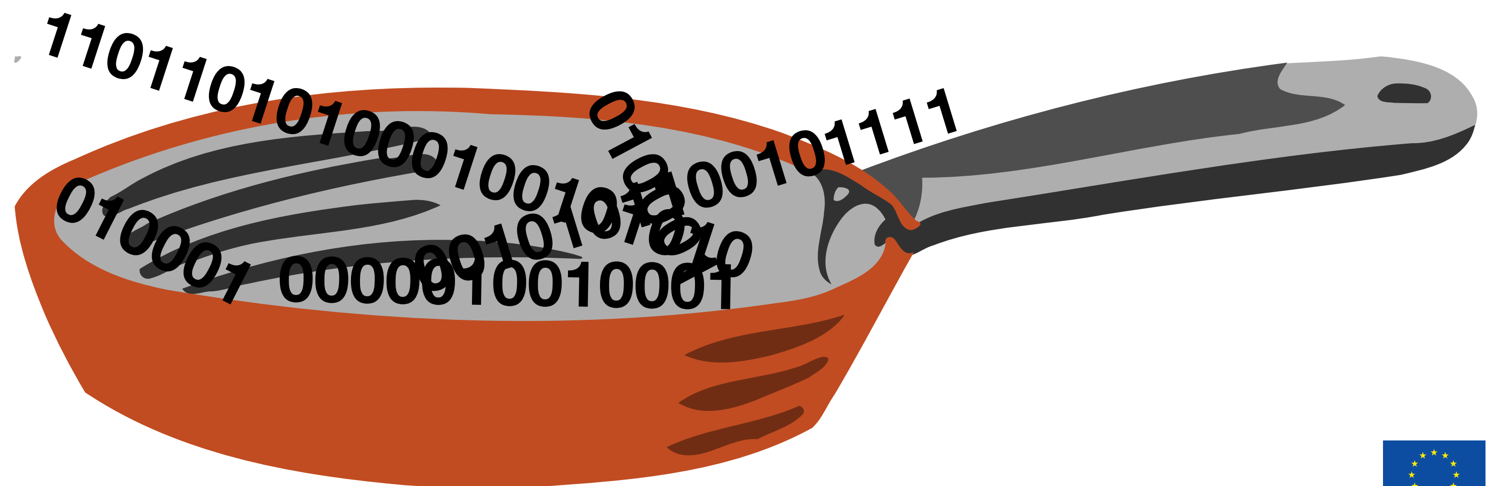
Efficient Reductions for k-Nearest Neighbor Search

Joint work with Tobias Christiani and Mikkel Thorup



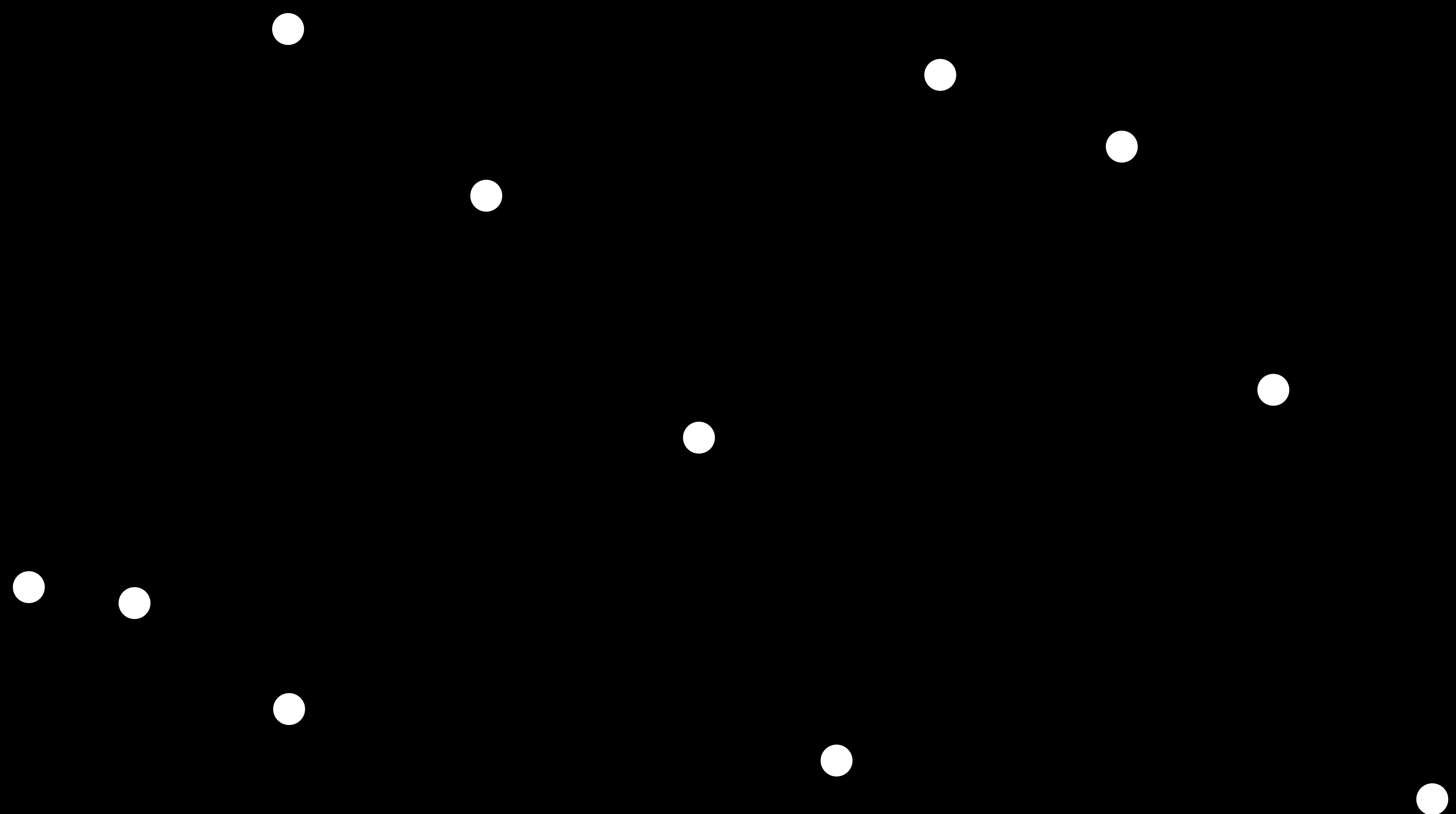
Rasmus Pagh

BARC and IT University of Copenhagen

Workshop on Sublinear Algorithms
and Nearest Neighbor Search

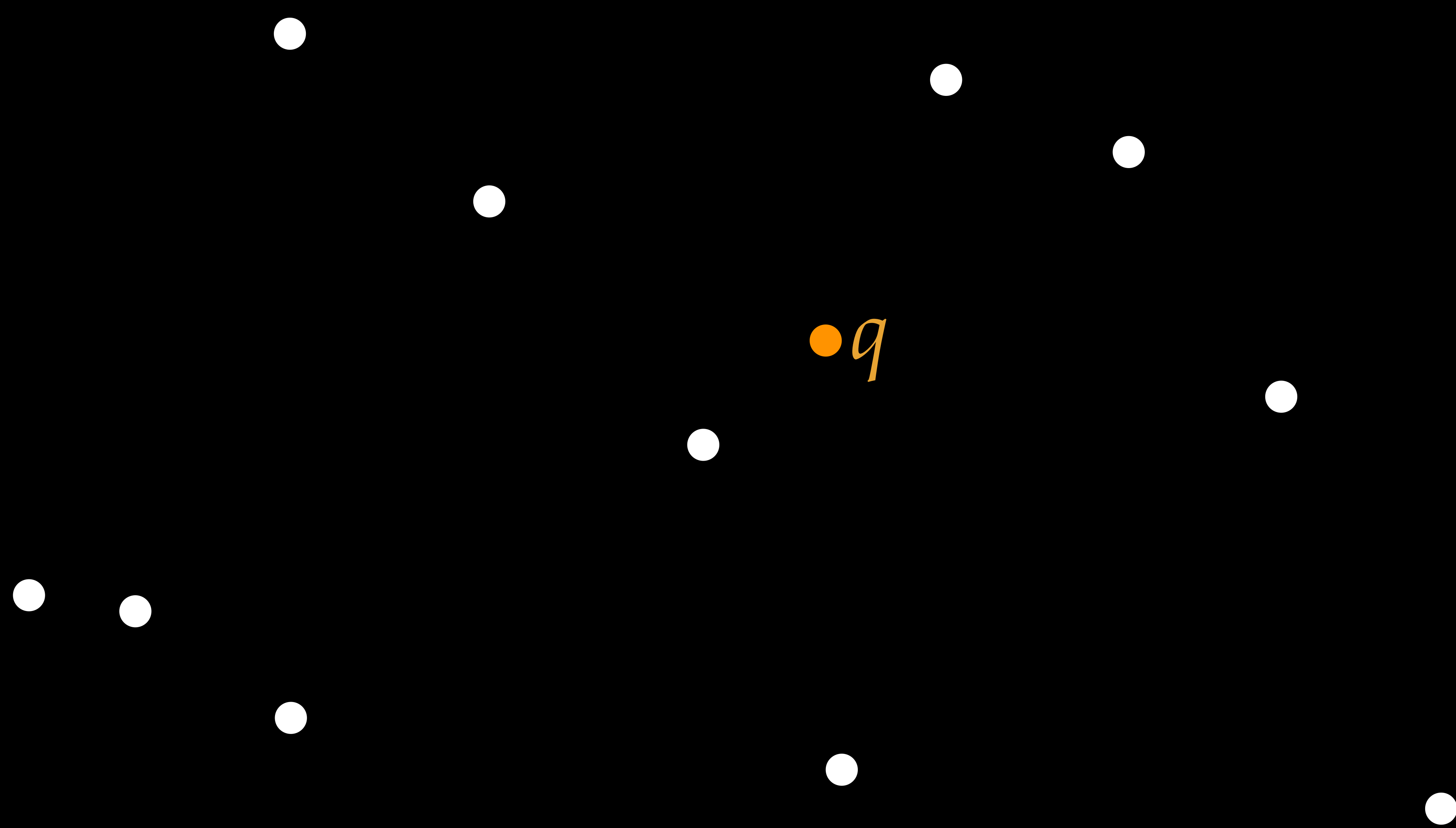
Simons Institute for Theory of Computing
November 29, 2018

Nearest neighbor search



$$P = \{x_1, \ldots, x_n\}$$

Nearest neighbor search



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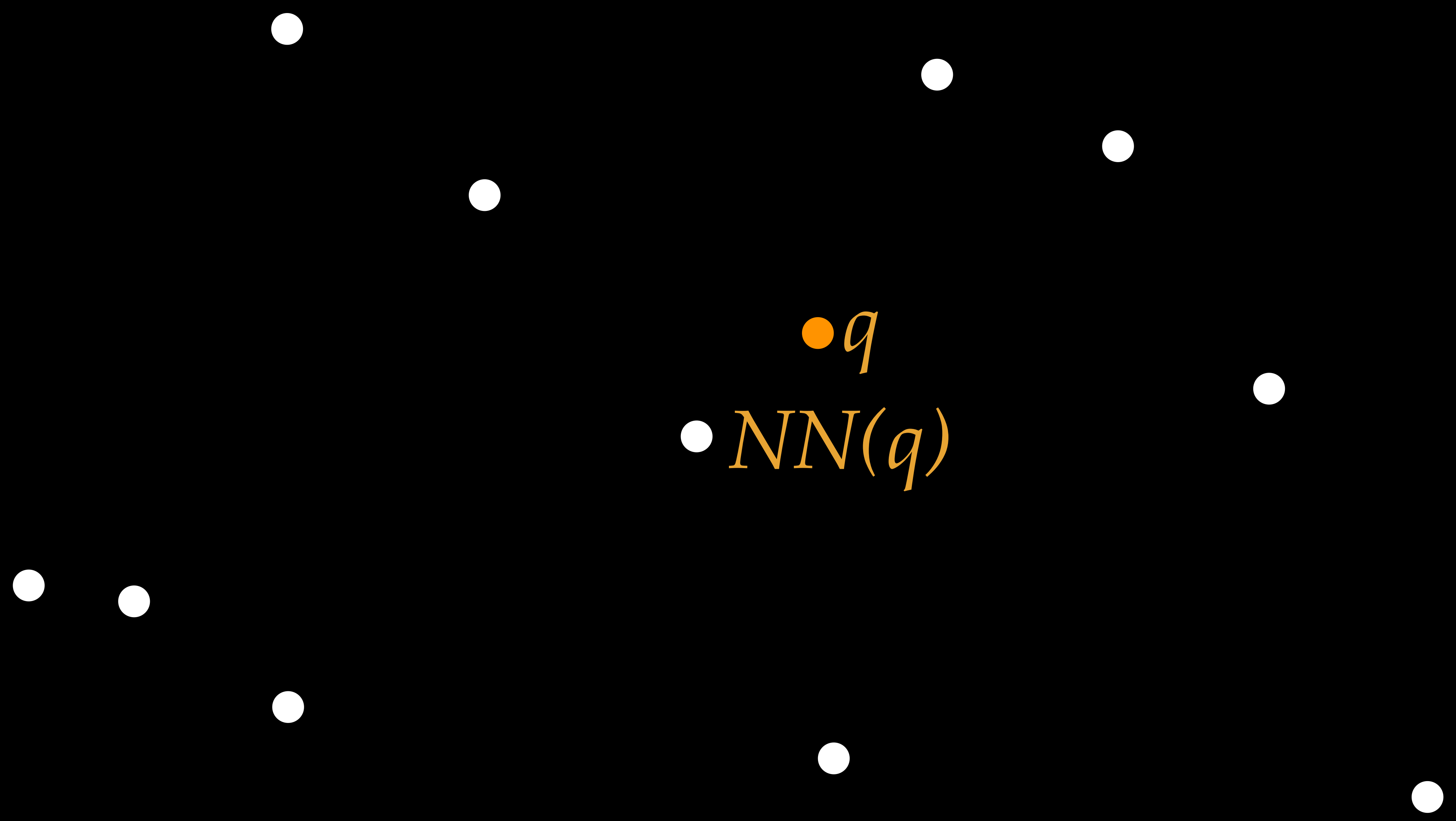

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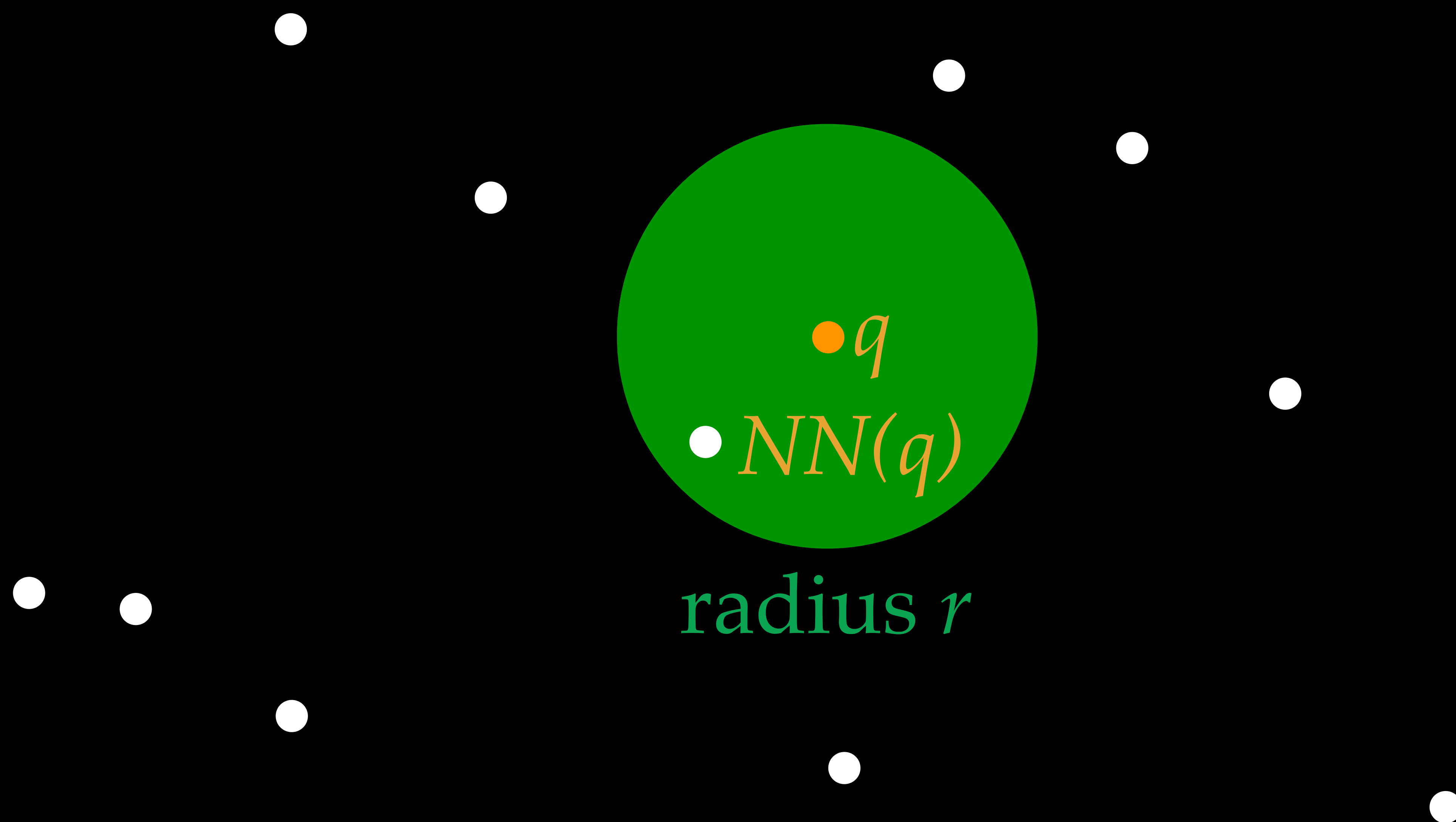
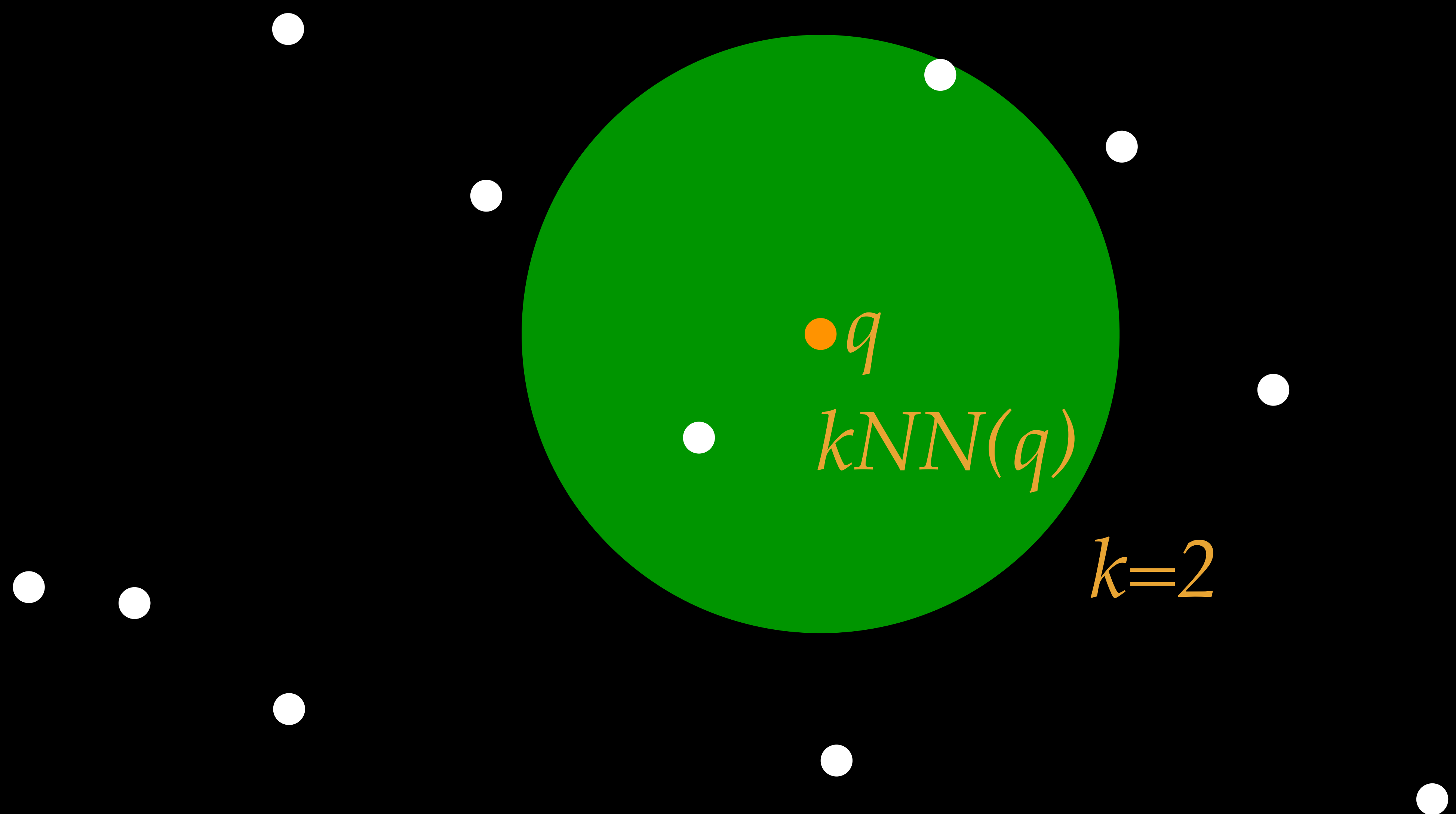
Near~~est~~ neighbor search



$$P = \{x_1, \ldots, x_n\}$$

k-nearest neighbor search



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Some application areas

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- Association rule mining
- Automation
- Bio-chemistry (finding motifs)
- Bio-informatics (homology search)
- Clustering
- Computer vision and pattern recognition
- Databases
- Data cleaning
- Data stream computation
- Data privacy
- First story detection (with application to Twitter)
- Identifying trends in time series
- Linear algebra
- Motion planning for robots
- Near-duplicate detection
- News personalization (collaborative filtering)
- Privacy preserving data mining
- Search engines for 3D models
- Sensor networks
- …

Hardness of NN search

- [Williams ’04], [Alman & Williams ’15]:
  NN search on $P \subseteq \{0,1\}^d$ in time $n^{0.99}\, 2^{o(d)}$ with preprocessing time poly(n) $2^{o(d)}$ $\Longrightarrow$
  k-SAT w. n variables can be solved in time c^n, $c < 2$

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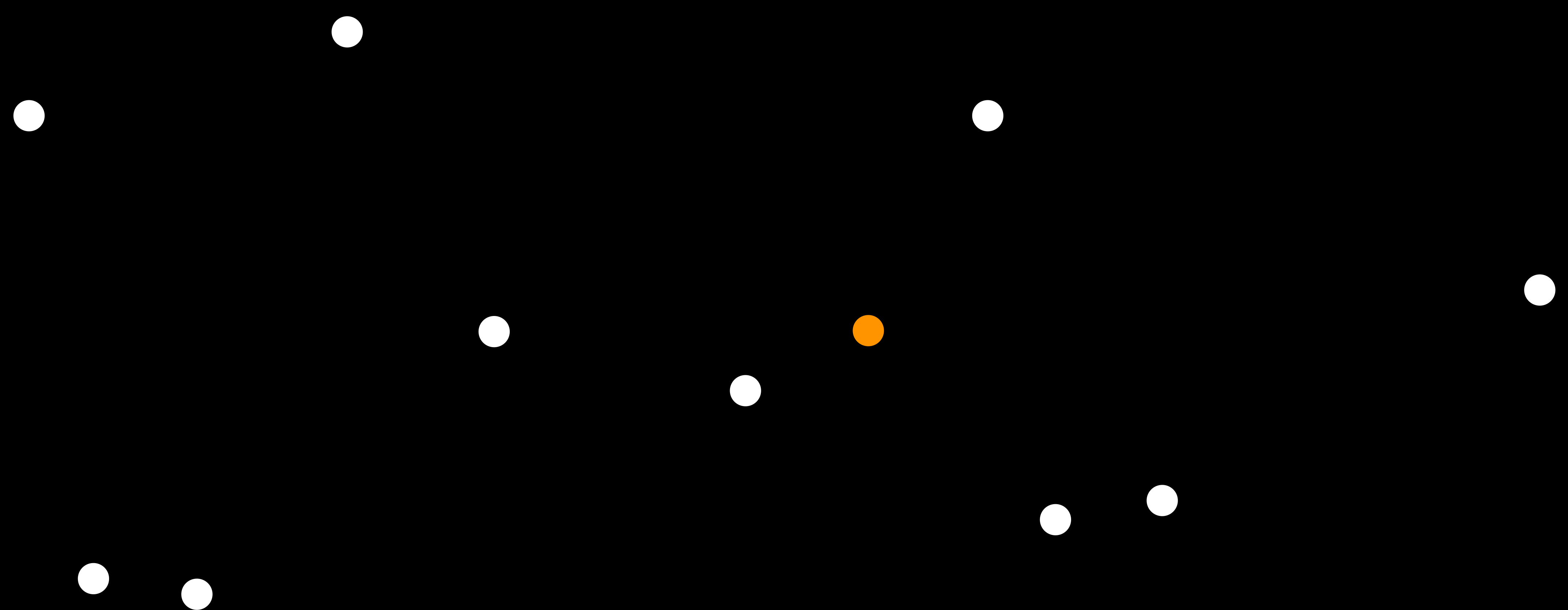
In practice: "Curse of dimensionality" makes NN search slow in high dimension.

Approximate nearest neighbor

Approximate nearest neighbors: towards removing the curse of dimensionality 3794 1998
P Indyk, R Motwani
Proceedings of the thirtieth annual ACM symposium on Theory of computing …



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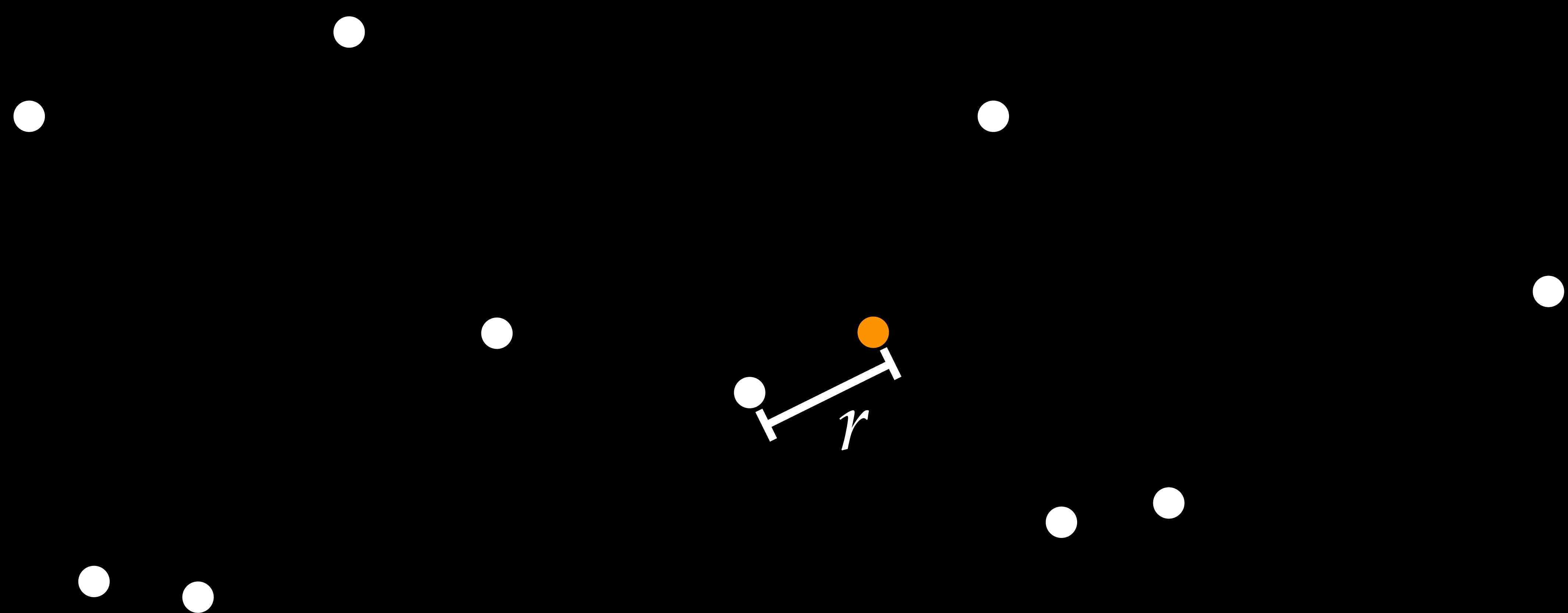

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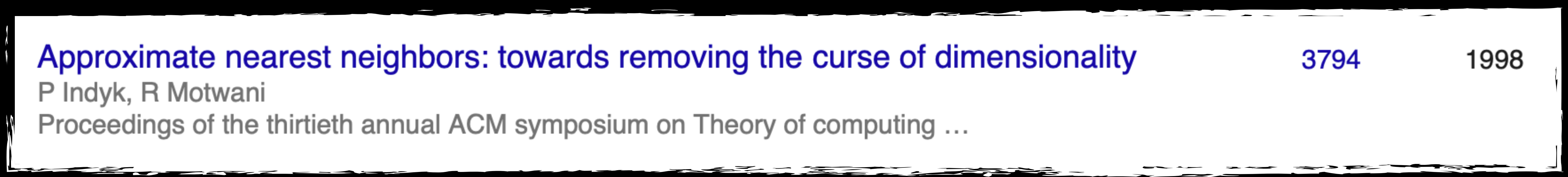
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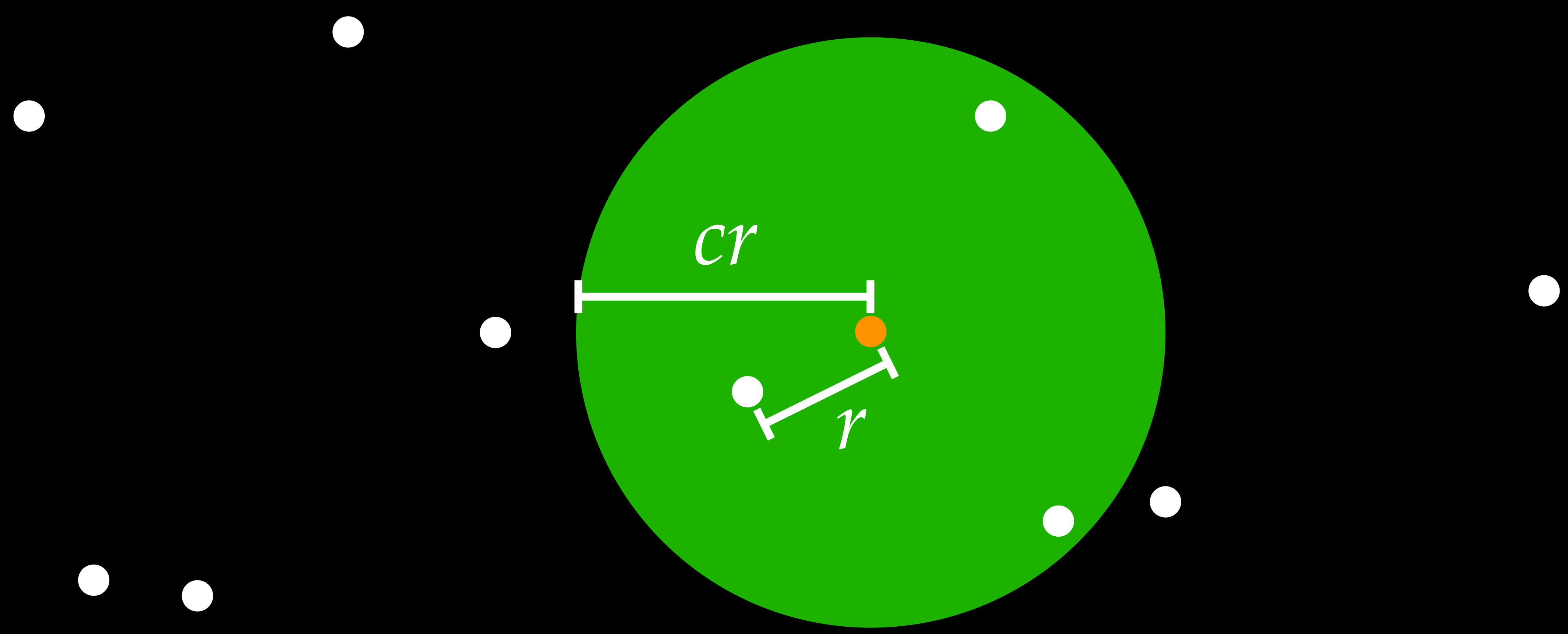

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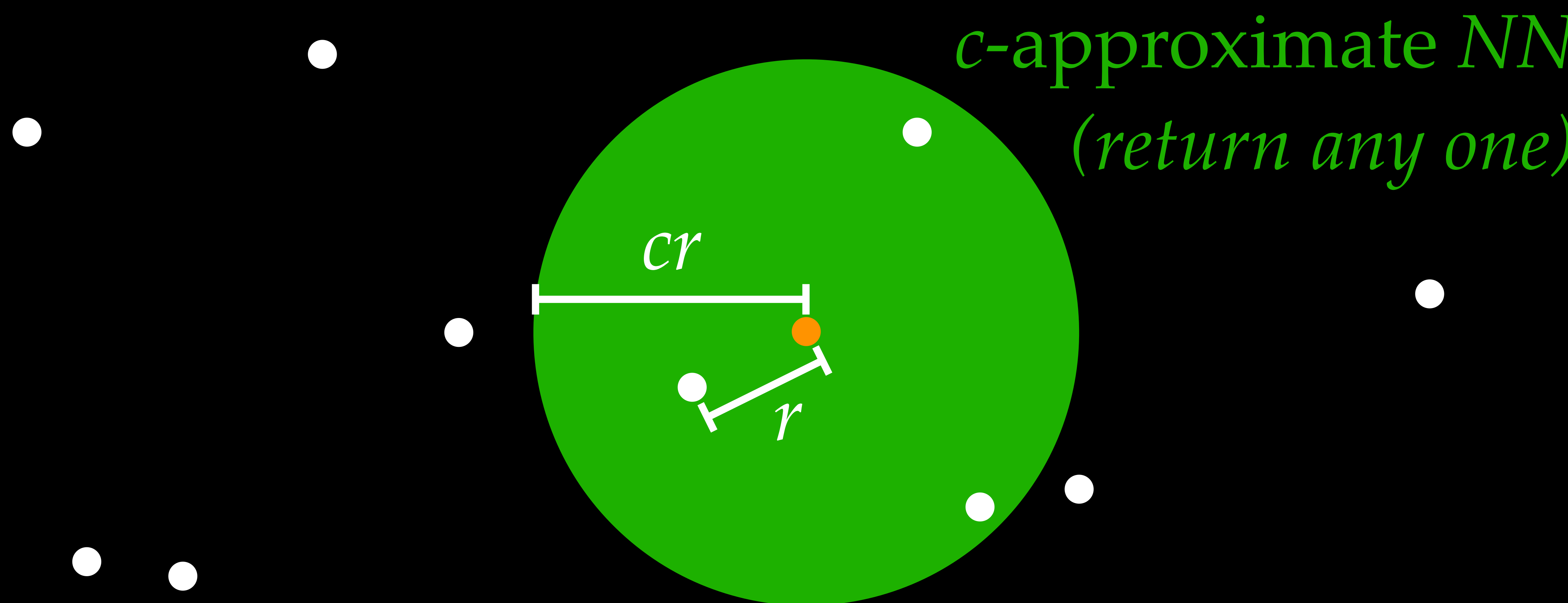

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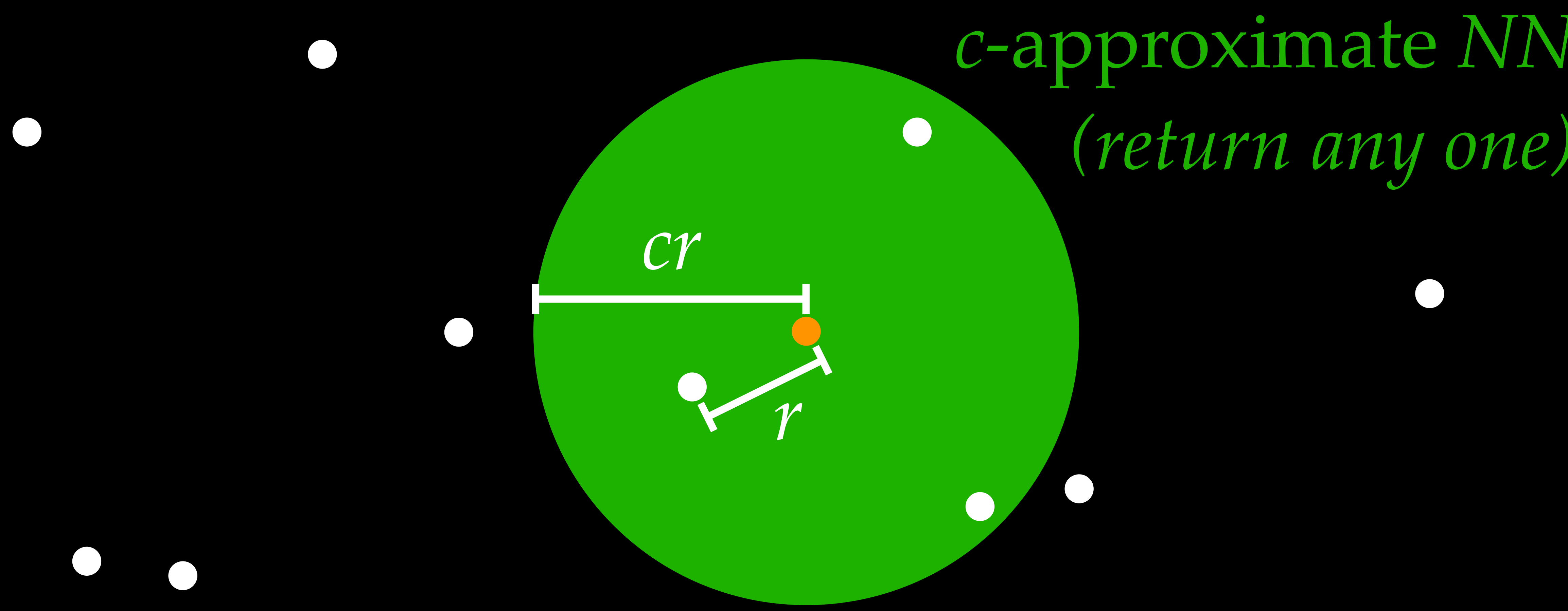
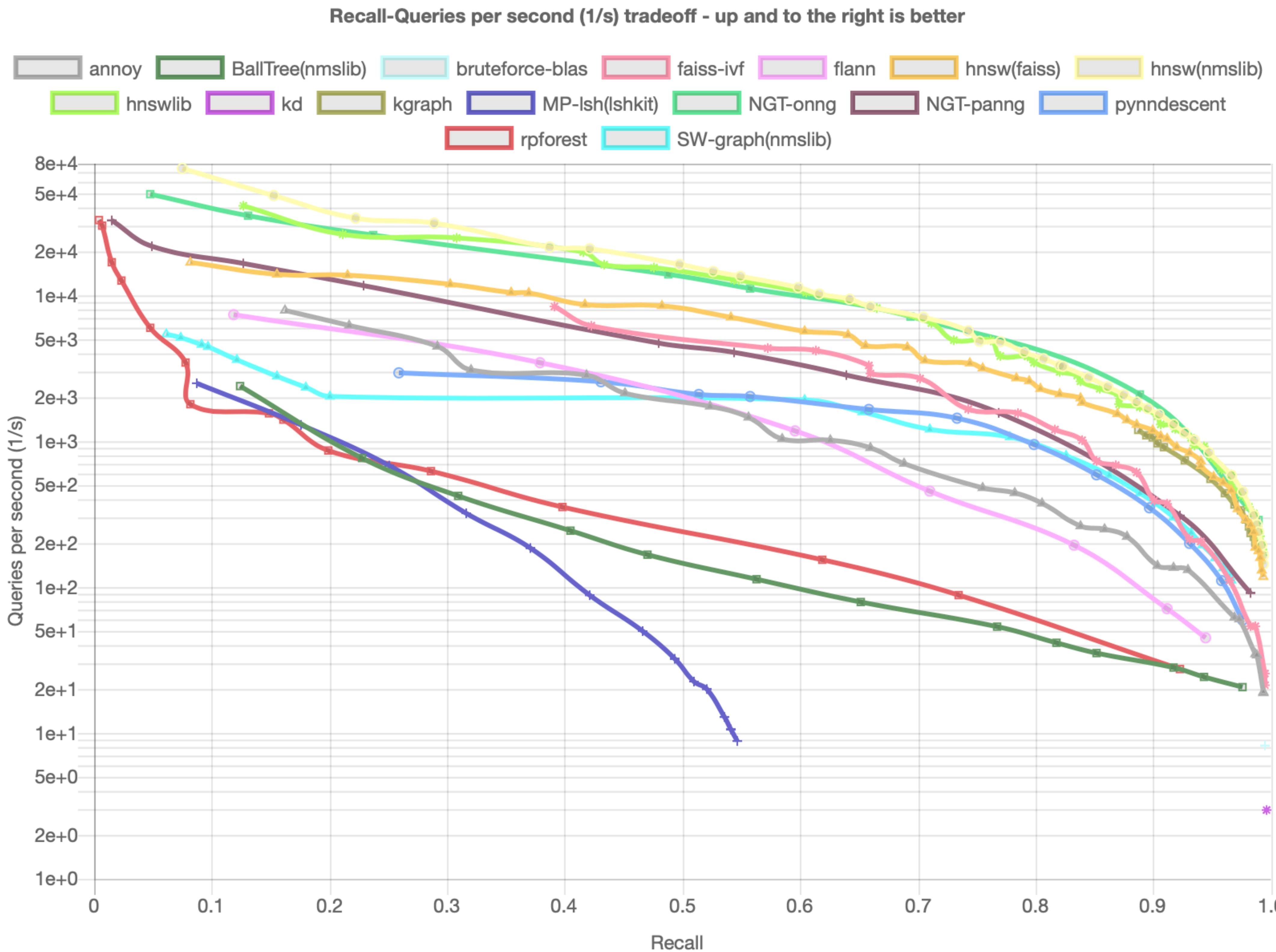
Time $n^{\rho(c)}$ and space $n^{1+\rho(c)}$, $\rho(c) < 1$ for $c > 1$



Approximate NN in practice



ann-benchmarks.com

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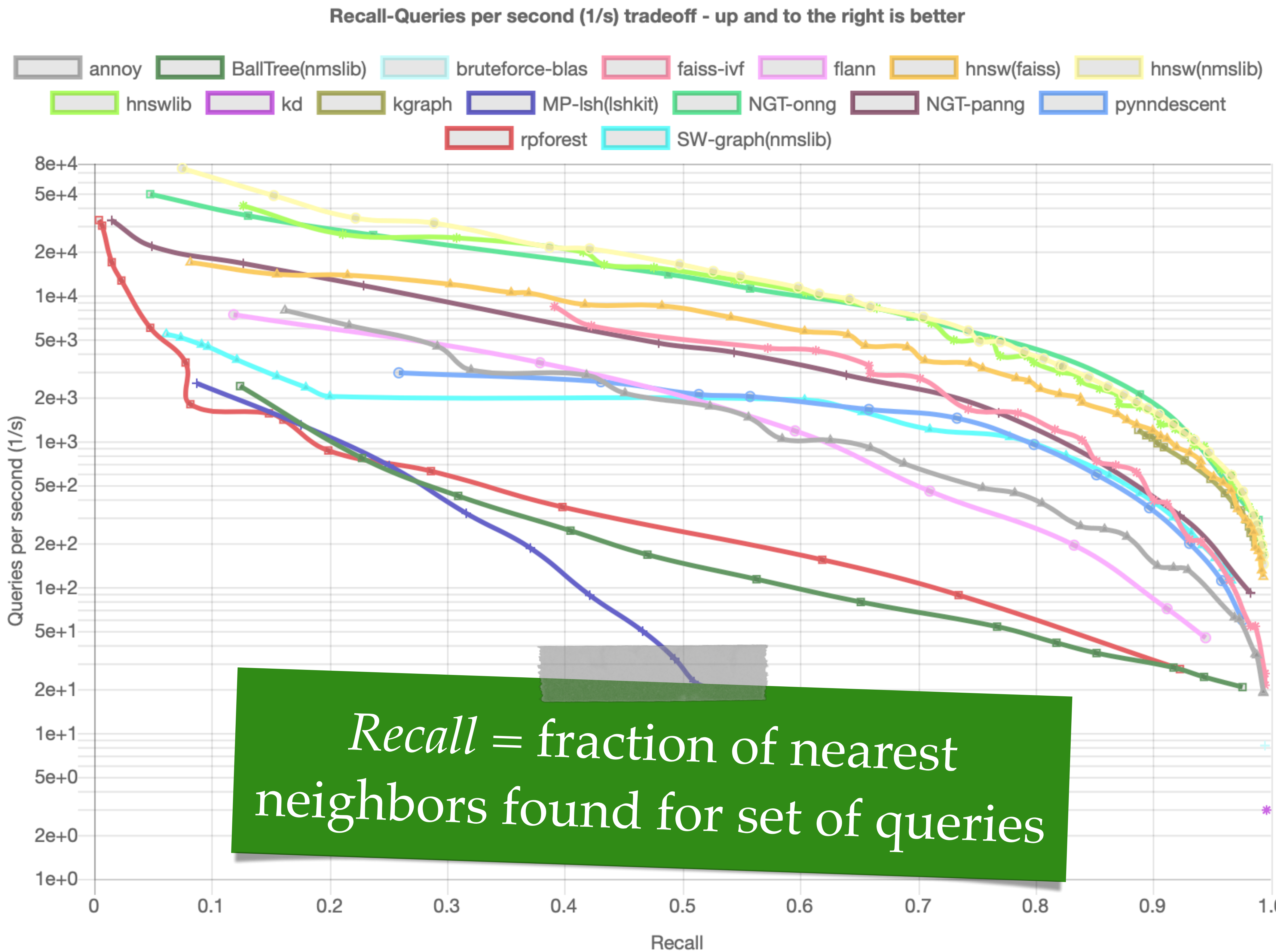

Recall = fraction of nearest neighbors found for set of queries

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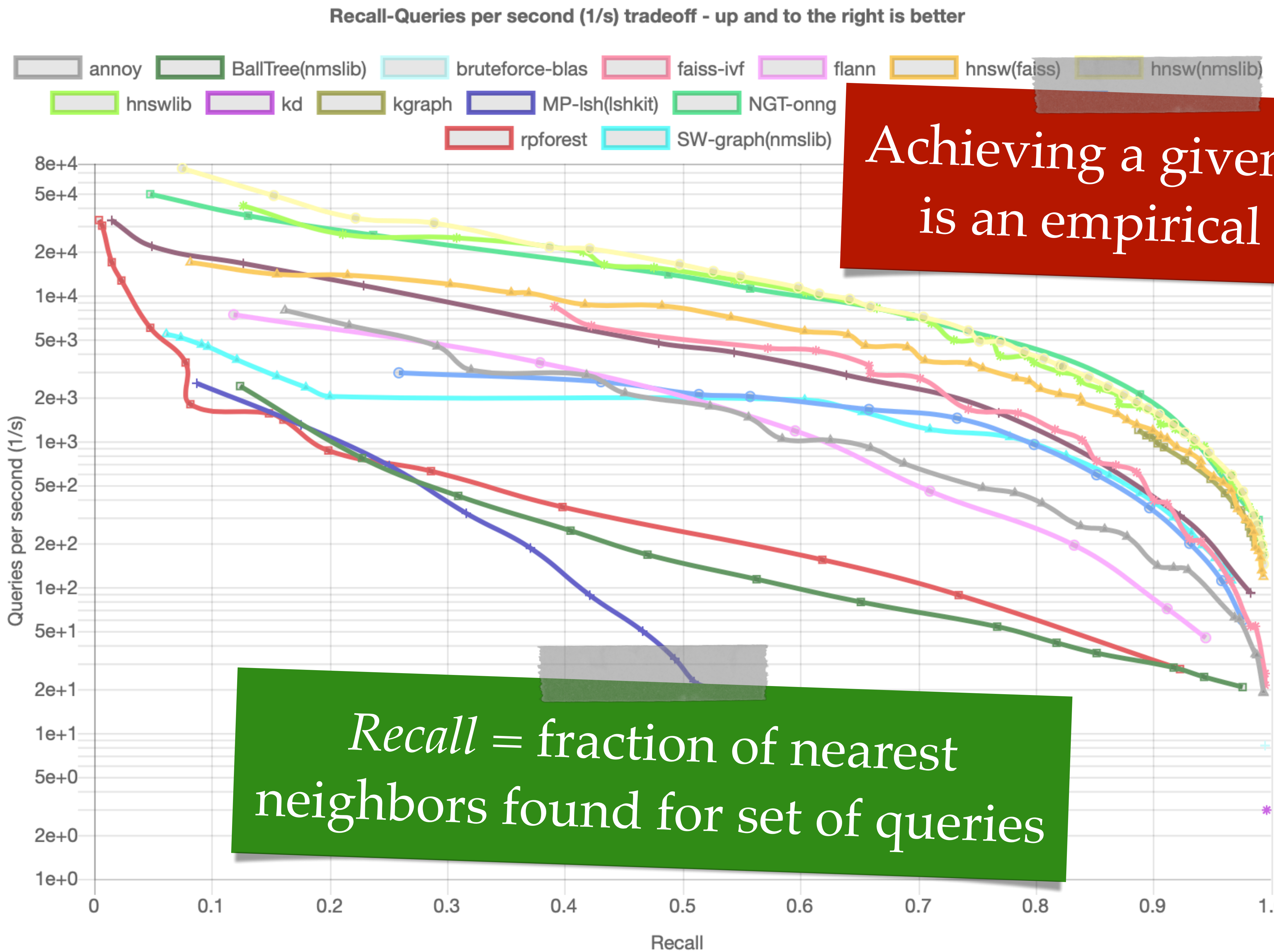

Achieving a given recall is an empirical task

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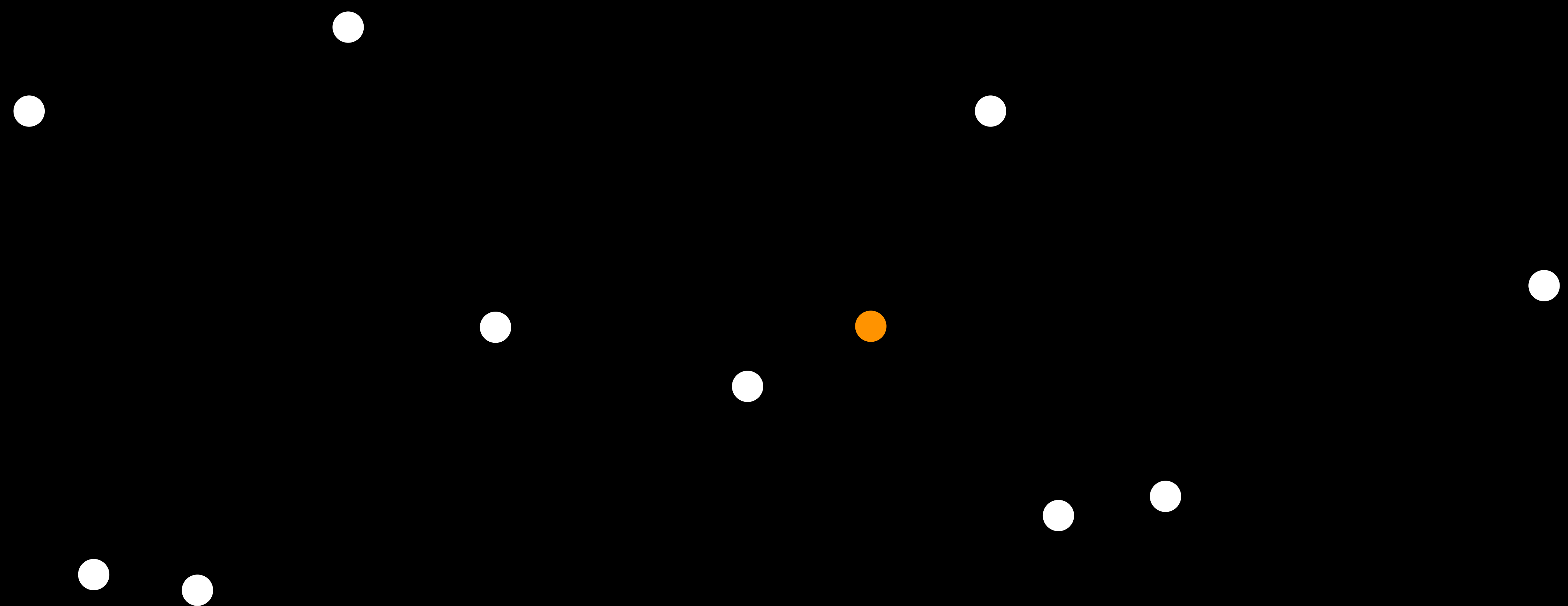
NN *recall* guarantee?

Black-box reduction: Choose c small enough to distinguish nearest neighbor from other points.



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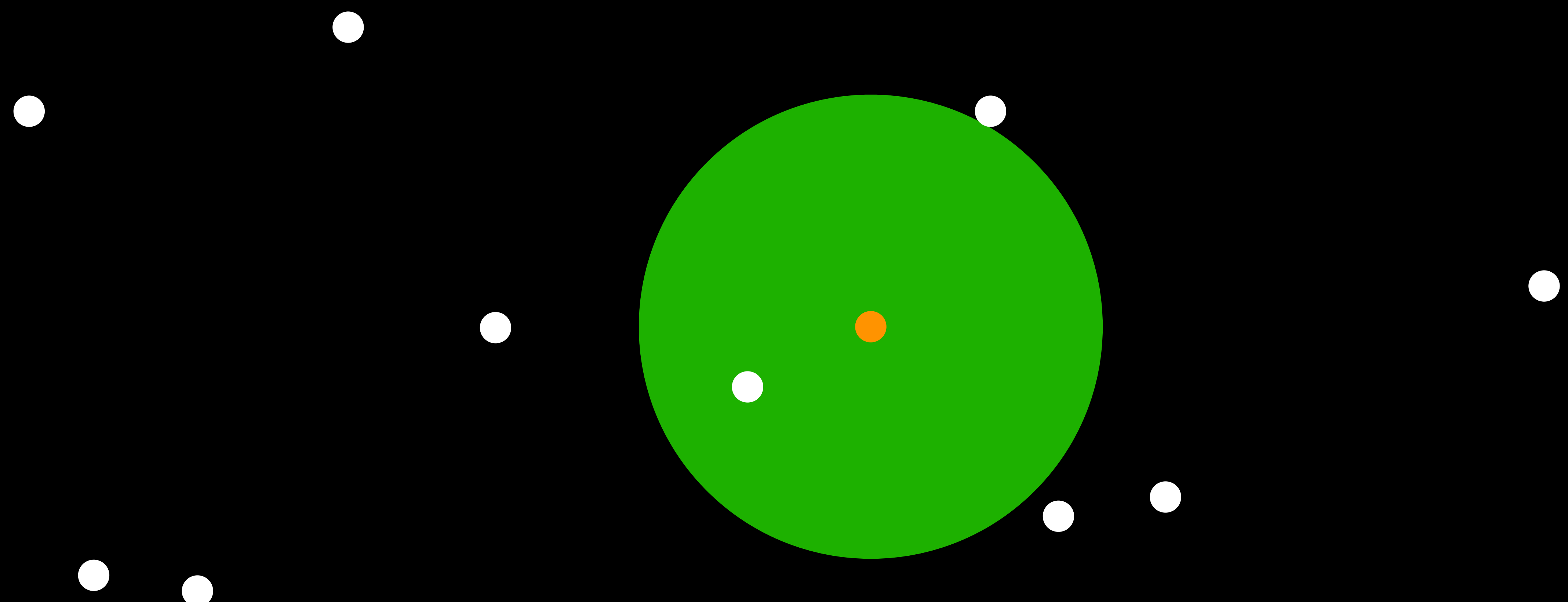

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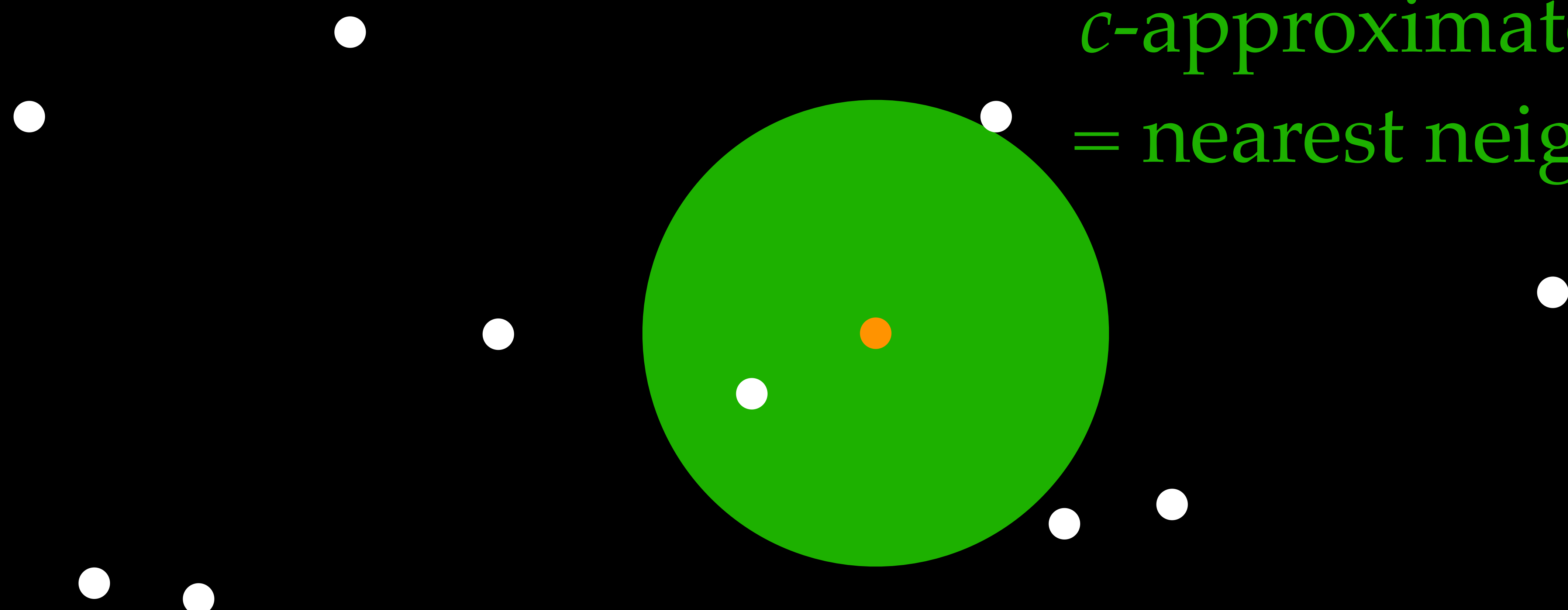
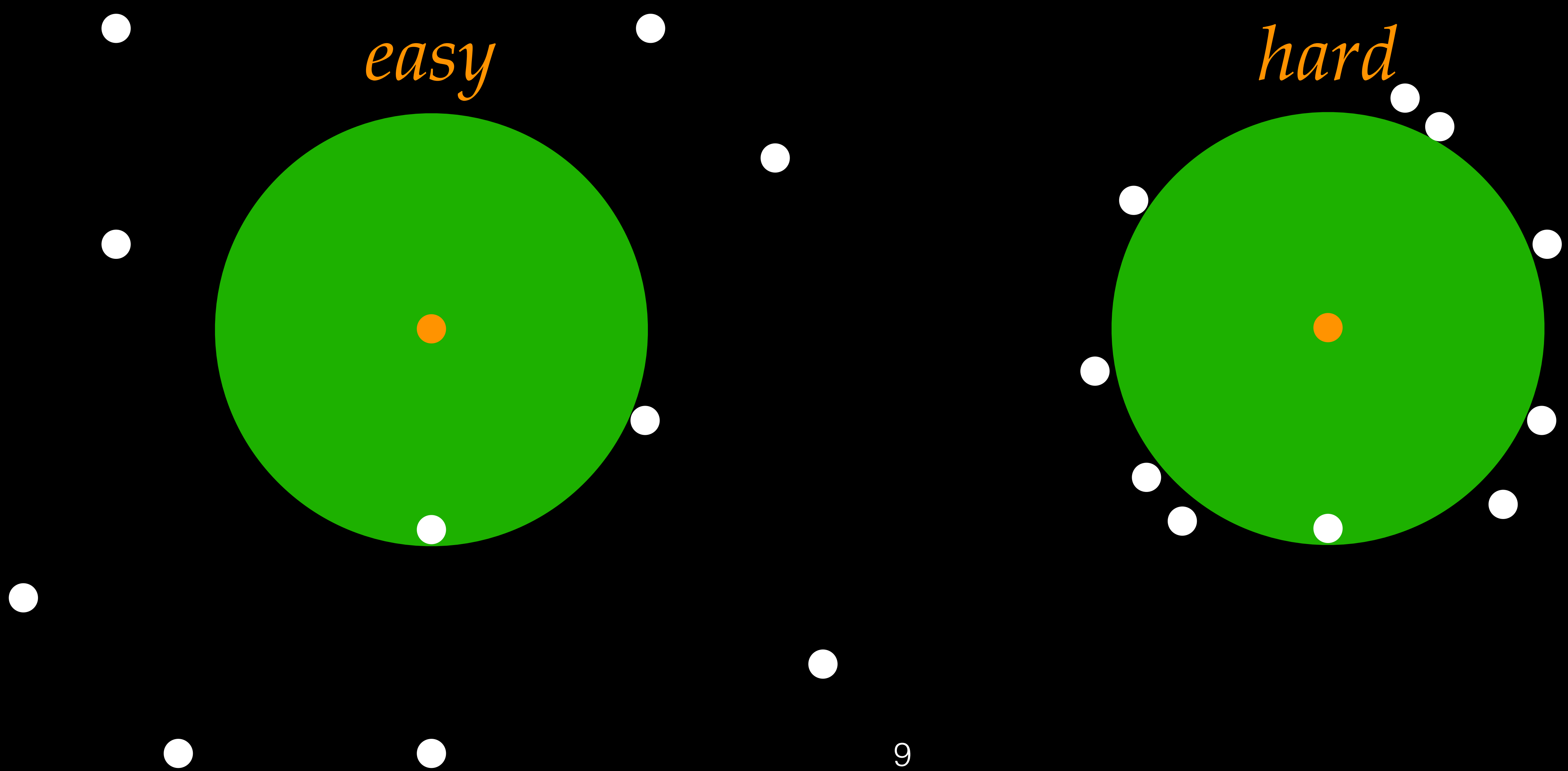


c-approximate *NN* = nearest neighbor

NN *recall* guarantee?

Black-box reduction does not distinguish easy and hard cases



[Panigrahy '06, Lv et al. '07]

LSH with multi-probing

- Building block: Linear space data structure (a hash table) that allows us to retrieve x_i with probability p_i.
    - Let p_1 = retrieval probability of nearest neighbor

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$$(1 - p_1)^L$$

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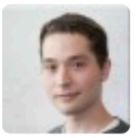
Need $L \approx \ln(1/\delta)/p_1$ for expected recall 1-δ

From FALCONN documentation



ilyaraz #1

152 commits 165,070 ++ 63,535 --

ludwigschmidt #2

90 commits 278,244 ++ 16,349 --

Choosing parameters

All in all, we have three parameters:

- K, the number of hash functions (space partitions) per hash table.
- L, the number of hash tables (each of which has K hash functions).
- T, the number of probes (total number of buckets probed across all hash tables).

Usually, it is a good idea to choose L first based on the available memory. Then, we have a trade-off between K and T: the larger K is, the more probes we need to achieve a given probability of success, and vice versa. The best way to choose K and T is usually the following parameter search: Try increasing values of K, and for each value of K, find the right number of probes T so that we get the desired accuracy on a set of sample queries. Varying the parameter T does not require rebuilding the hash table (as opposed to K and L). Moreover, we can search over T using a binary search. Usually, this means that we can find the optimal parameter setting fairly quickly.

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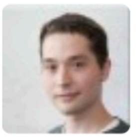

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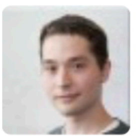

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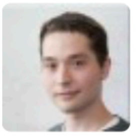

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In theory: "Only polylog n different parameter choices"

[Dong et al. ’08]

Adaptive stopping

Idea:

- Suppose that after searching t hash tables the nearest neighbor retrieved so far is x^*.
- Let p^* denote the probability that x* is retrieved in a hash table.
- If $t > \ln(1/\delta)/p^*$ then stop and return x^*.

[Dong et al. ’08]

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Issue: Need way of computing p^*.

Abstract view

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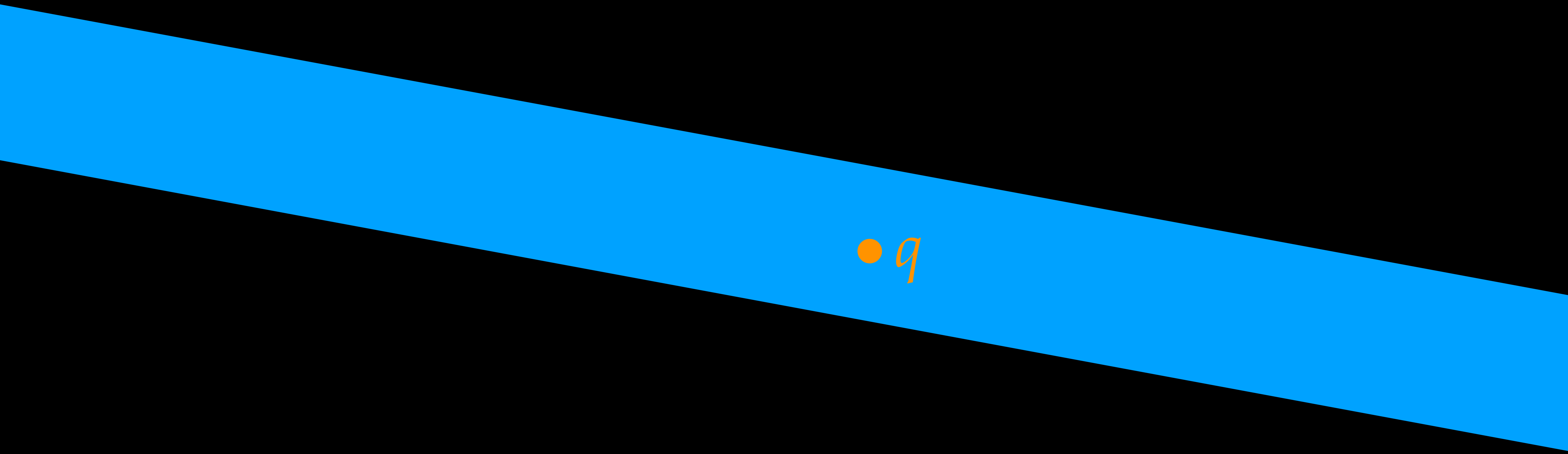

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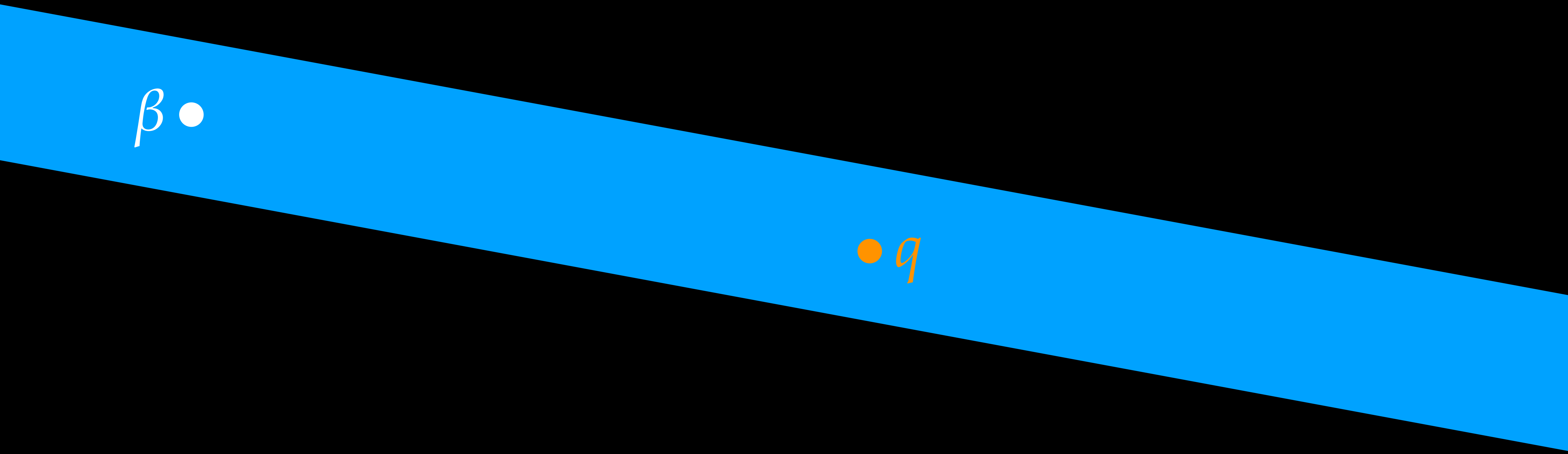

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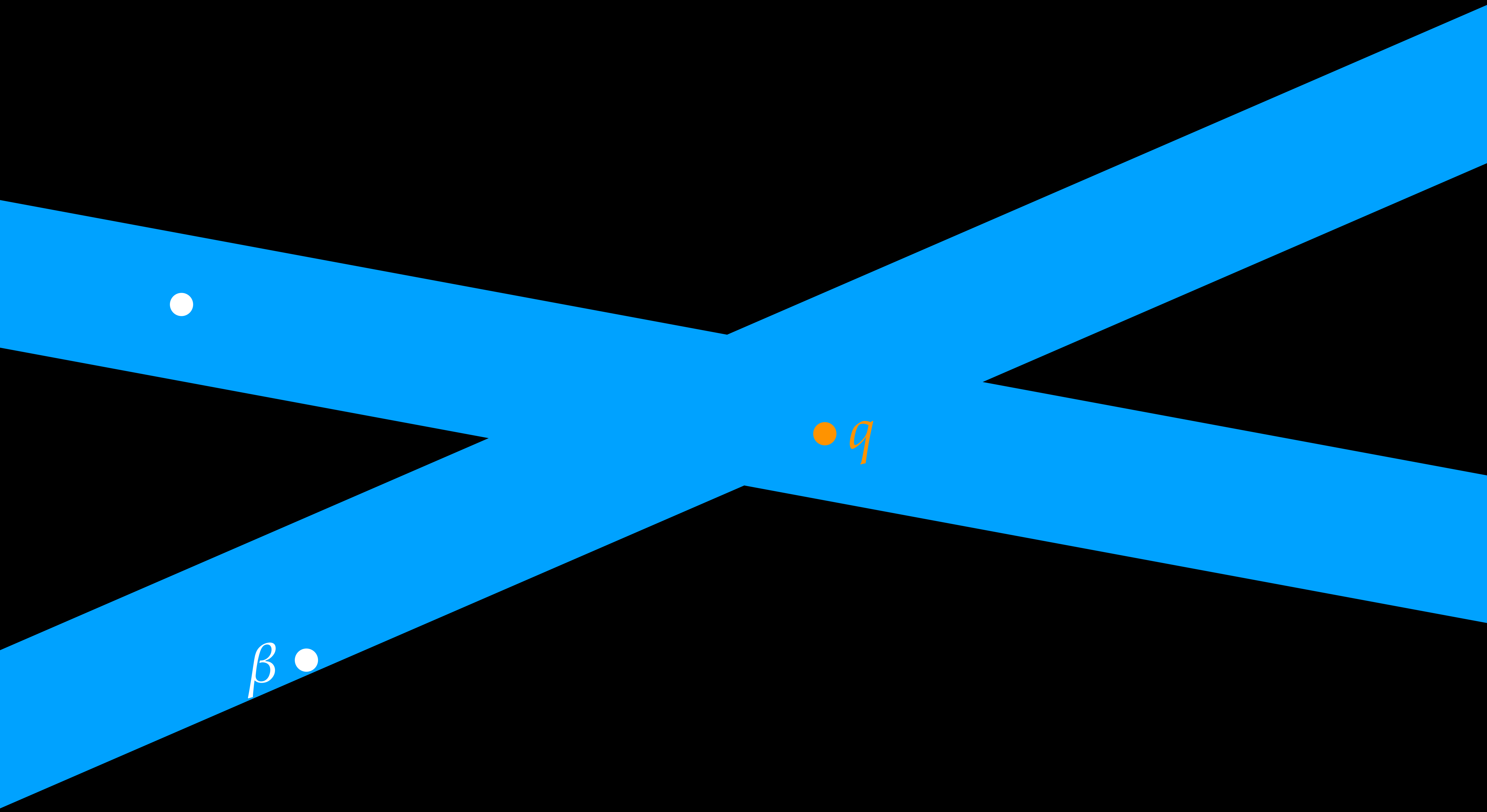

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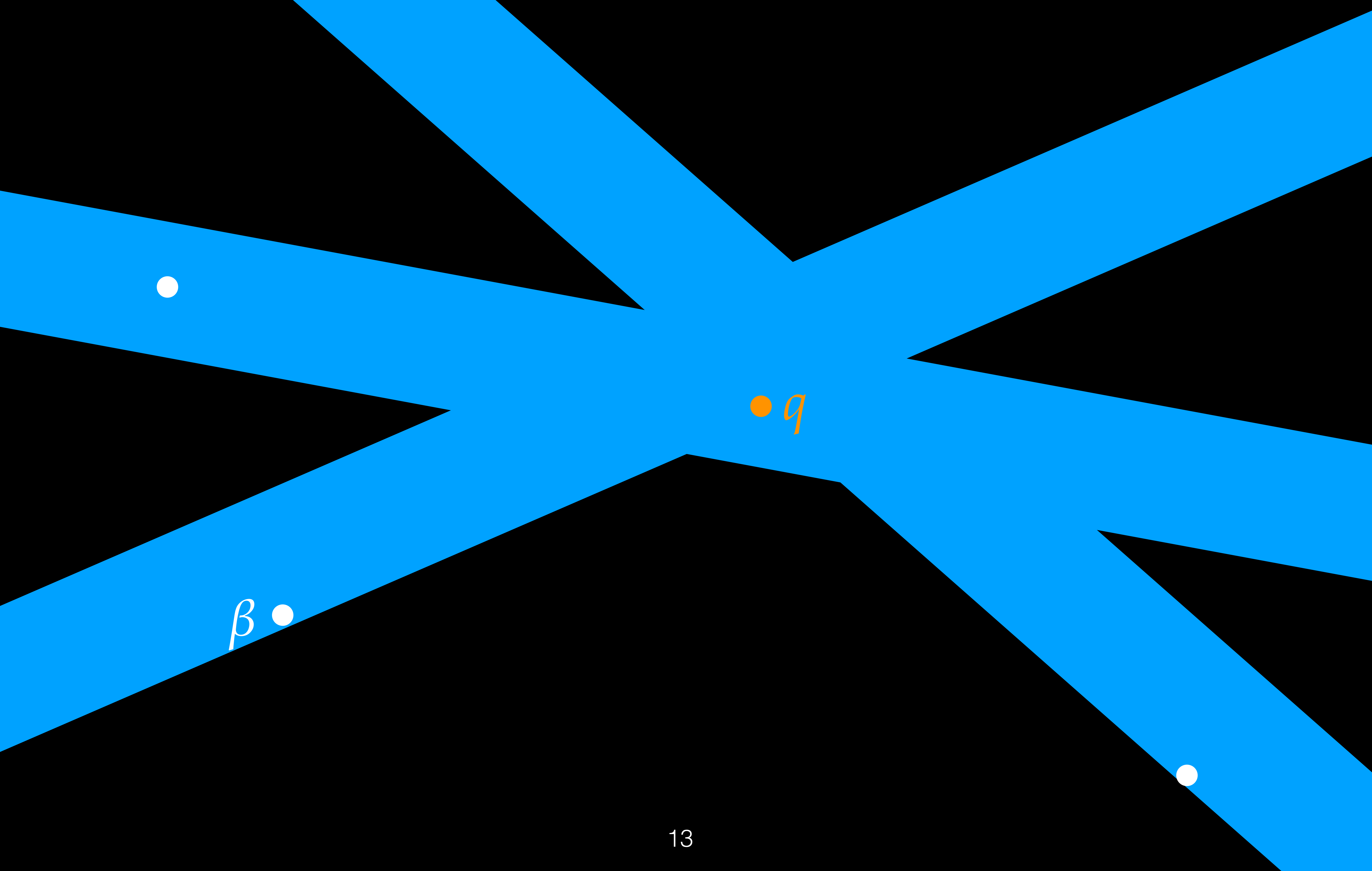

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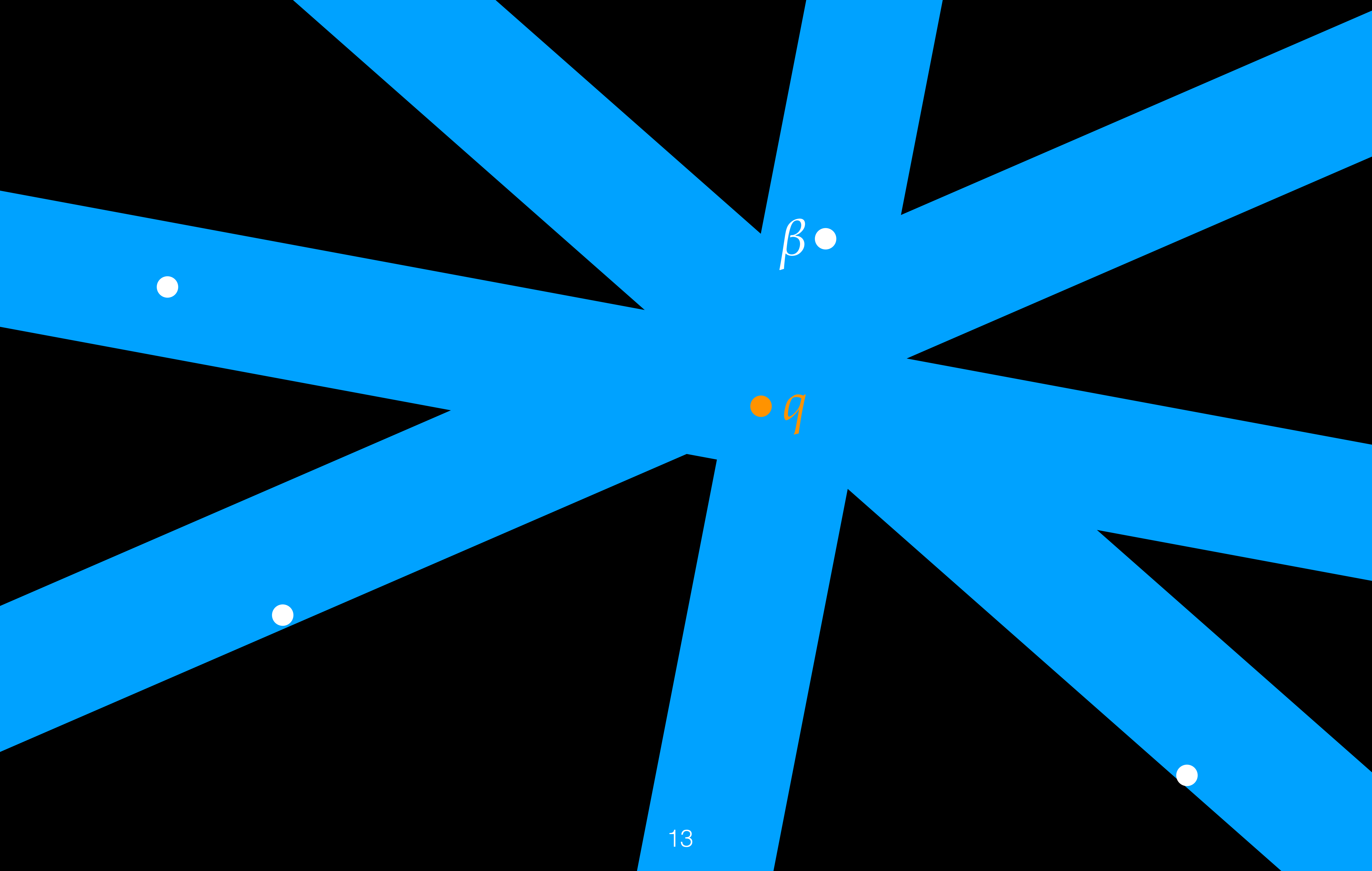

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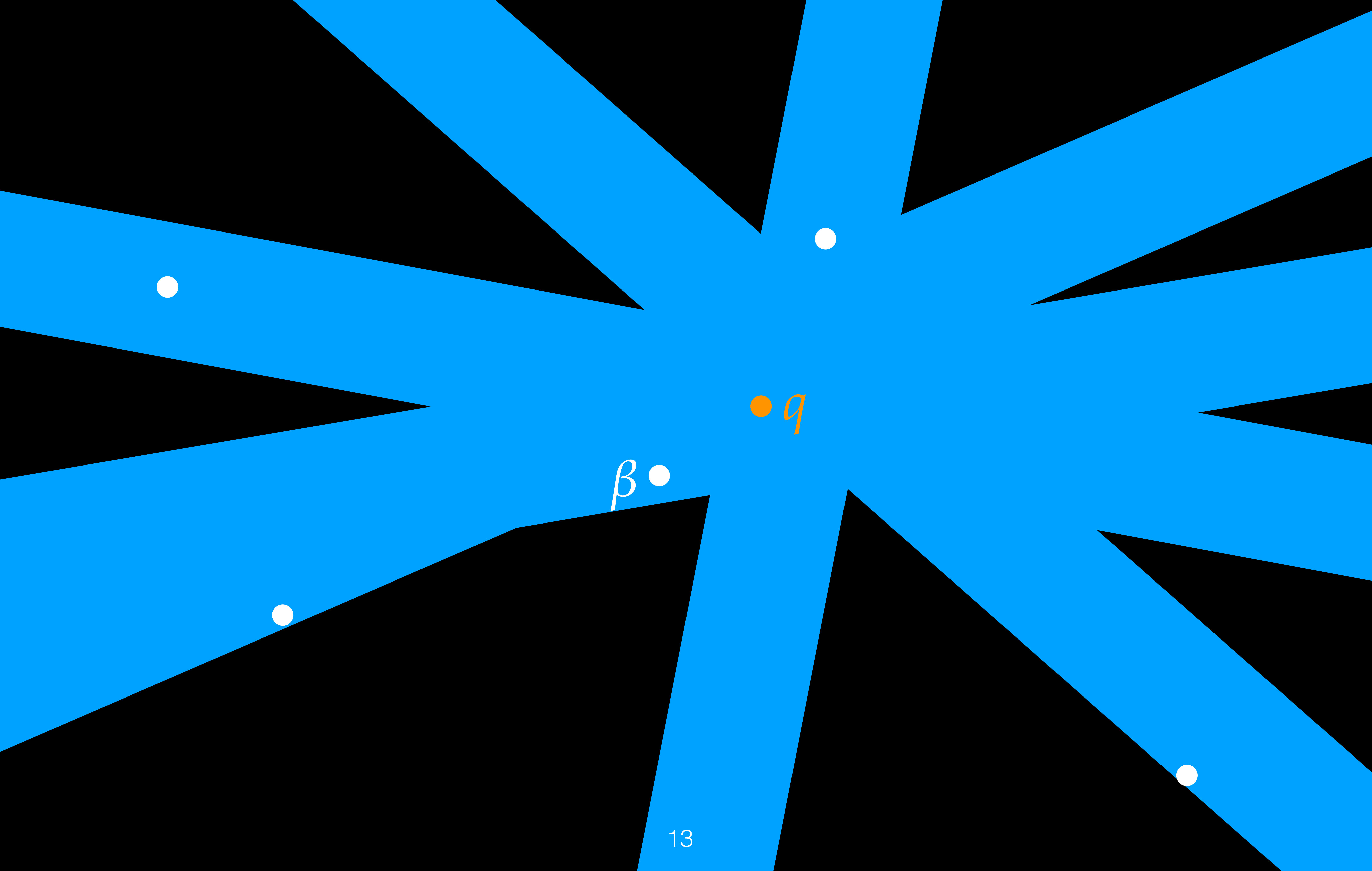

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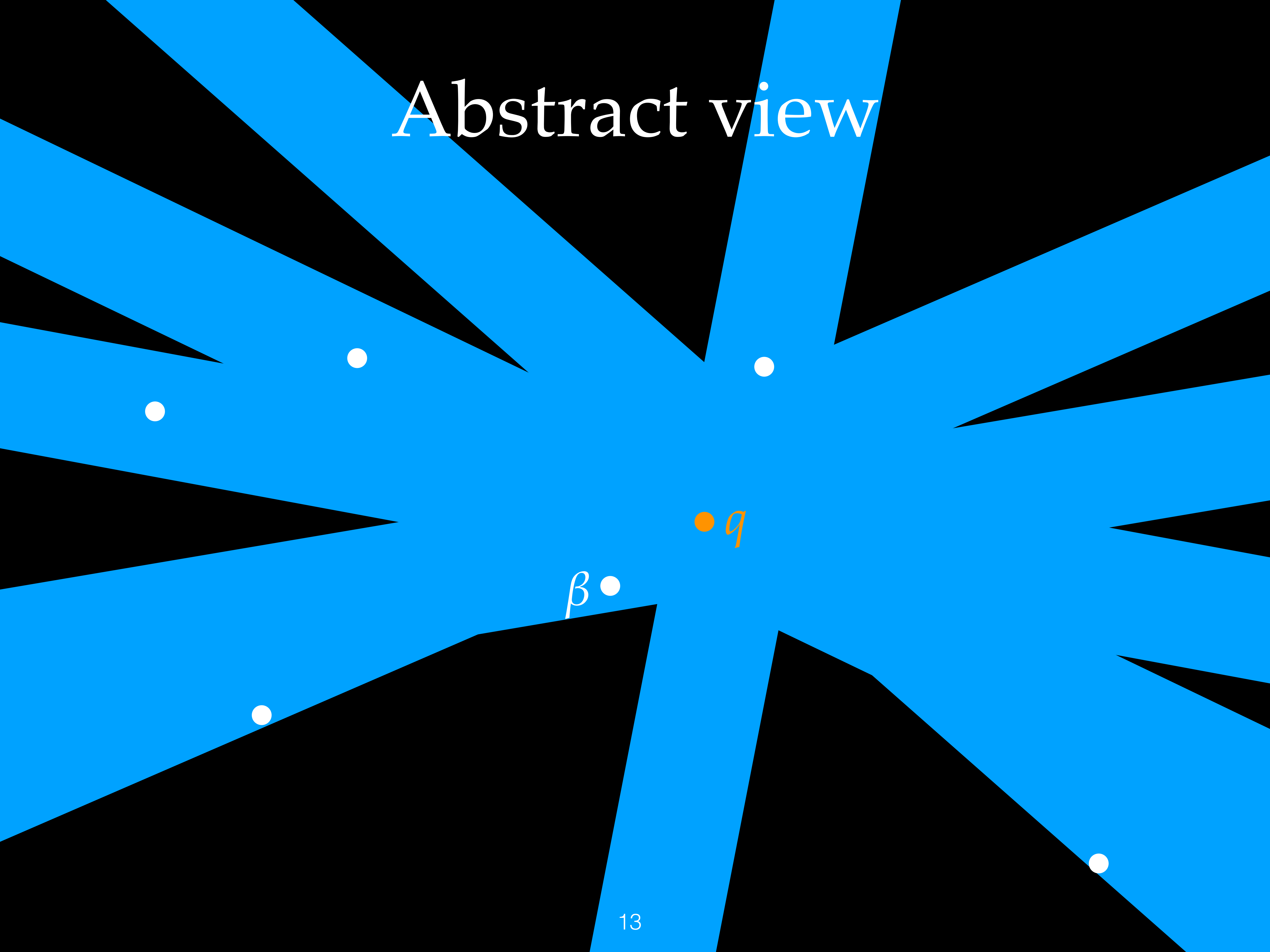

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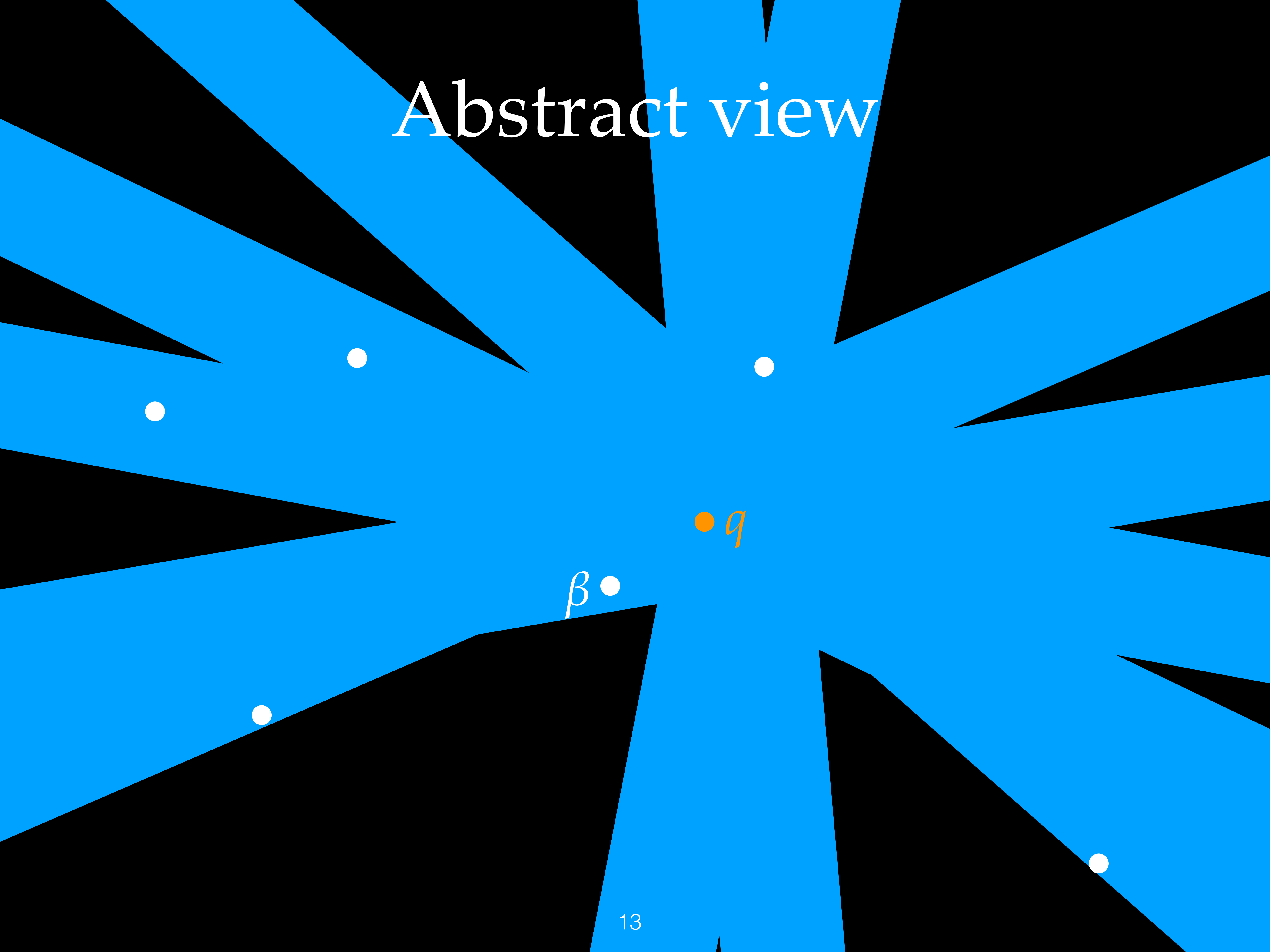

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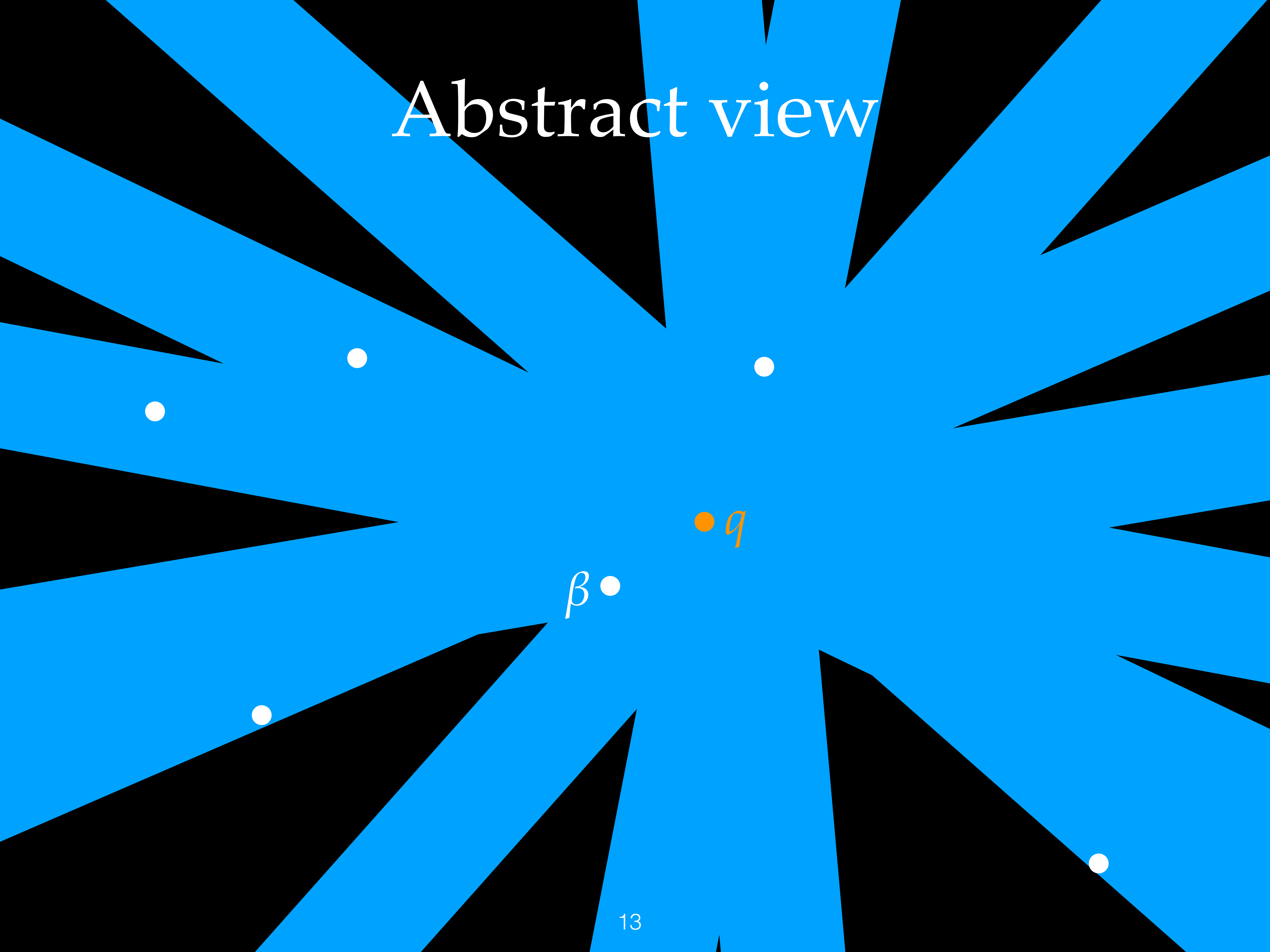

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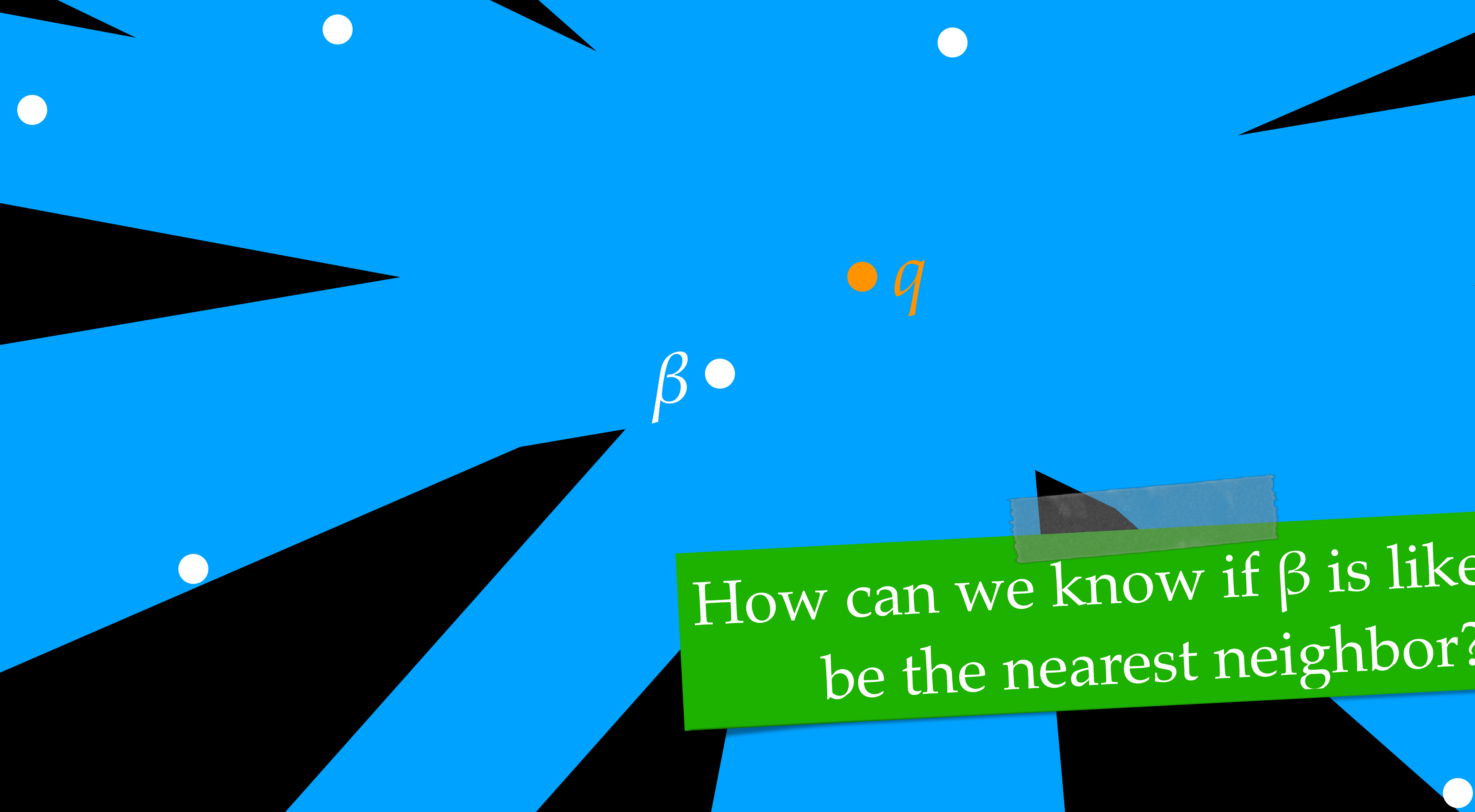

How can we know if β is likely to be the nearest neighbor?

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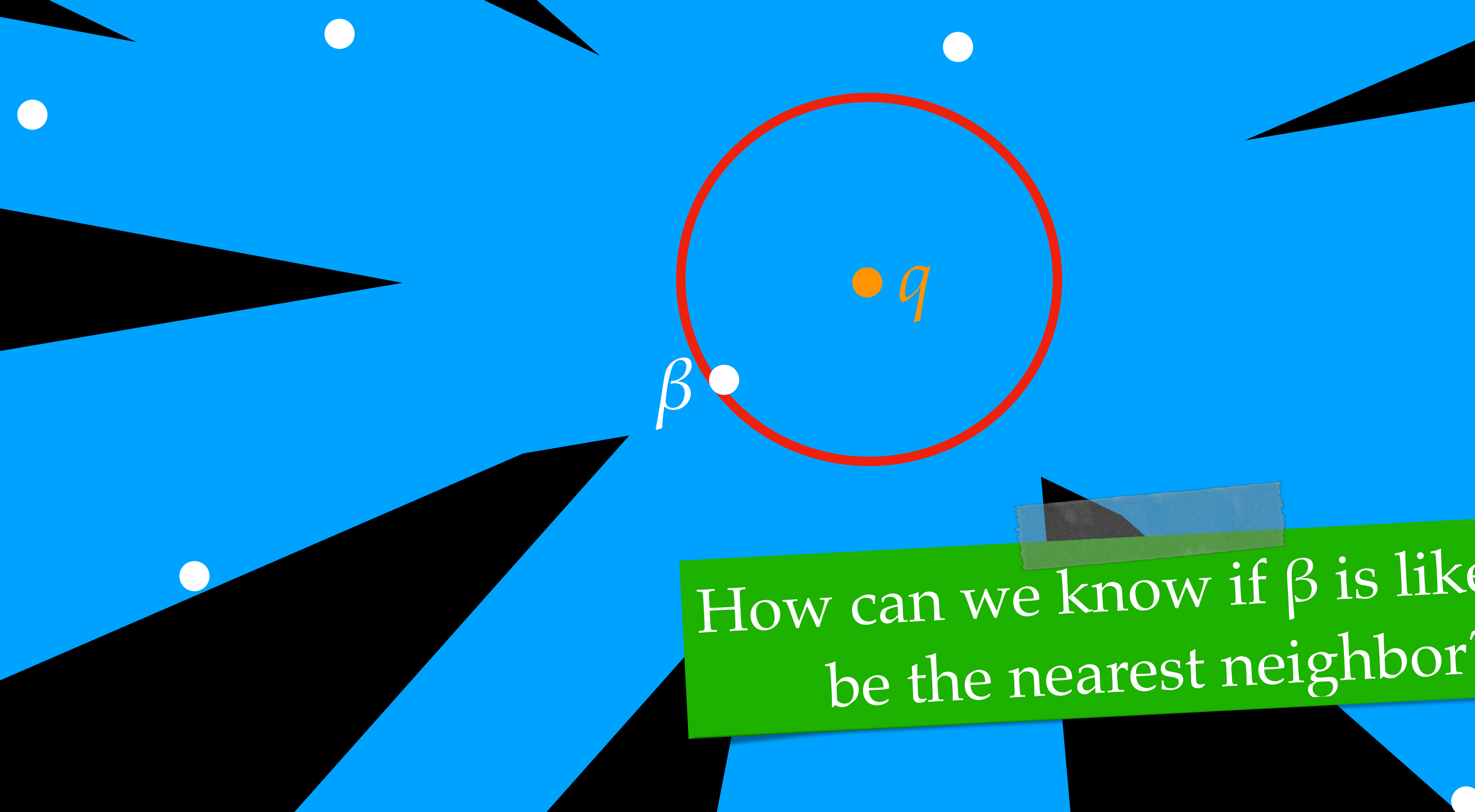

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Confirmation sampling

- Notation: Repetition i produces *one* nearest neighbor candidate y_i, independently for each i.
- Let β_i be the nearest neighbor of q in $Y_i = \{y_1,\ldots,y_i\}$.

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Claim: If nearest neighbor is most likely to be a candidate, the probability of returning a different point is at most 2^{-t}.

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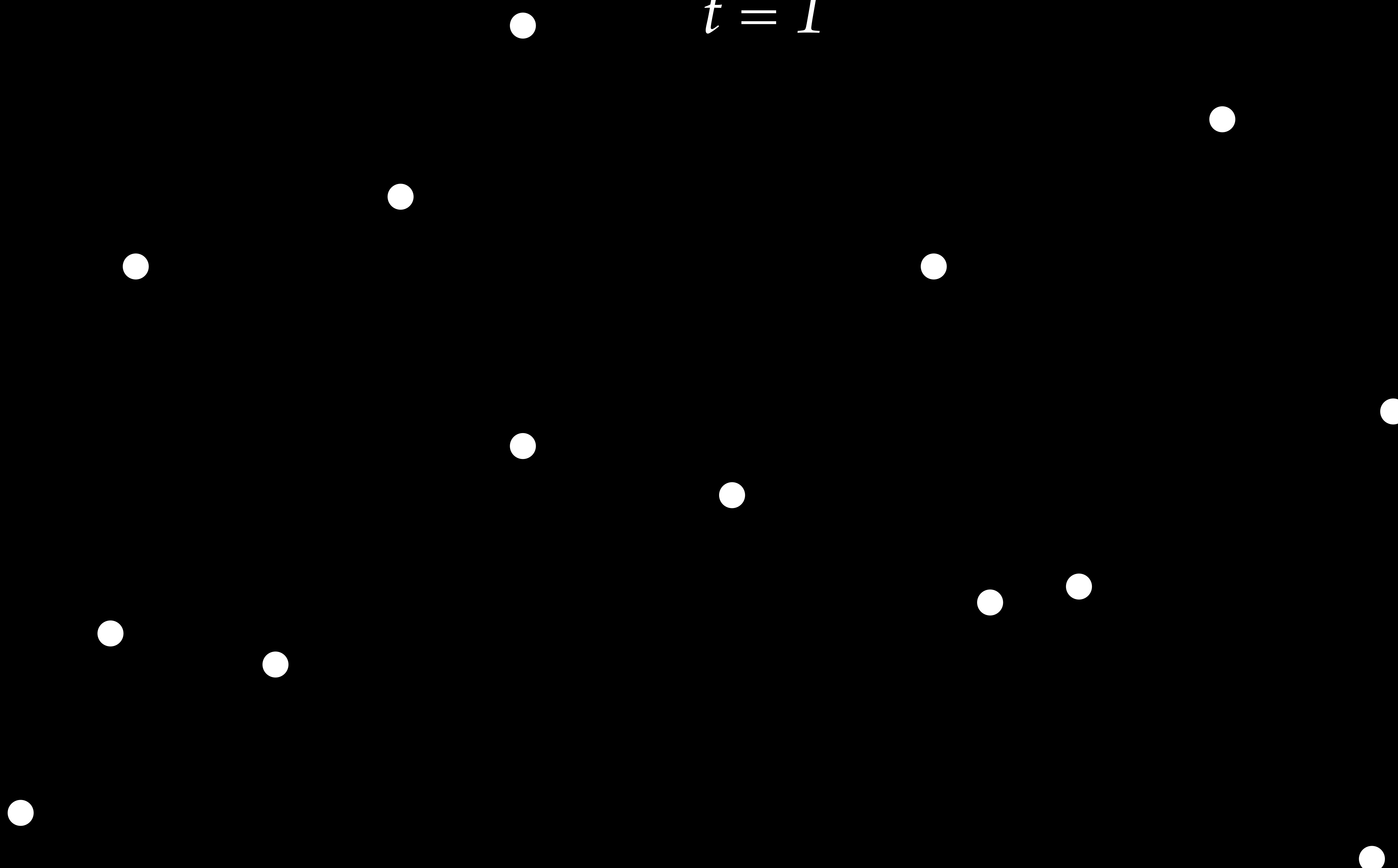
Confirmation sampling

$t = 1$



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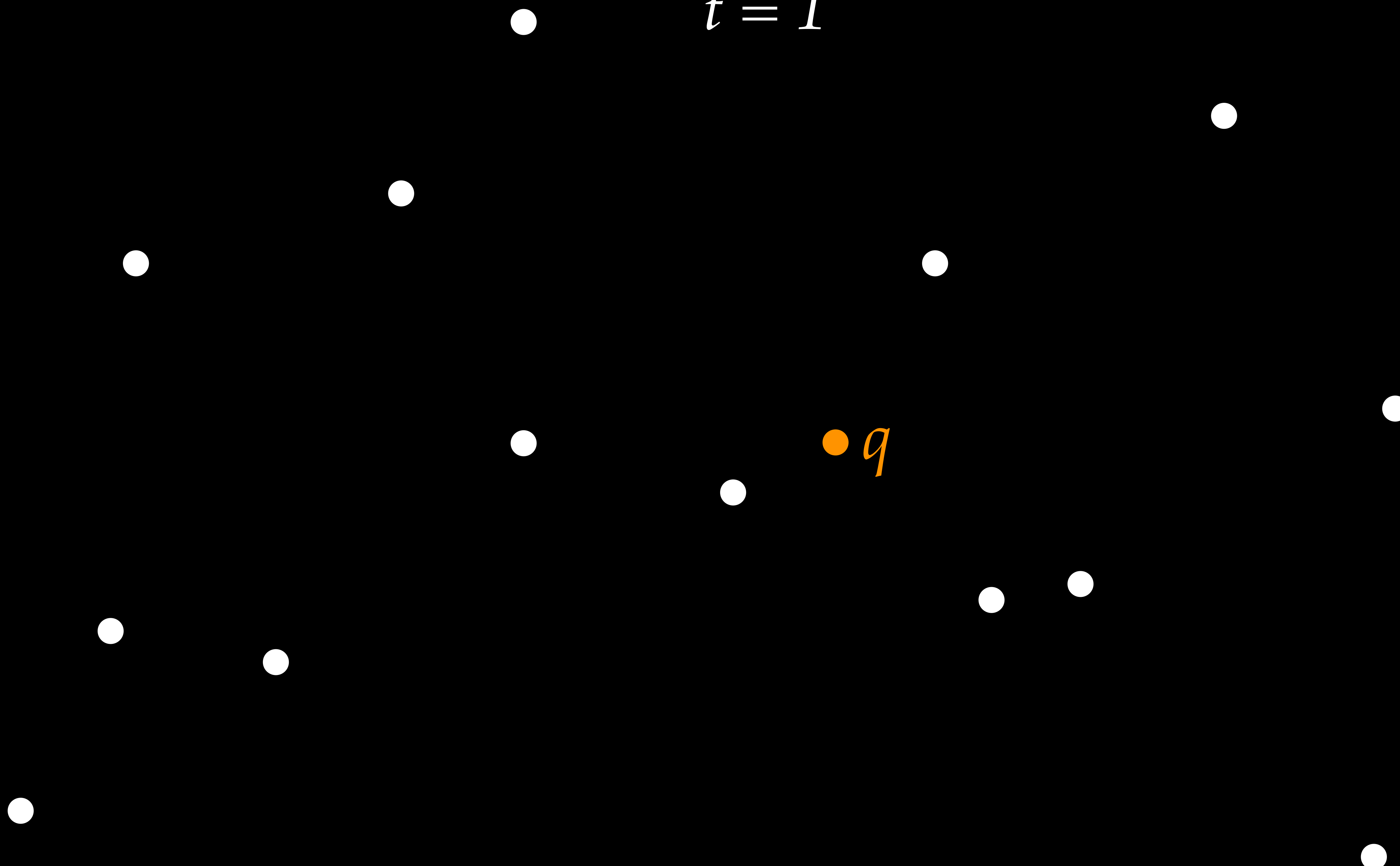

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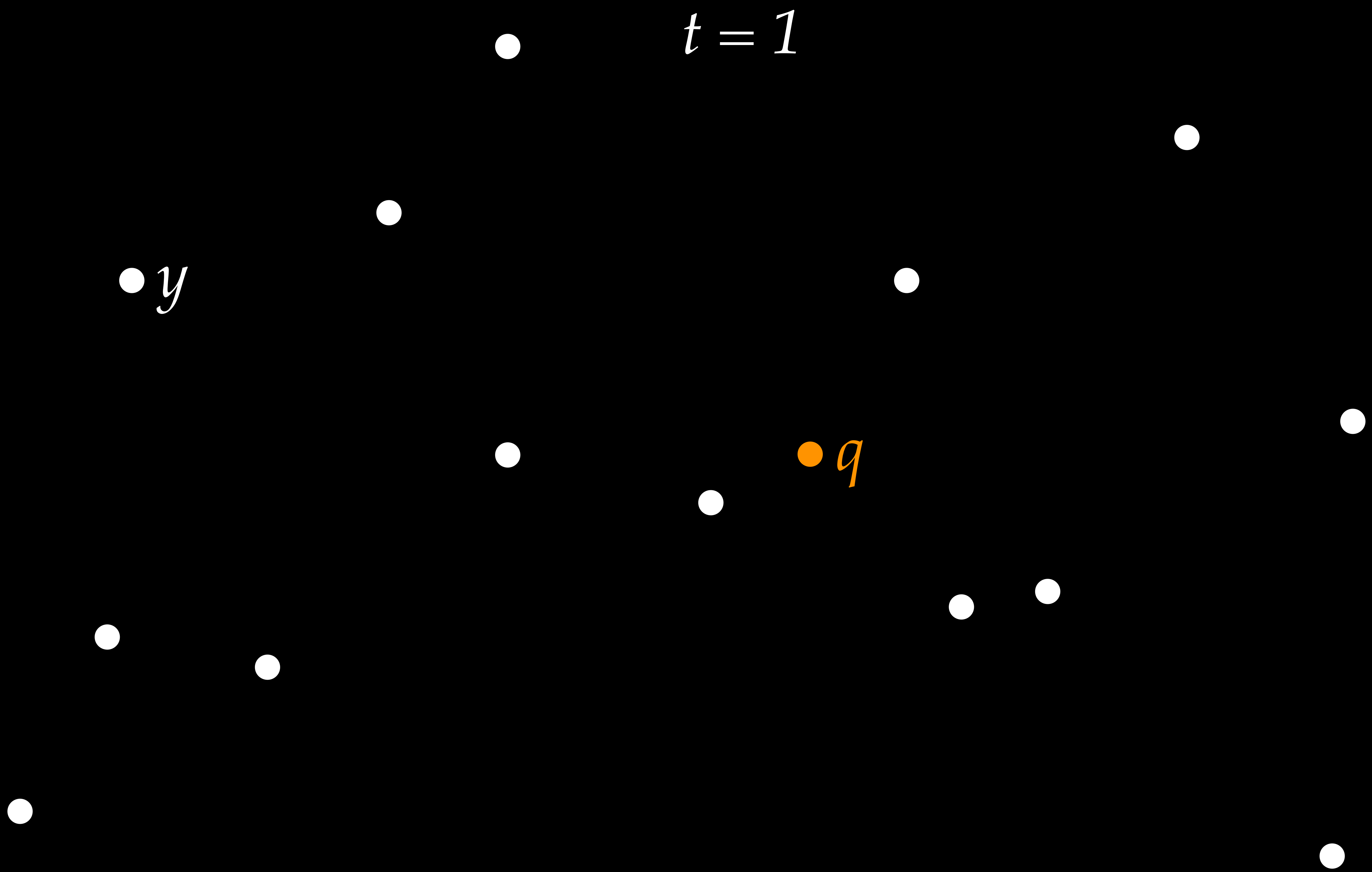

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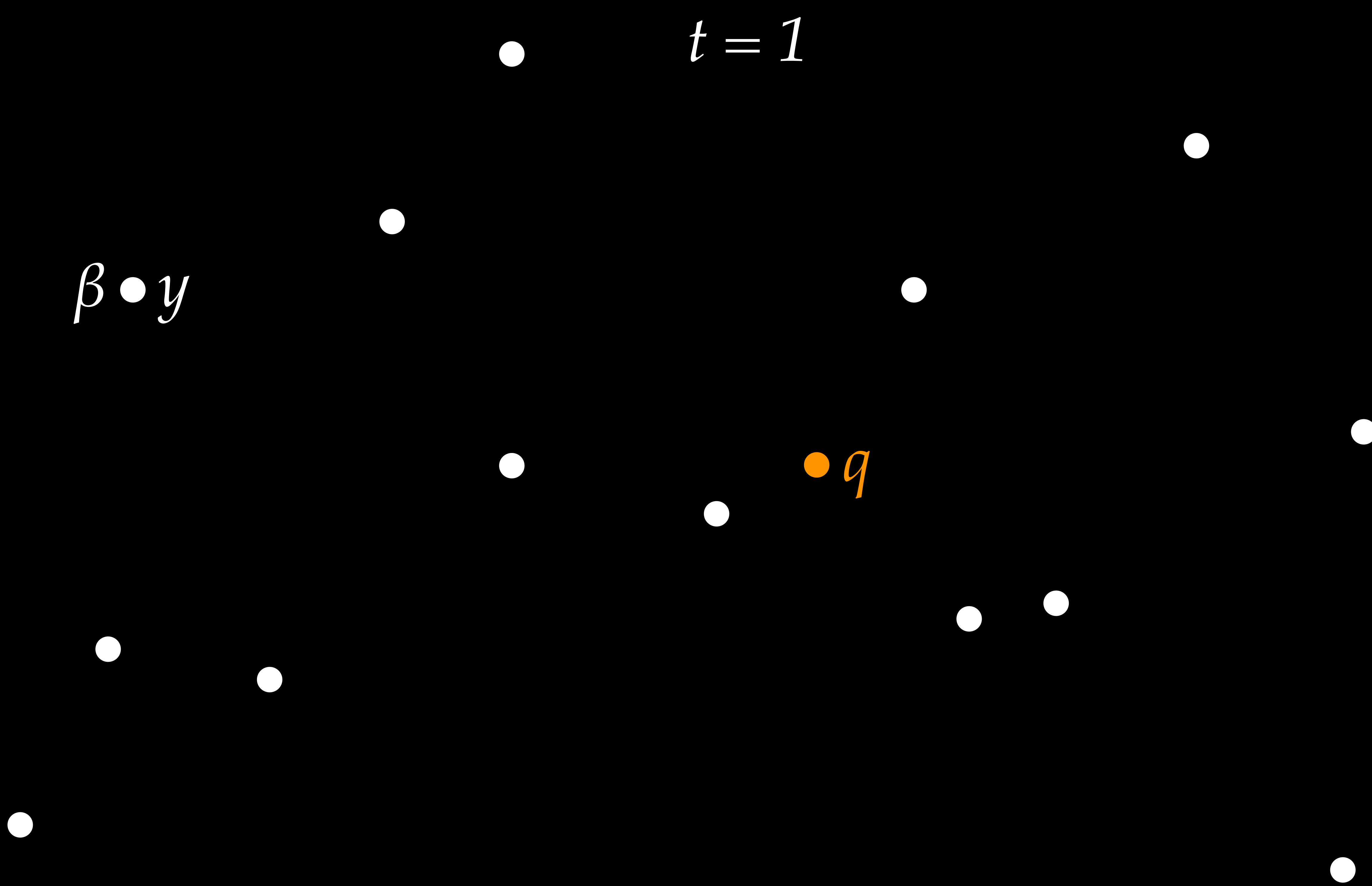

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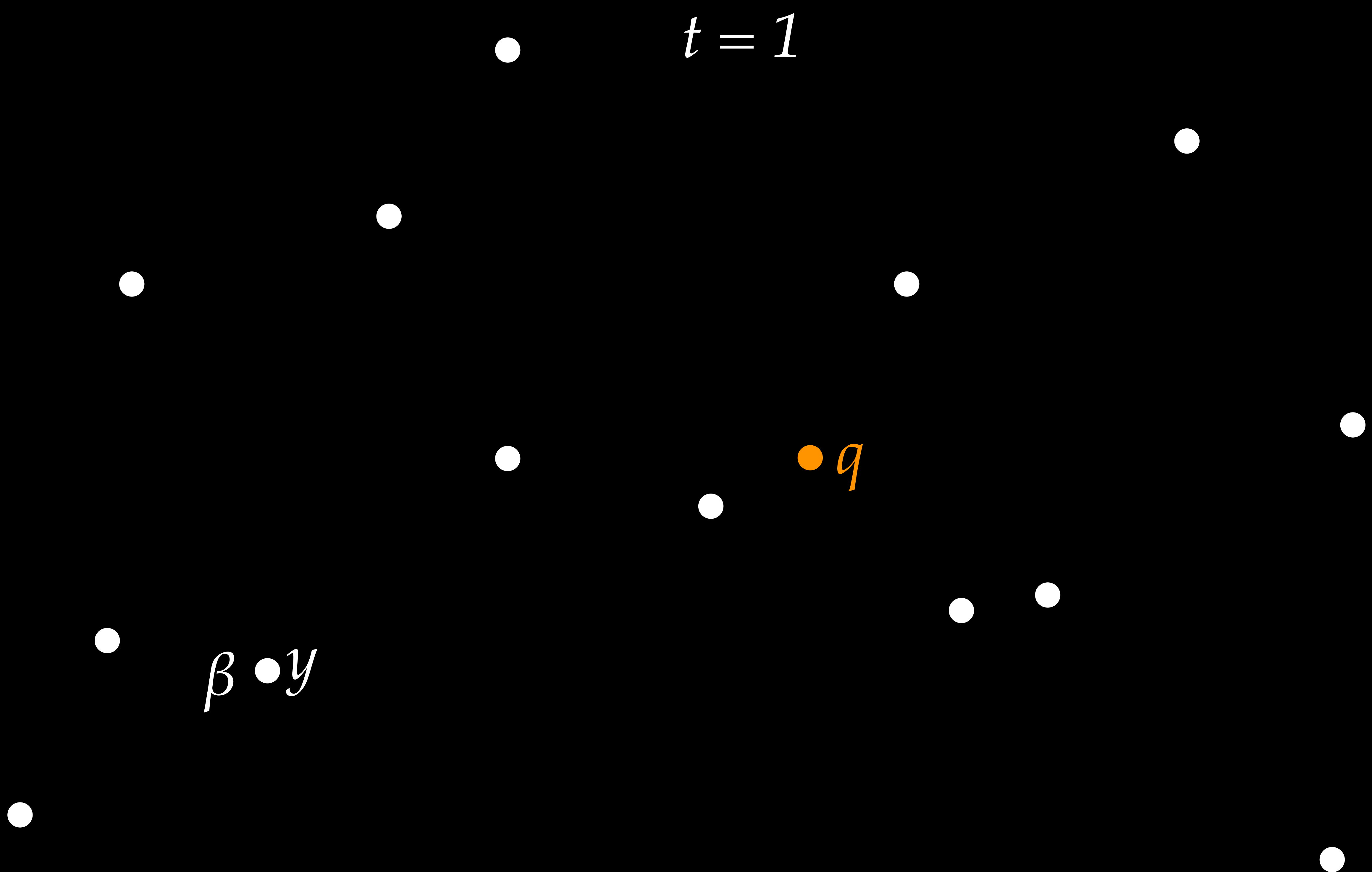

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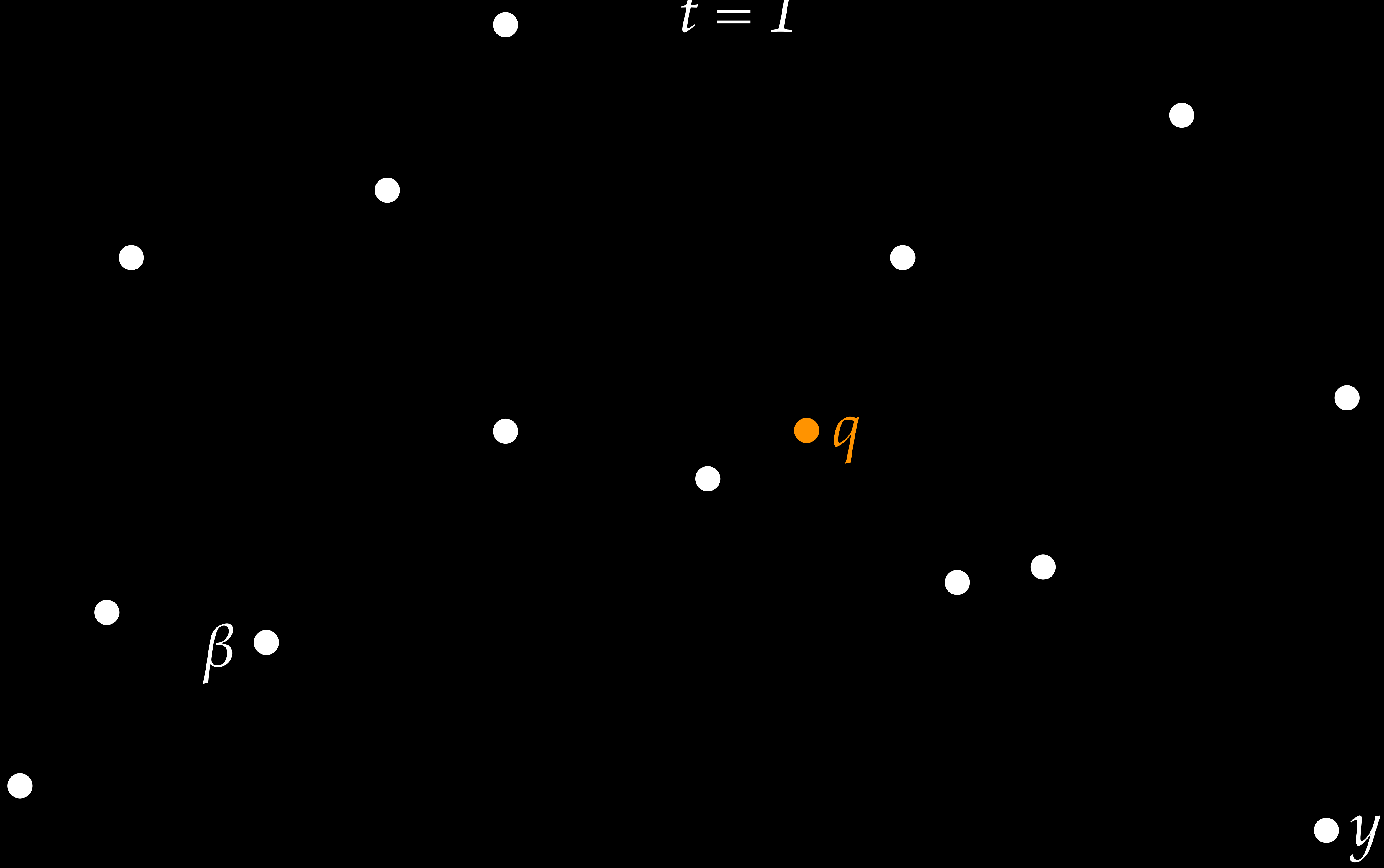

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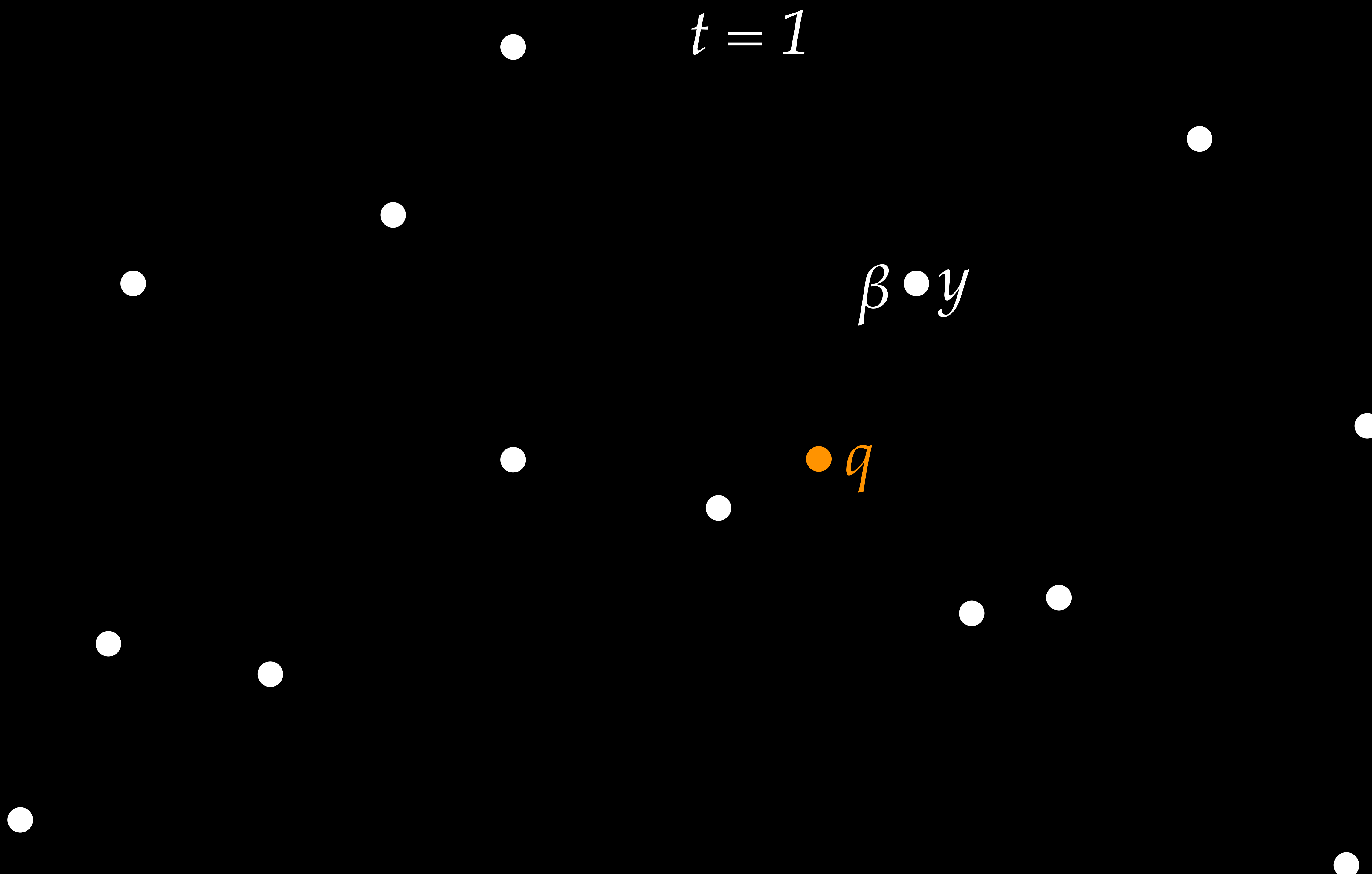

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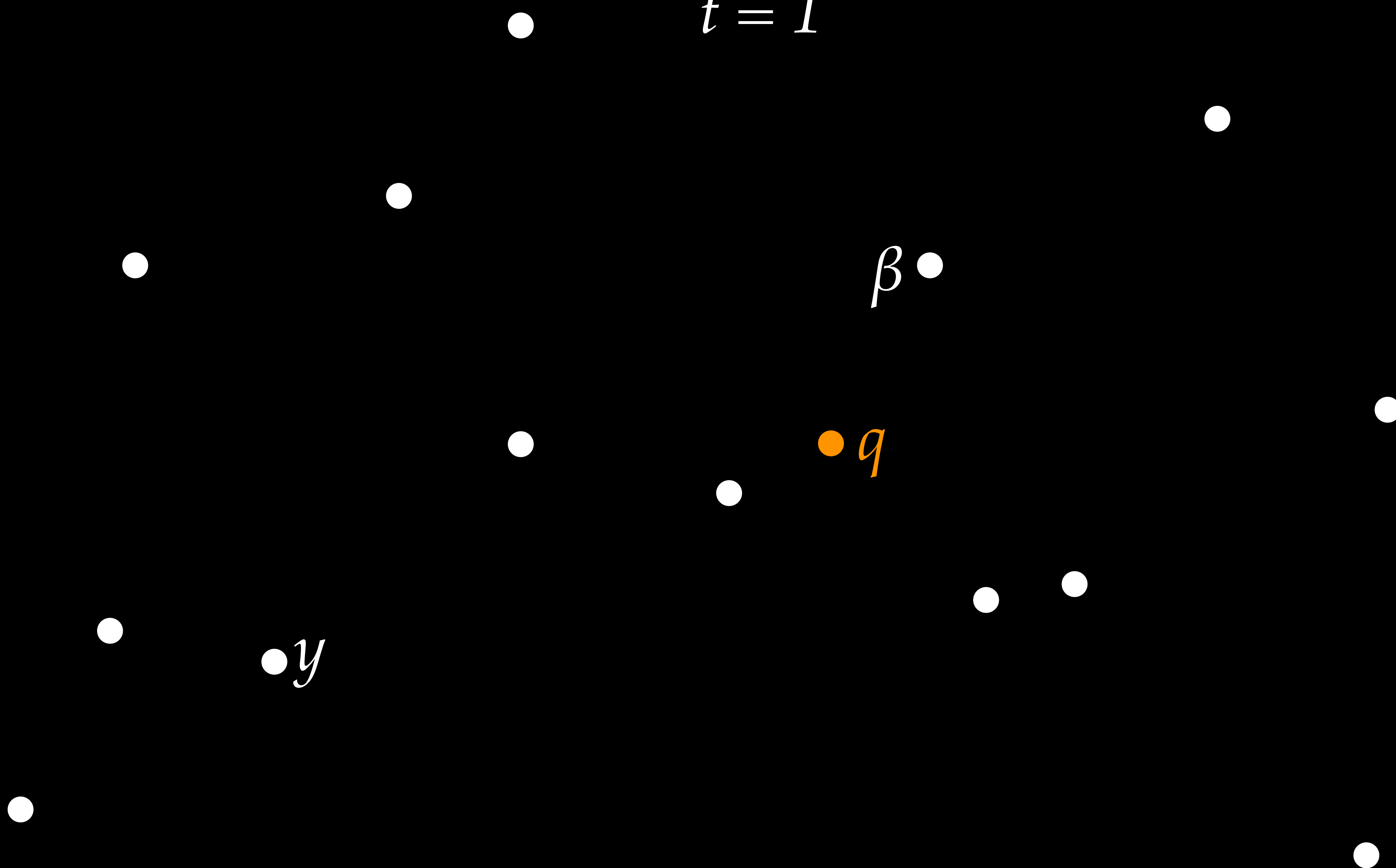

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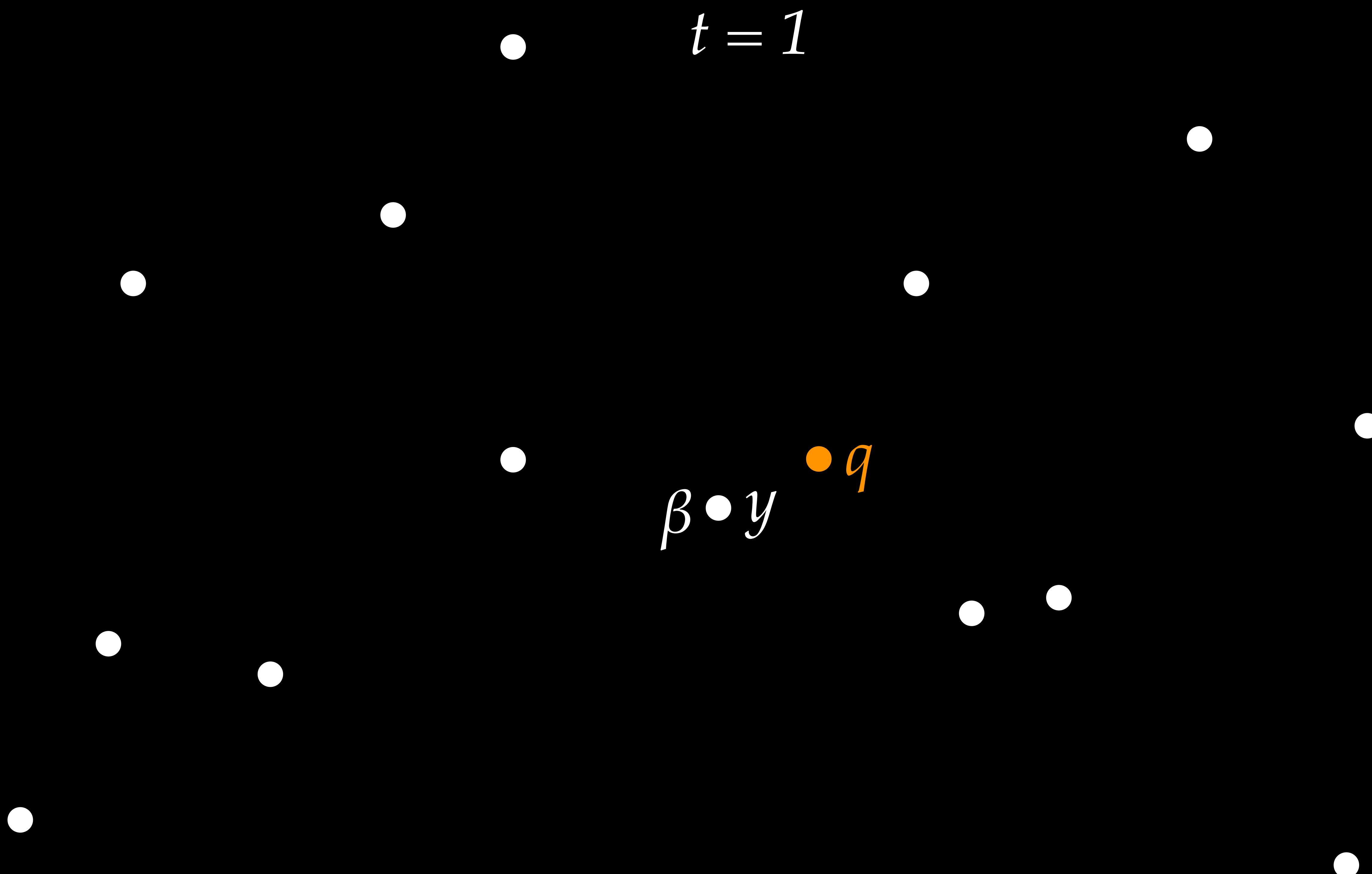

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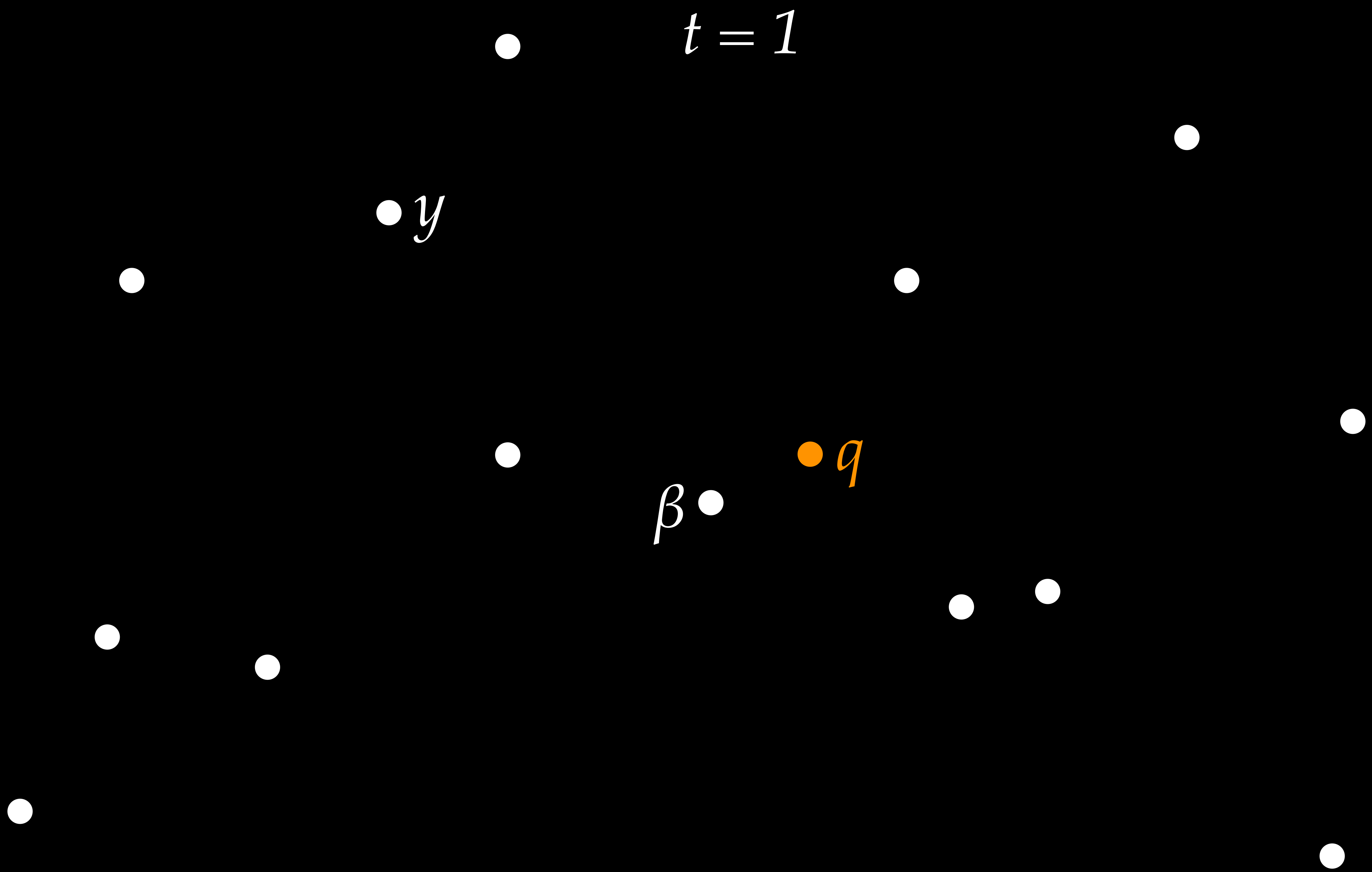
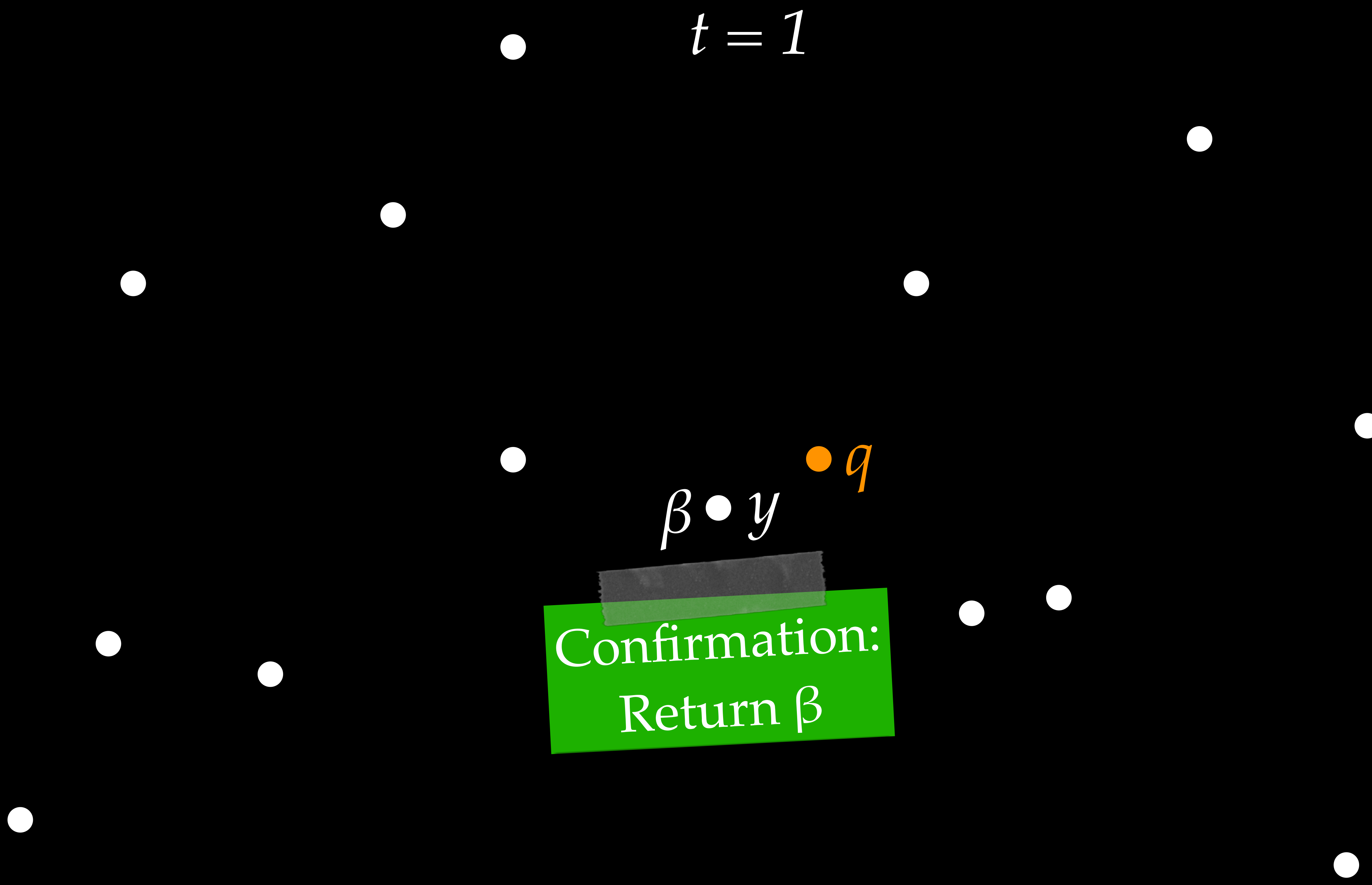


Confirmation sampling



Why confirmation sampling works

- Suppose x_1 is the nearest neighbor.
- For $i > 1$, if $y_i = \beta_{i\text{-}1}$ but $y_i \neq x_1$ we say step i is a *false confirmation*.

Why confirmation sampling works

- Suppose x_1 is the nearest neighbor.
- For $i > 1$, if $y_i = \beta_{i\text{-}1}$ but $y_i \neq x_1$ we say step i is a *false confirmation*.
- Consider the first t steps where we either sample x_1 or produce a false confirmation:
  - If sampling x_1 is more likely than sampling $\beta_{i\text{-}1} \neq x_1$, the probability of false confirmation is at most 1/2 in each step.
  - Probability of t false confirmations is at most 2^{-t}.

Abstract confirmation sampling

Algorithm 1: $\textsc{ConfirmationSampling}(\mathcal{Q}, t, \prec)$

$\beta \leftarrow \infty$, $\mathsf{count} \leftarrow 0$
while $\mathsf{count} < t$ **do**
    sample $X \sim \mathcal{Q}$
    if $X = \beta$ **then**
        $\mathsf{count} \leftarrow \mathsf{count} + 1$
    else if $X \prec \beta$ **then**
        $\beta \leftarrow X$
        $\mathsf{count} \leftarrow 0$
return β

Algorithm 1: $\textsc{ConfirmationSampling}(\mathcal{Q}, t, \prec)$

```
β ← ∞, count ← 0
while count < t do
    sample X ~ Q
    if X = β then
        count ← count + 1
    else if X ≺ β then
        β ← X
        count ← 0
return β
```

Theorem 3. *Let $\mathcal{Q}$ denote a probability distribution with finite support S. For $x_1 = \min(S)$ and $X \sim \mathcal{Q}$ let $p_1 = \Pr[X = x_1]$ and let $p_2 = \max\{\Pr[X = x] \mid x \in S \setminus \{x_1\}\}$ be the largest sampling probability among elements of S other than x_1. Then:*

$$\Pr[\textsc{ConfirmationSampling}(\mathcal{Q}, t) \neq x_1] \leq (1 - p_1)\left(\frac{p_2}{p_1 + p_2}\right)^t$$

The expected number of samples made by $\textsc{ConfirmationSampling}$ *is bounded by* $(t+1)/p_1$.

Application to nearest neighbor

Theorem 1. *Suppose there is a sequence of independent, randomized data structures* $\mathcal{D}_1, \mathcal{D}_2, \ldots,$ *such that on query* q, $\mathcal{D}_i$ *returns the nearest neighbor of* q *in* P *with probability* at least p_q *and each other point in* P *with probability* at most p_q. *Let* $\delta > 0$ *be given. There is an algorithm that depends on* δ *but not on* p_q *that on input* q *queries data structures* $\mathcal{D}_1, \ldots, \mathcal{D}_{j_q}$, *performs* j_q *distance computations, where* $\mathbb{E}[j_q] = O(\ln(1/\delta)/p_1)$, *and returns the nearest neighbor of* q *with probability at least* $1 - \delta$.

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- Finding the nearest neighbor quickly boils down to minimizing the product of the expected time for querying $\mathcal{D}_i$ and $1/p_1$.

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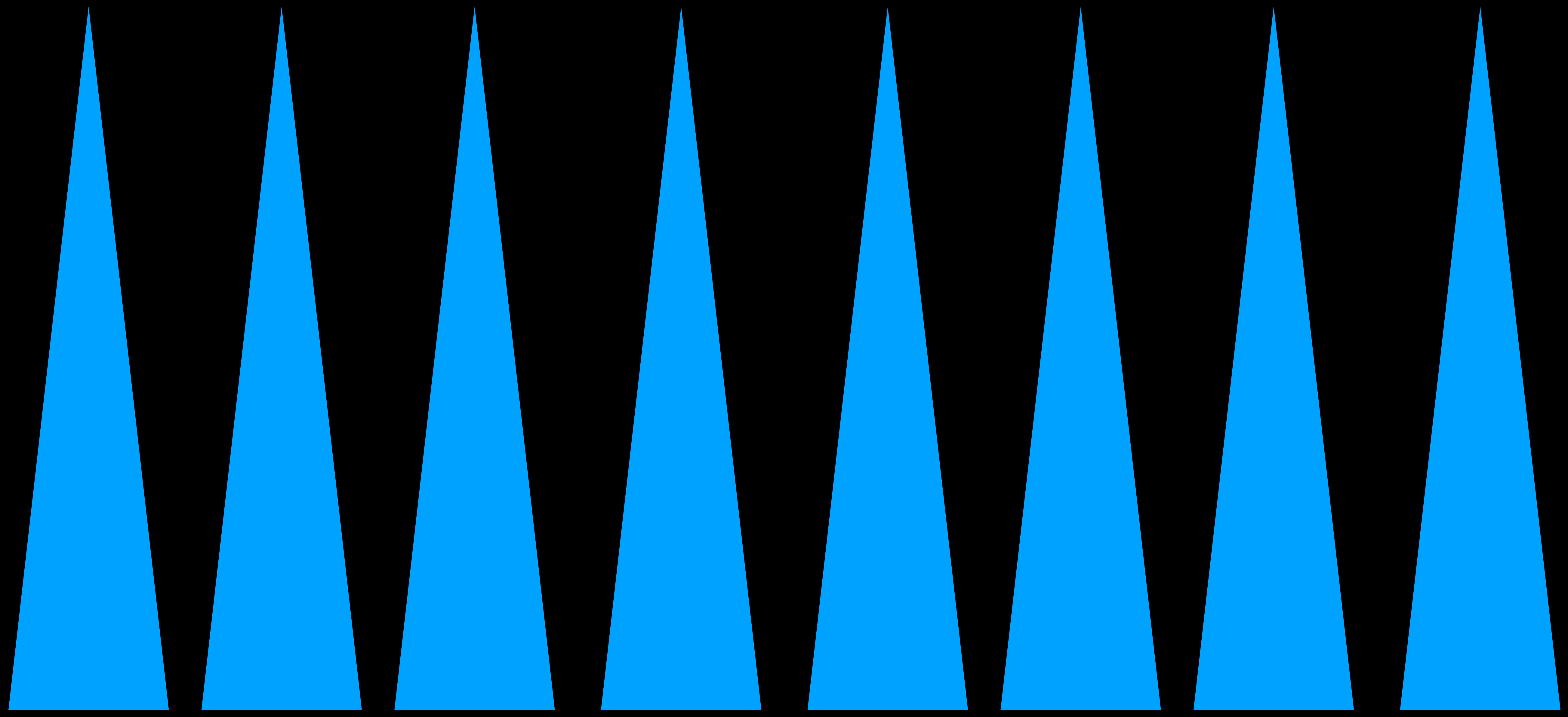
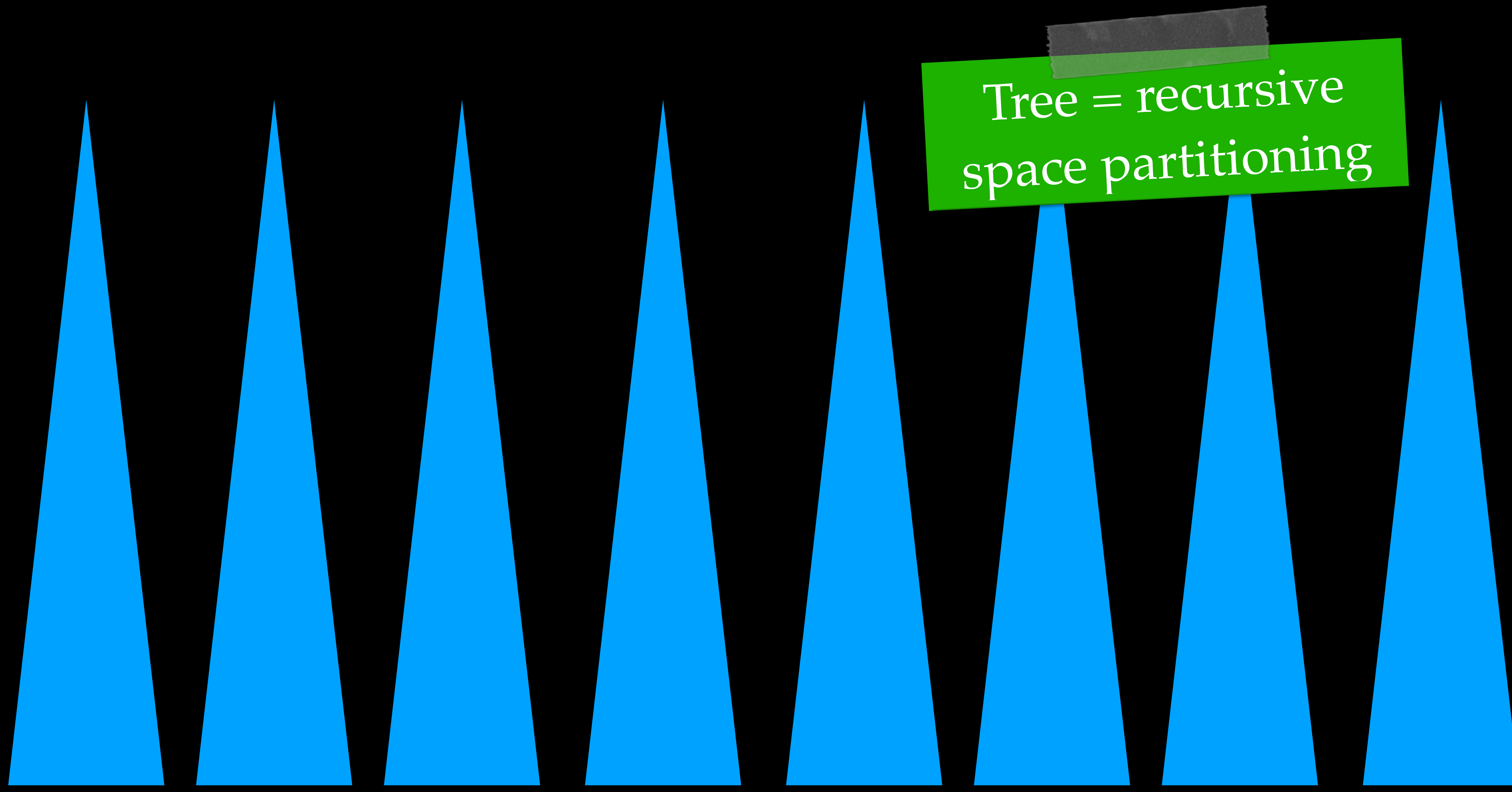
- Finding the nearest neighbor quickly boils down to minimizing the product of the expected time for querying $\mathcal{D}_i$ and $1/p_1$.

- **Question**: Can this be done optimally without knowledge of the distance to the nearest neighbor?

Partial answer for LSH forest



Partial answer for LSH forest



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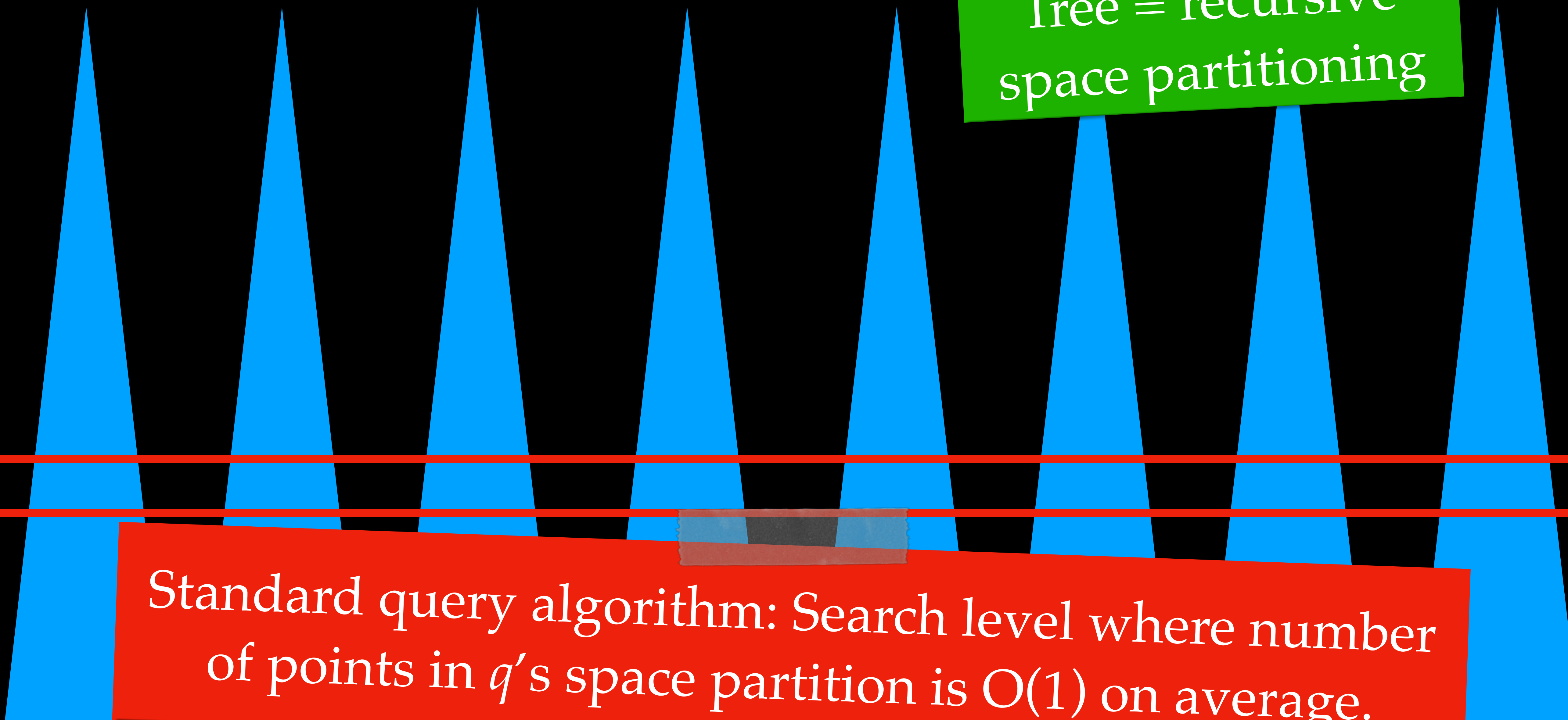

Tree = recursive space partitioning

Standard query algorithm: Search level where number of points in q's space partition is O(1) on average.

Partial answer for LSH forest

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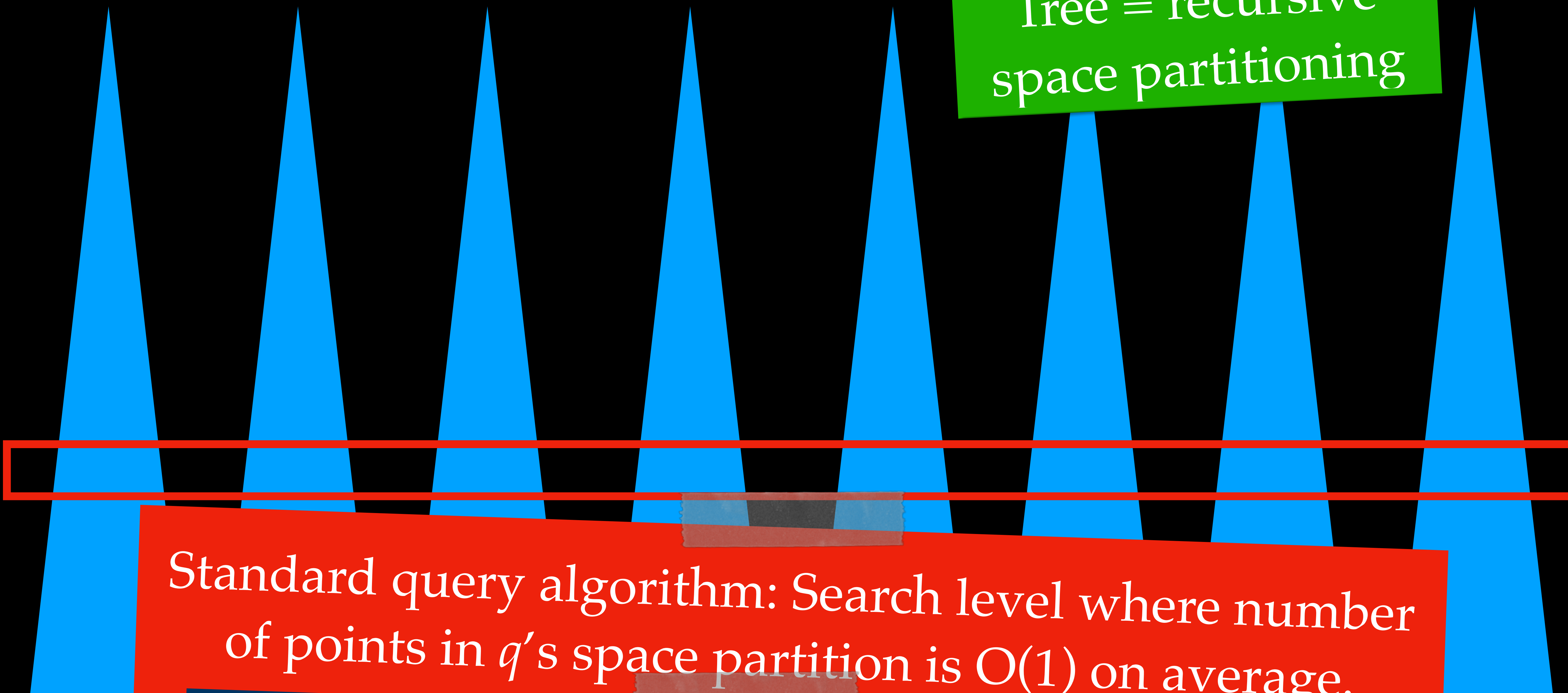
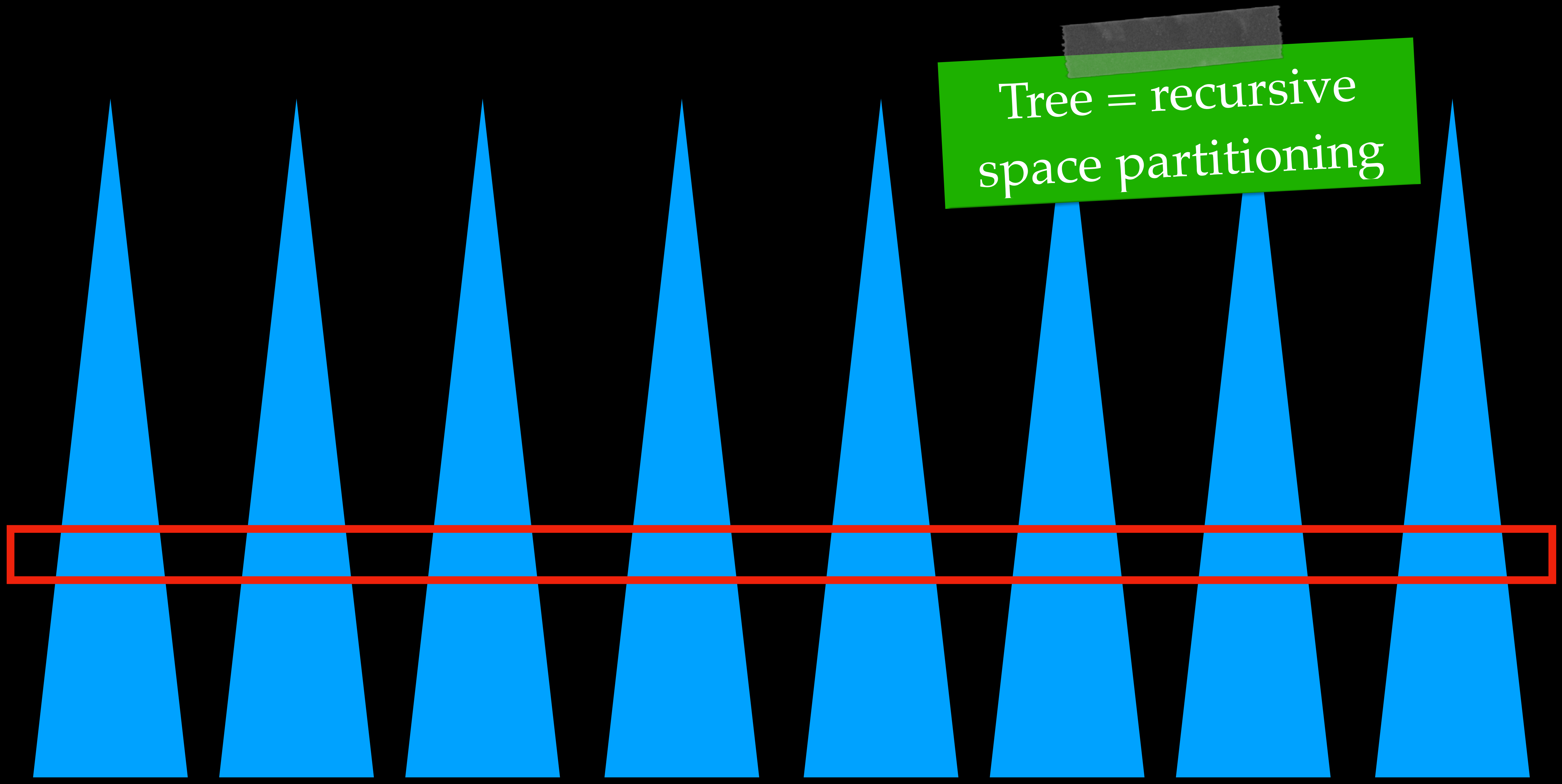


Standard query algorithm: Search level where number of points in q's space partition is O(1) on average.

Works if number of trees is high enough, depending on distance to nearest neighbor.

Partial answer for LSH forest



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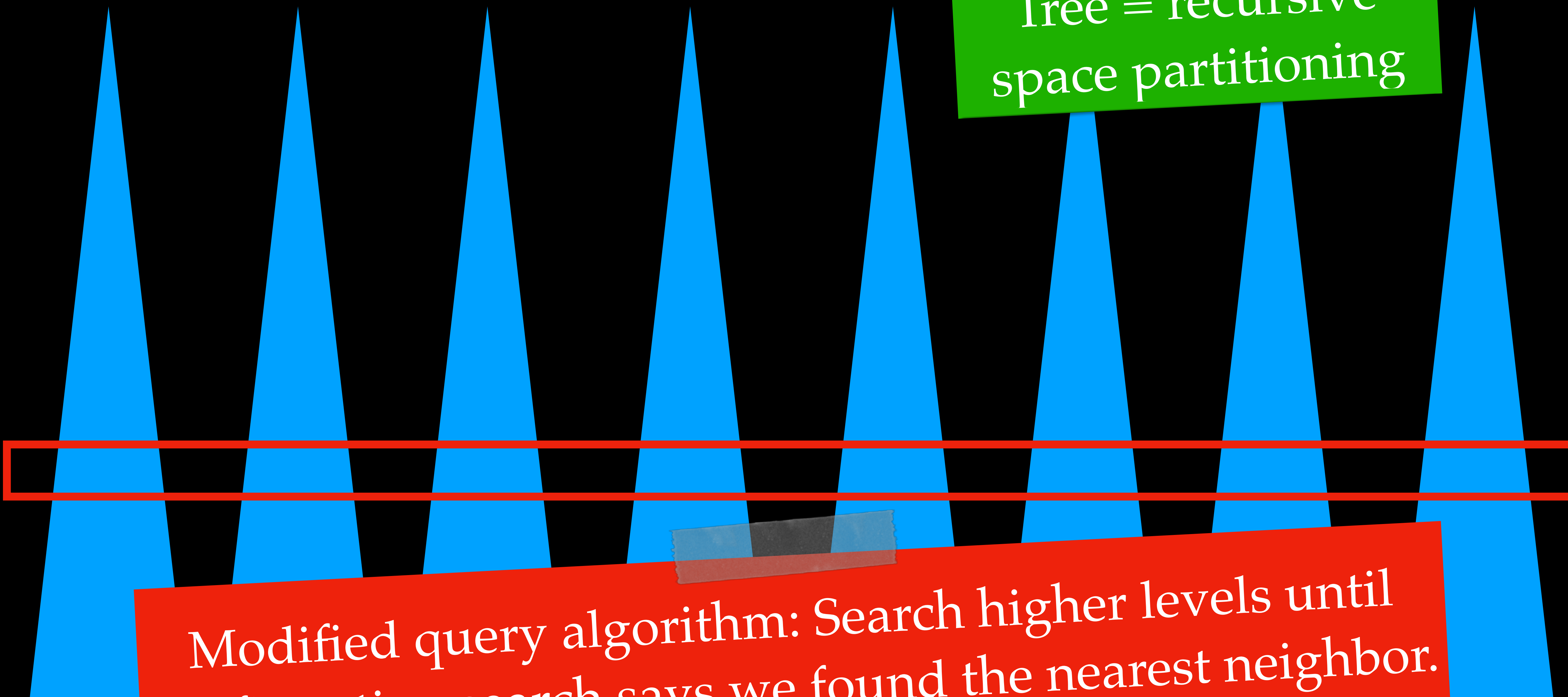
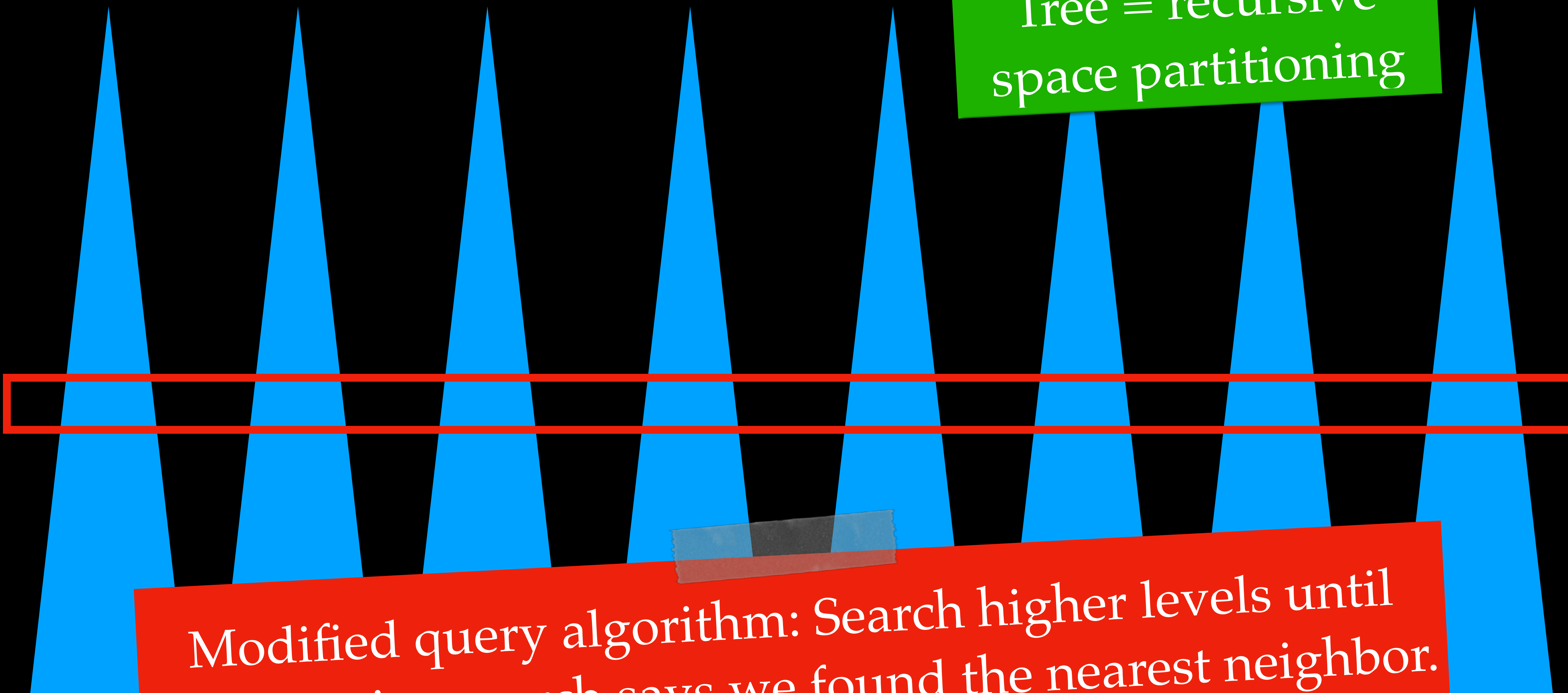


Tree = recursive space partitioning

Modified query algorithm: Search higher levels until confirmation search says we found the nearest neighbor.

Partial answer for LSH forest

Tree = recursive space partitioning



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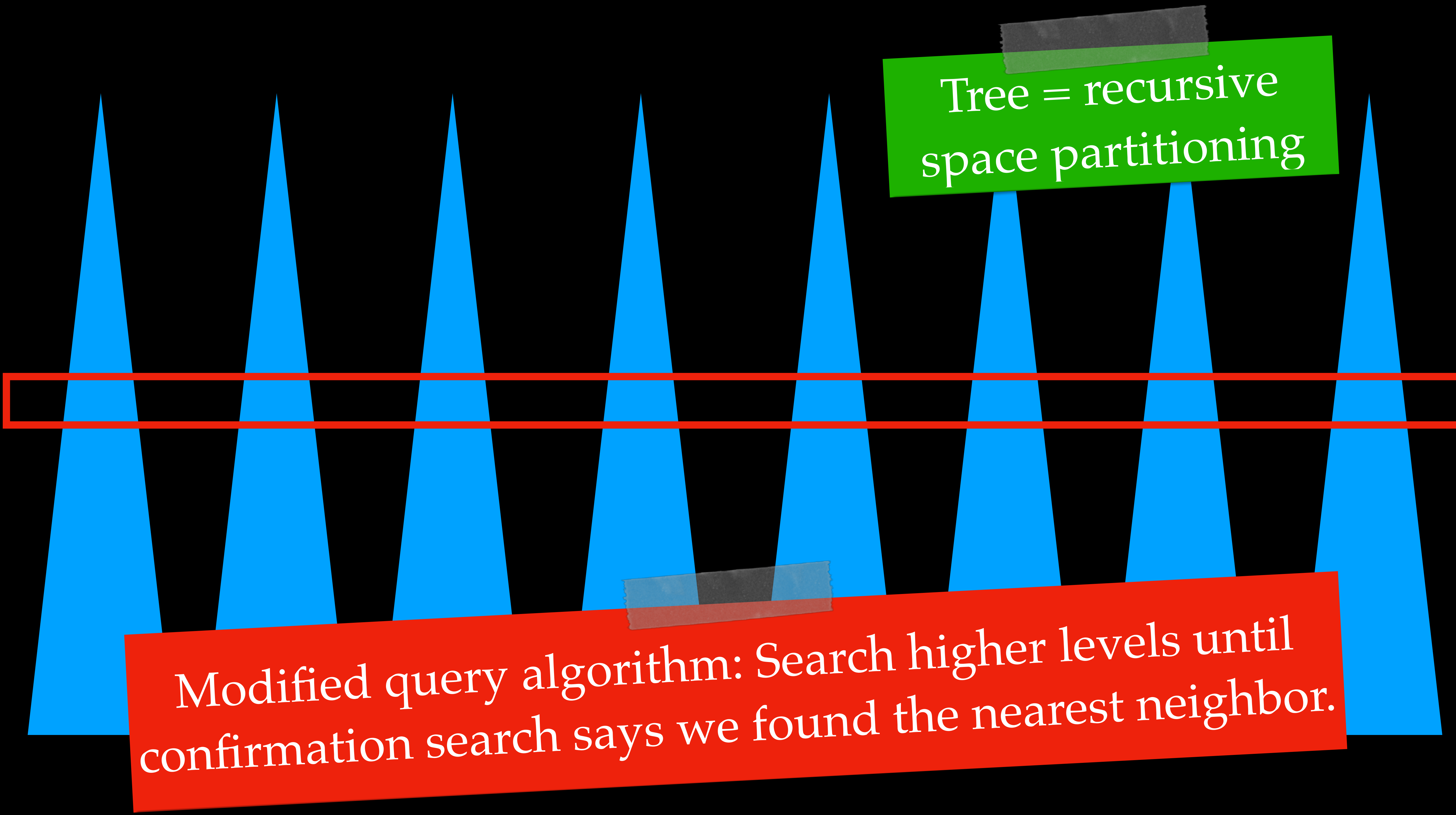

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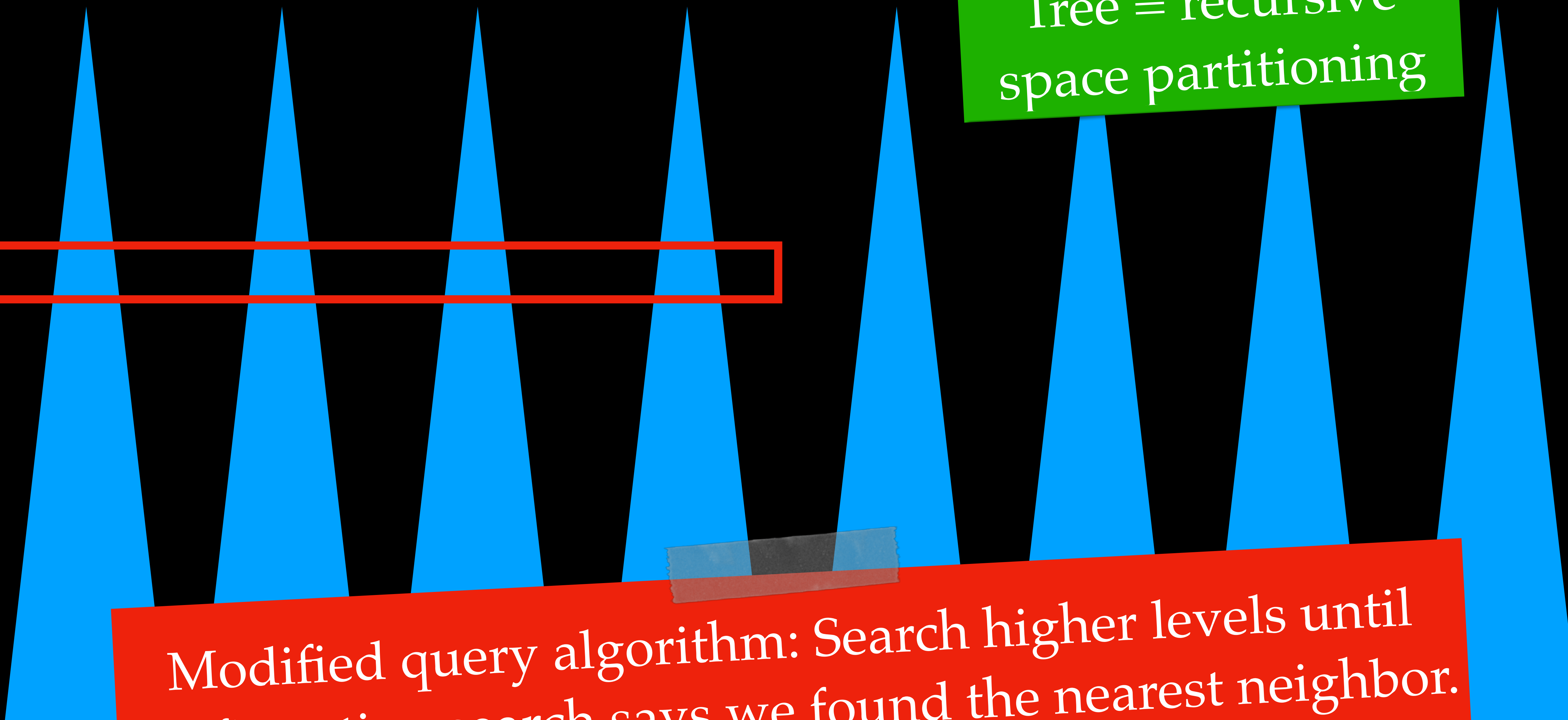
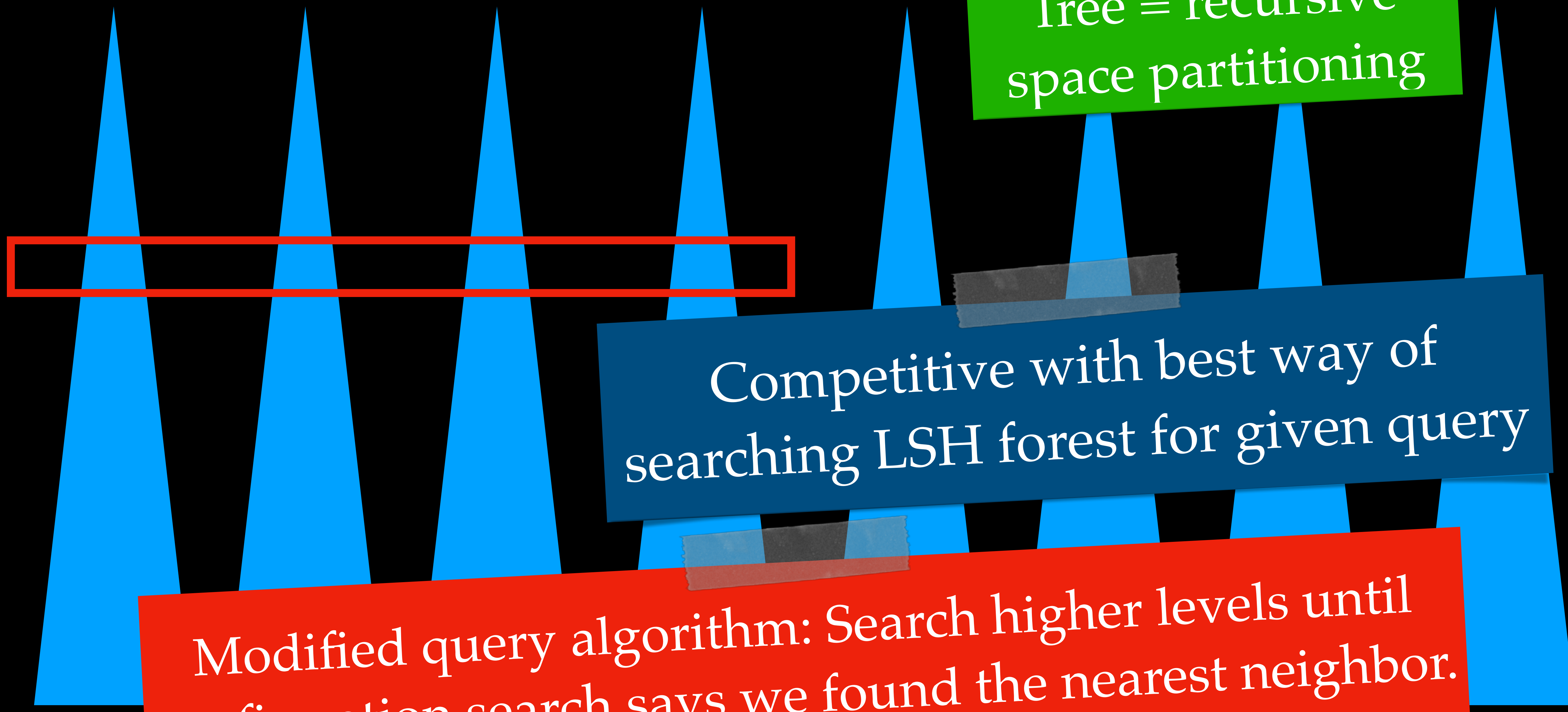


Tree = recursive space partitioning

Modified query algorithm: Search higher levels until confirmation search says we found the nearest neighbor.

Also consider partially searching a level.

Partial answer for LSH forest



Tree = recursive space partitioning

Competitive with best way of searching LSH forest for given query

Modified query algorithm: Search higher levels until confirmation search says we found the nearest neighbor.

Also consider partially searching a level.

Open question

- Is it possible to achieve space and time that is $O(1)$-competitive with the best LSH scheme, adapted to the *query and to the data distribution*, for a given expected recall?