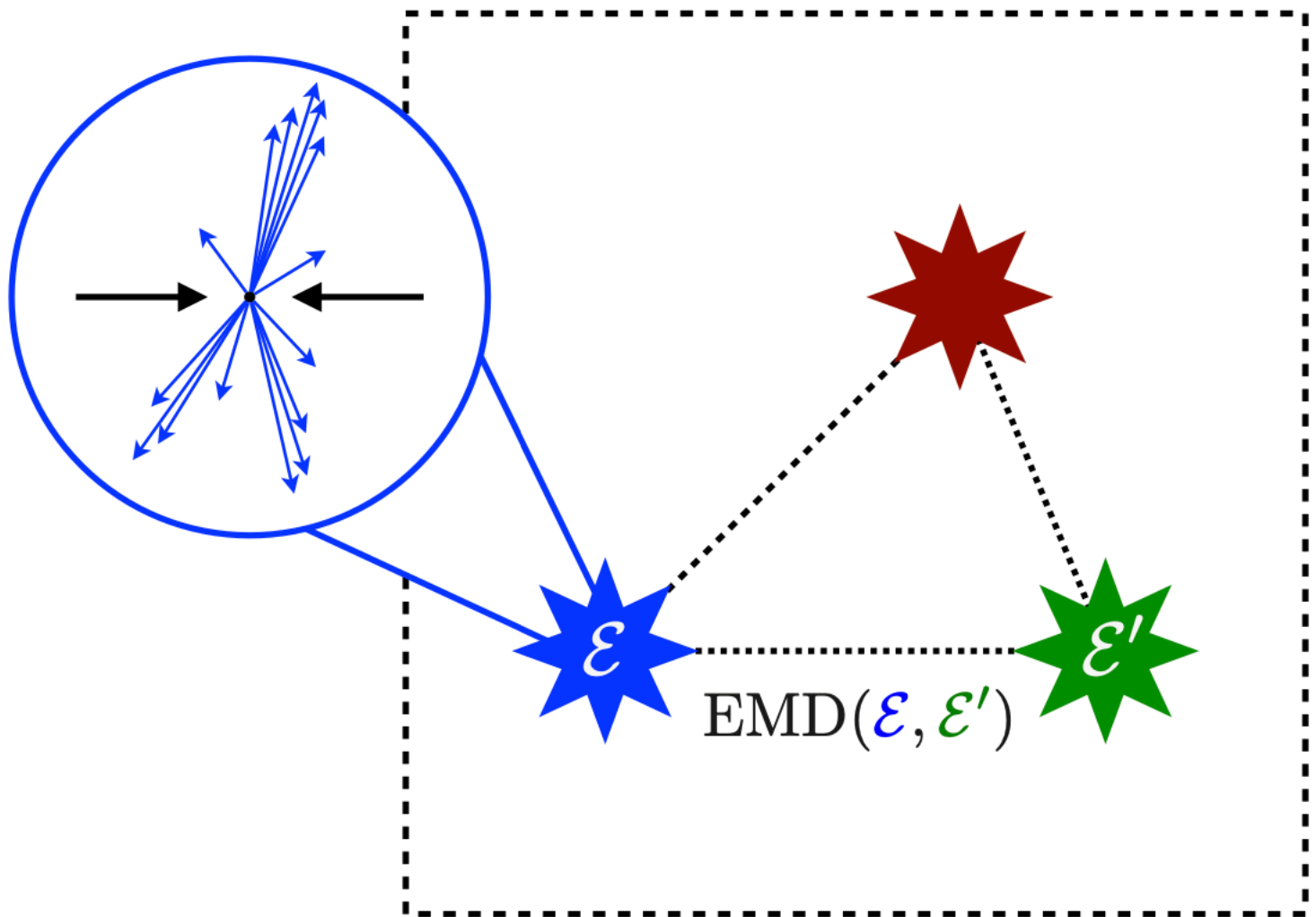


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Figures from talk by Jesse Thaler, University of Chicago and Caltech AI+Science: <https://www.youtube.com/watch?v=BMBSAWUxBn4>

# Future directions for HEP applications

## Does quantum dynamics make sense on this metric space?

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energy (GeV)

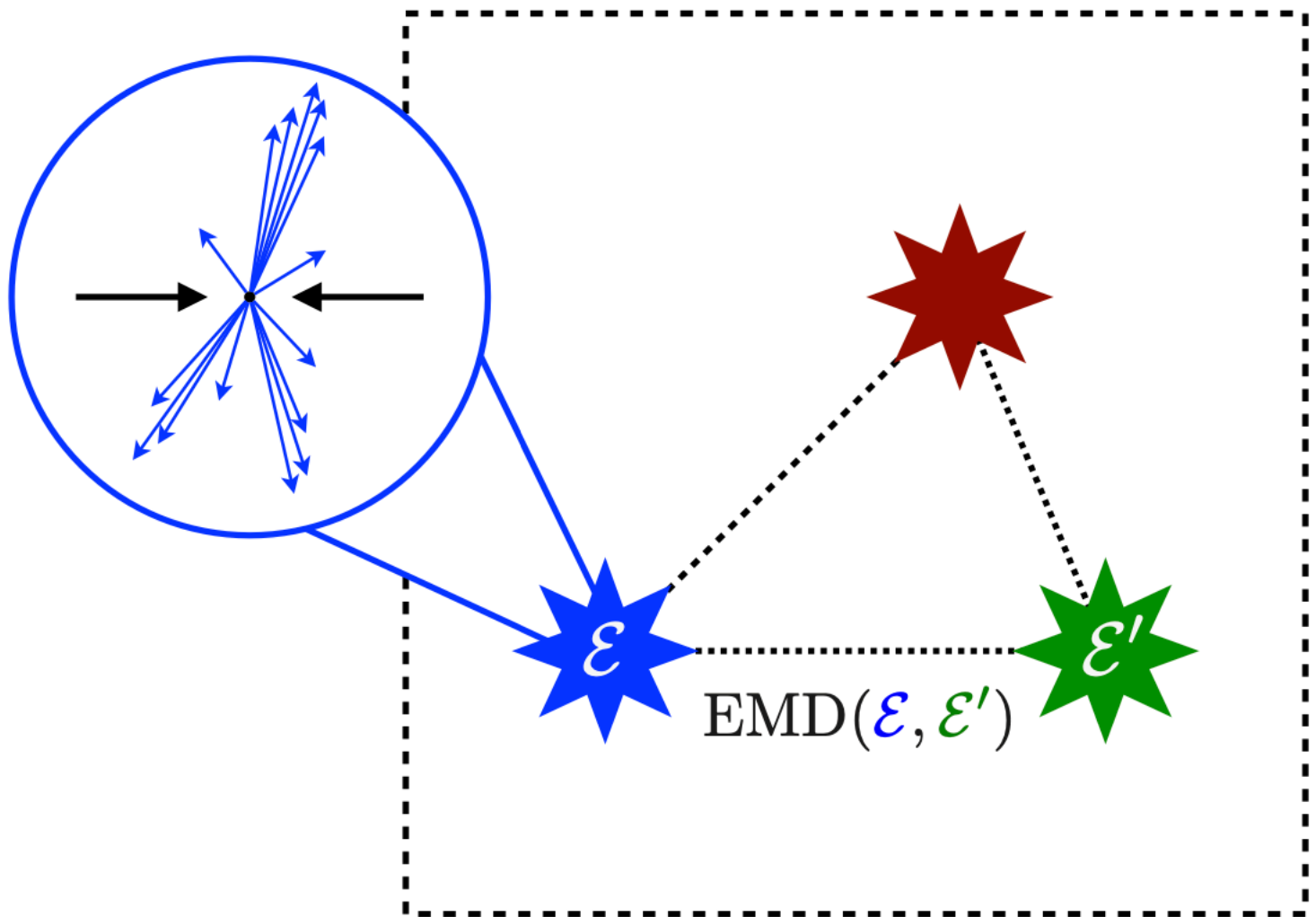


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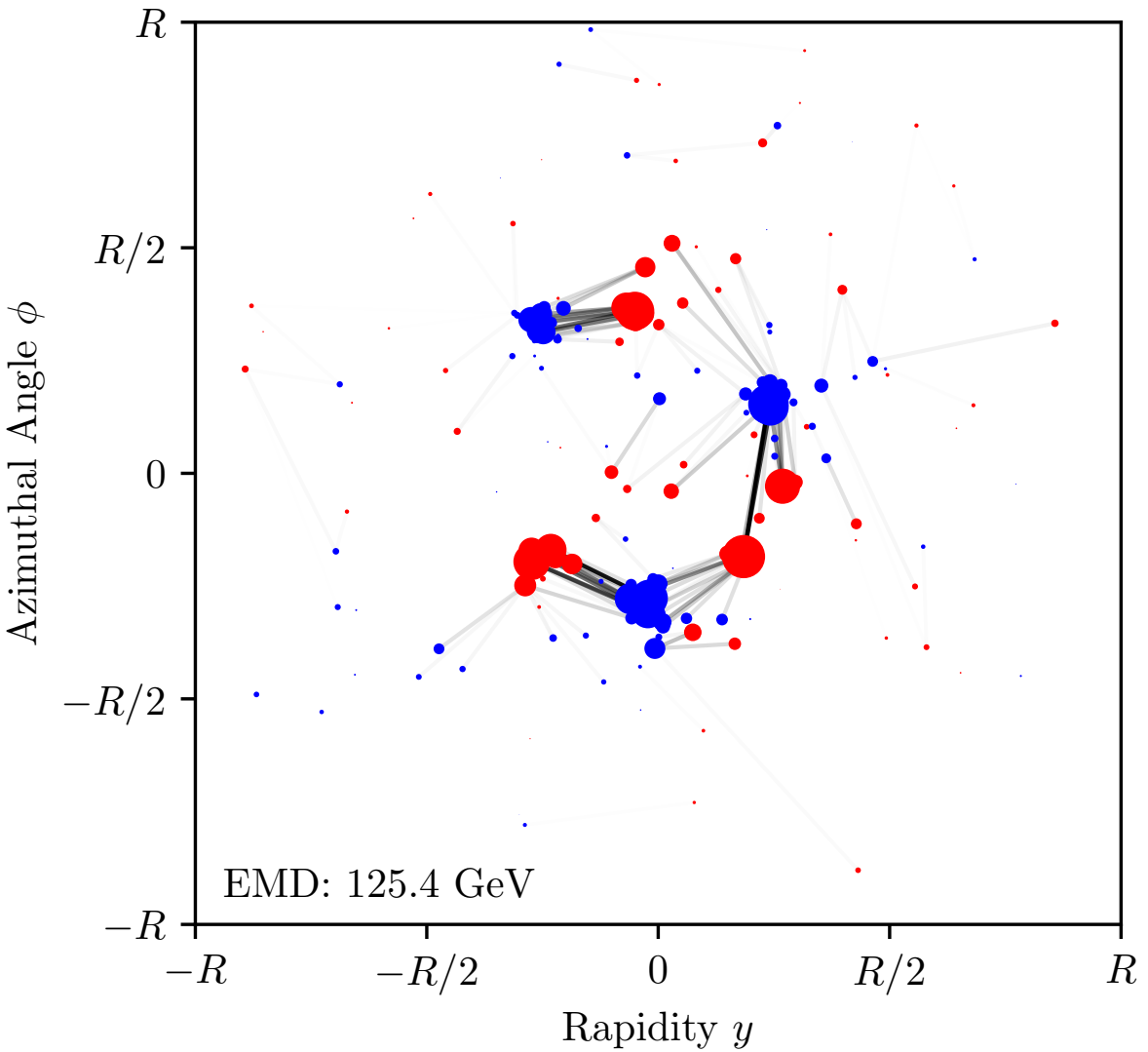
cost to move energy

cost to create energy

Metric\* space of possible events



$\mathcal{E} \rightarrow \mathcal{E}'$



\* for R sufficiently large  
i.e.,  $R \geq$  jet radius for conical jets



# Future directions for HEP applications

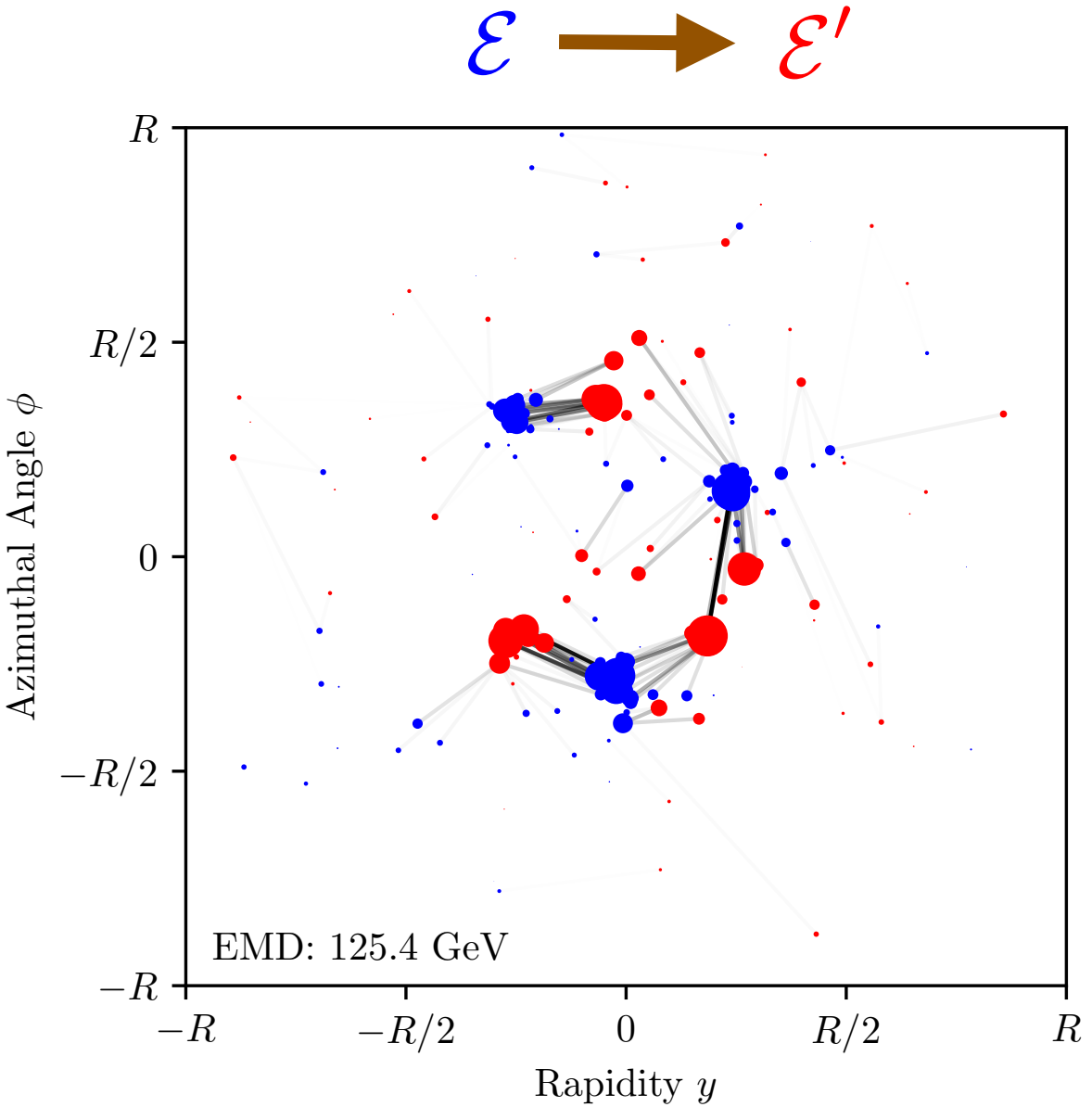
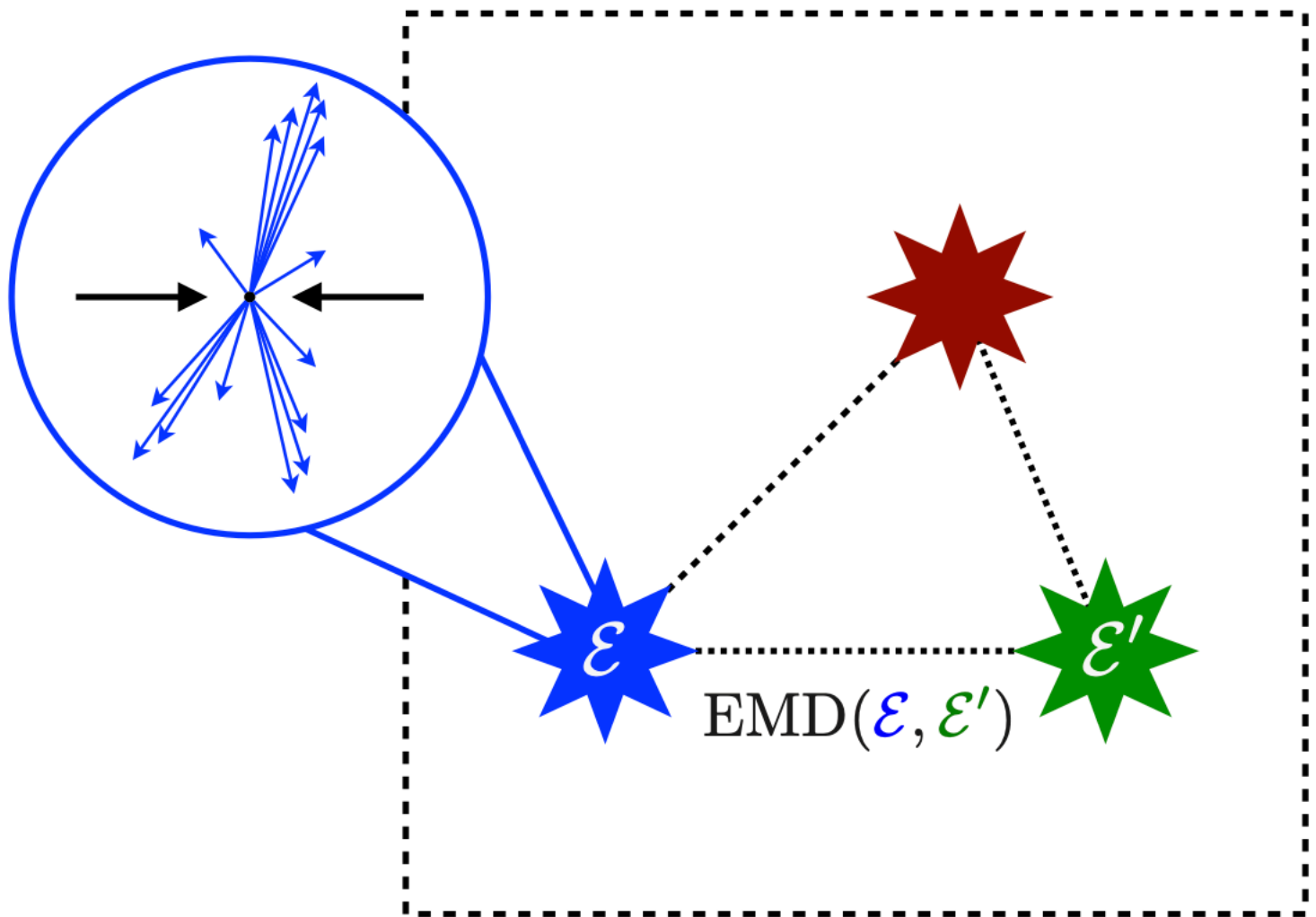
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  - We quantized the geodesic flow. Optimal transport has dynamical (PDE) descriptions as well.

energy (GeV) ↓

$$\text{EMD}(\mathcal{E}, \mathcal{E}') := \min_{\{f_{i,j} \geq 0\}} \underbrace{\sum_{i=1}^N \sum_{j=1}^{N'} f_{i,j} \frac{\text{dist}(\hat{n}_i, \hat{n}_j)}{R}}_{\text{cost to move energy}} + \underbrace{\left| \sum_{i=1}^N E_i + \sum_{j=1}^{N'} E_j \right|}_{\text{cost to create energy}}$$

Metric\* space of possible events



\* for  $R$  sufficiently large  
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# Future directions for HEP applications

## Does quantum dynamics make sense on this metric space?

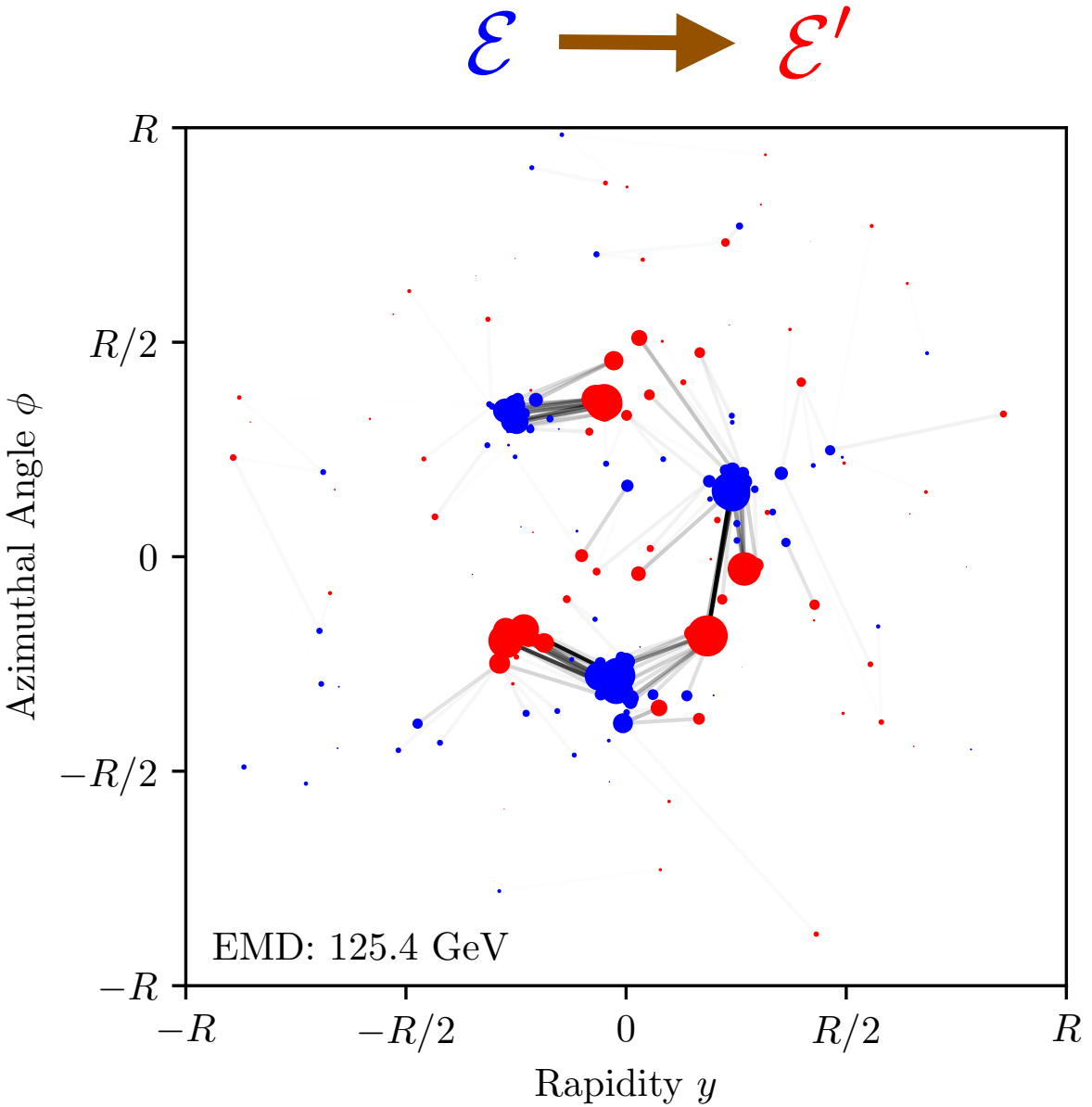
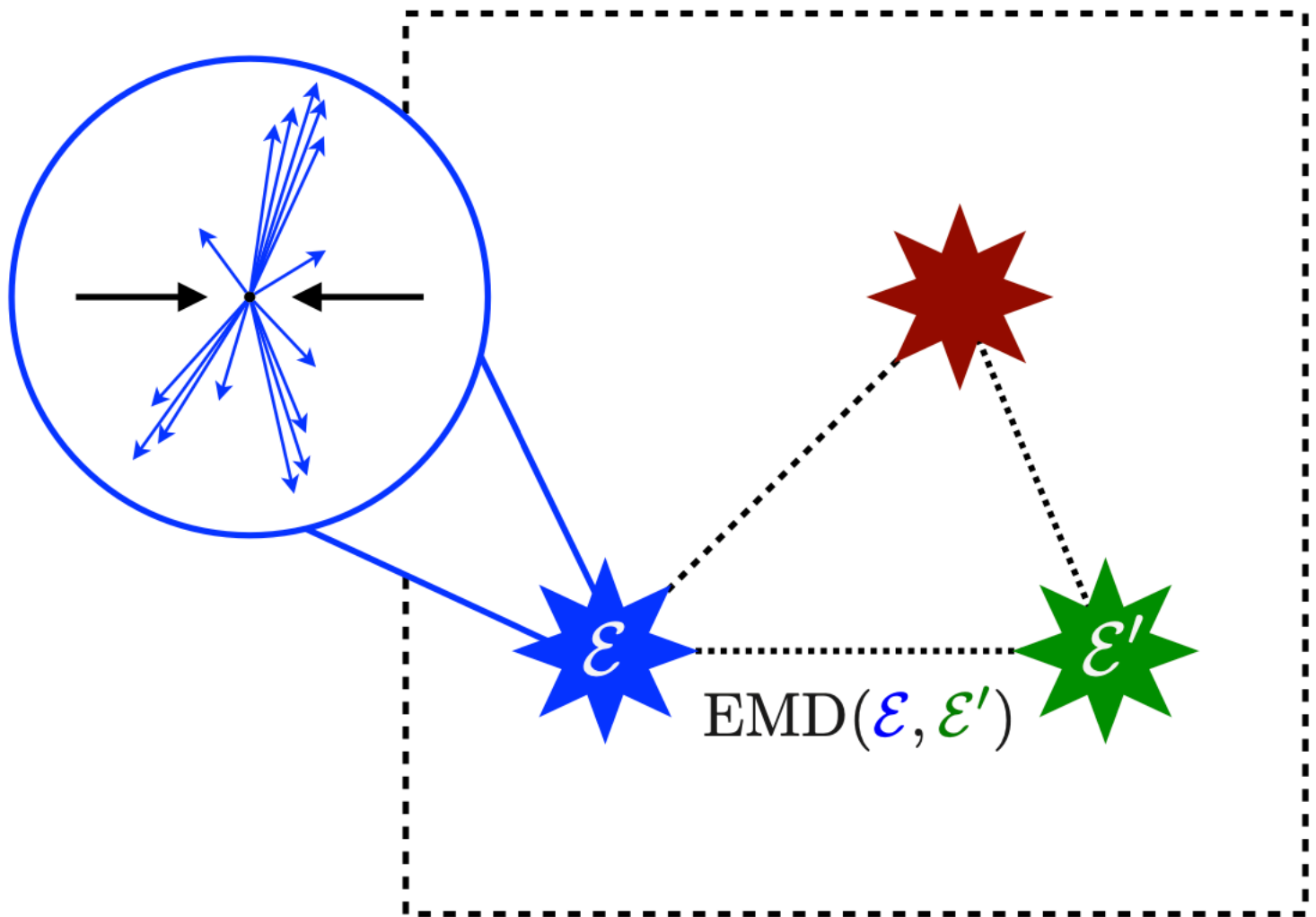
- Not a Riemannian manifold!
  - but maybe formally it is?
- What is the analogous quantum-classical correspondence principle?
- What is the **quantization** of the energy flow  $\text{EMD}(\cdot, \cdot)$ ?
  - We quantized the geodesic flow. Optimal transport has dynamical (PDE) descriptions as well.
- The **EMD** is solvable quickly, but **optimal transport plans are harder**. Could **quantization** resolve optimal transport plans more rapidly?

energy (GeV) ↓

$$\text{EMD}(\mathcal{E}, \mathcal{E}') := \min_{\{f_{i,j} \geq 0\}} \sum_{i=1}^N \sum_{j=1}^{N'} f_{i,j} \frac{\text{dist}(\hat{n}_i, \hat{n}_j)}{R} + \left| \sum_{i=1}^N E_i + \sum_{j=1}^{N'} E_j \right|$$

cost to move energy
cost to create energy

Metric\* space of possible events



\* for R sufficiently large  
i.e.,  $R \geq$  jet radius for conical jets



## What about quantum algorithms?

We have a rigorous convergence theory and classical algorithm.

```
1: Inputs:  $X_N = \{v_1, \dots, v_N\}, v^*, \epsilon > 0, \alpha \geq 1, t > 0$ 
2: Output: Propagated state  $[\psi_h^\zeta](t)$ 
3: procedure PROPAGATE
4:   for  $i, j = 1 : N$  do  $[T_\epsilon]_{i,j} \leftarrow k(\|v_i - v_j\|^2/\epsilon)$ 
5:    $D_\epsilon \leftarrow$  diagonal matrix  $\left(\sum_{j=1}^N [T_\epsilon]_{i,j}\right)_{1 \leq i \leq N}$ 
6:    $\Delta_{\epsilon,N} \leftarrow \frac{4(I_N - D_\epsilon^{-1}T_\epsilon)}{\epsilon}$ 
7:    $U_{\epsilon,N}^t \leftarrow \exp(-it\sqrt{\Delta_{\epsilon,N}})$ 
8:    $\hbar \leftarrow \epsilon^{\frac{1}{2+\alpha}}$ 
9:    $p_0 \leftarrow v_j - v^*$  for  $v_j$  closest to point  $v^*$ 
10:  while  $1 \leq \ell \leq N$  do
11:     $[\psi_h^\zeta]_\ell \leftarrow e^{-\|v_\ell - v^*\|^2/2\hbar} e^{\frac{i}{\hbar}(v_\ell - v^*)^\top p_0/\|p_0\|}$ 
12:  return  $[\psi_h^\zeta](t) = U_{\epsilon,N}^t[\psi_h^\zeta]$ 
```

## What about quantum algorithms?

We have a rigorous convergence theory and classical algorithm.

- Uses only quantum primitives: unitary operators acting on localized wavepackets.

```
1: Inputs:  $X_N = \{v_1, \dots, v_N\}, v^*, \epsilon > 0, \alpha \geq 1, t > 0$ 
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**We have a rigorous convergence theory and classical algorithm.**

- Uses only quantum primitives: unitary operators acting on localized wavepackets.
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- Fast implementation of  $U_{\epsilon,N}^t$  has widespread implications for **quantum algorithms for manifold learning**.

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# Thank you

## Manifold learning via quantum dynamics

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[arXiv:2112.11161](https://arxiv.org/abs/2112.11161)

## Shining light on data: Geometric data analysis through quantum dynamics

Akshat Kumar,<sup>1\*</sup> Mohan Sarovar<sup>2\*</sup>

[arXiv:2212.00682](https://arxiv.org/abs/2212.00682)

## ON A QUANTUM-CLASSICAL CORRESPONDENCE: FROM GRAPHS TO MANIFOLDS

AKSHAT KUMAR

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