Technische Universiteit
Eindhoven
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New directions in approximate nearest neighbors for the angular distance

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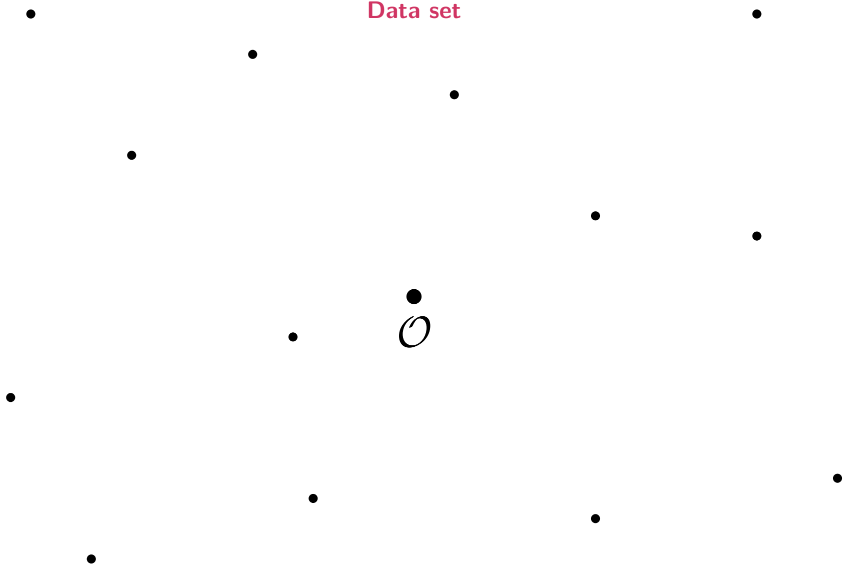
(January 13, 2016)

Nearest neighbor searching

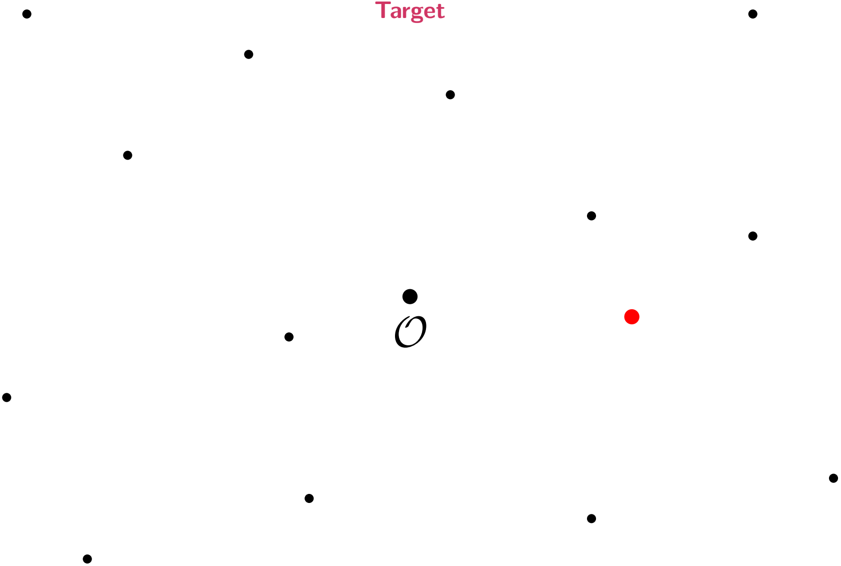
Nearest neighbor searching

Data set



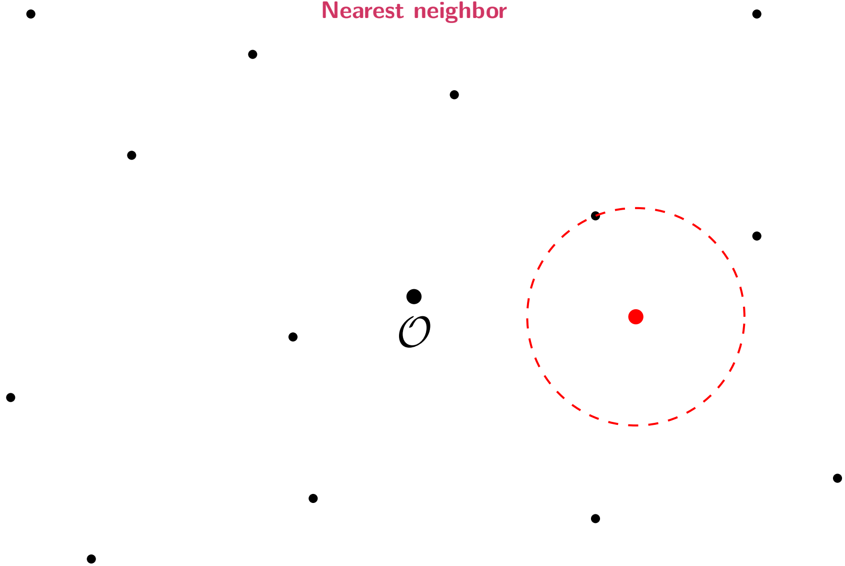
Nearest neighbor searching

Target



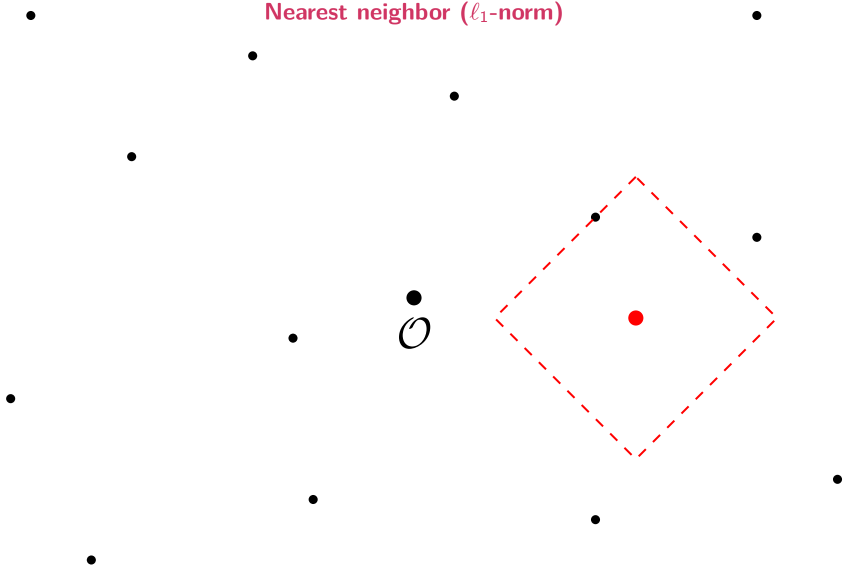
Nearest neighbor searching

Nearest neighbor



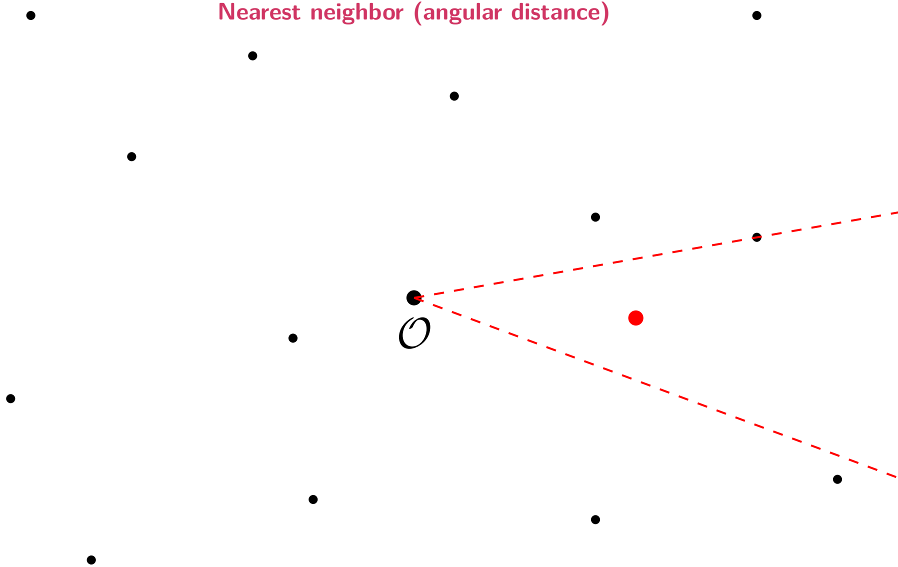
Nearest neighbor searching

Nearest neighbor (ℓ_1-norm)



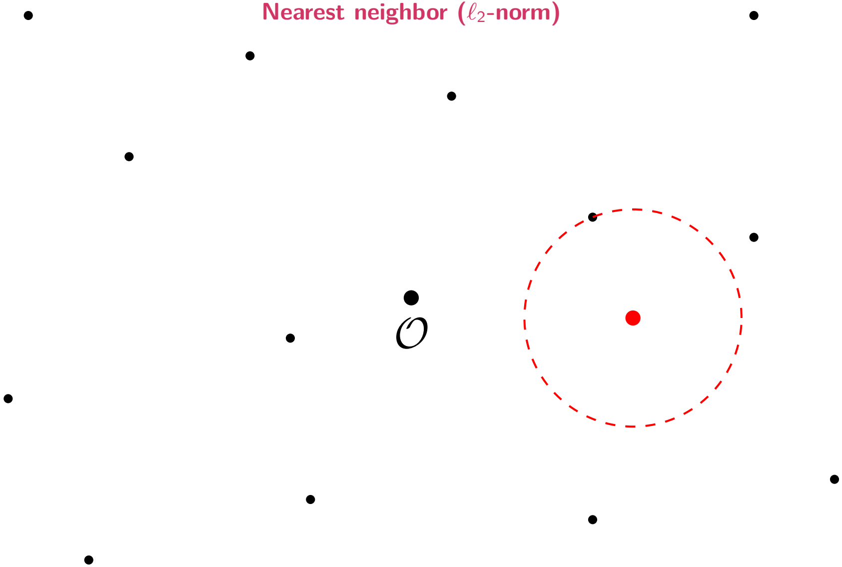
Nearest neighbor searching

Nearest neighbor (angular distance)



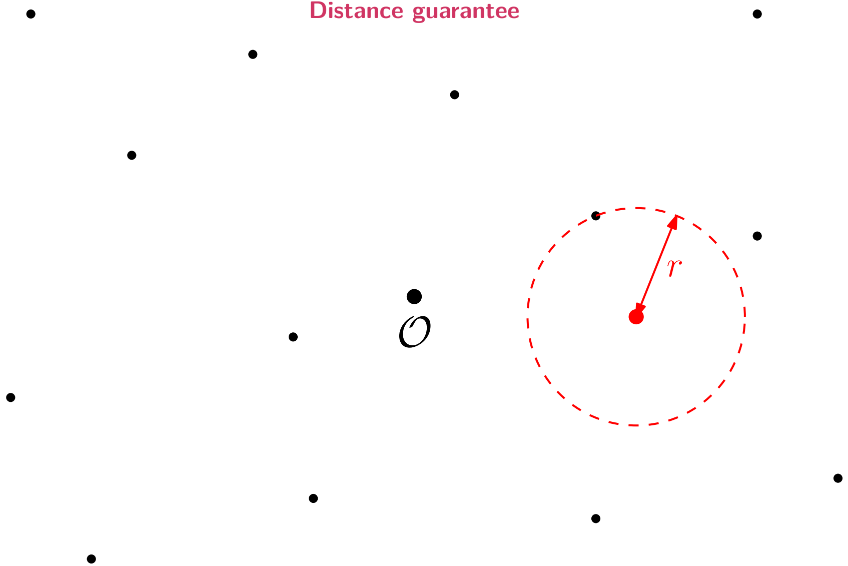
Nearest neighbor searching

Nearest neighbor (ℓ_2-norm)



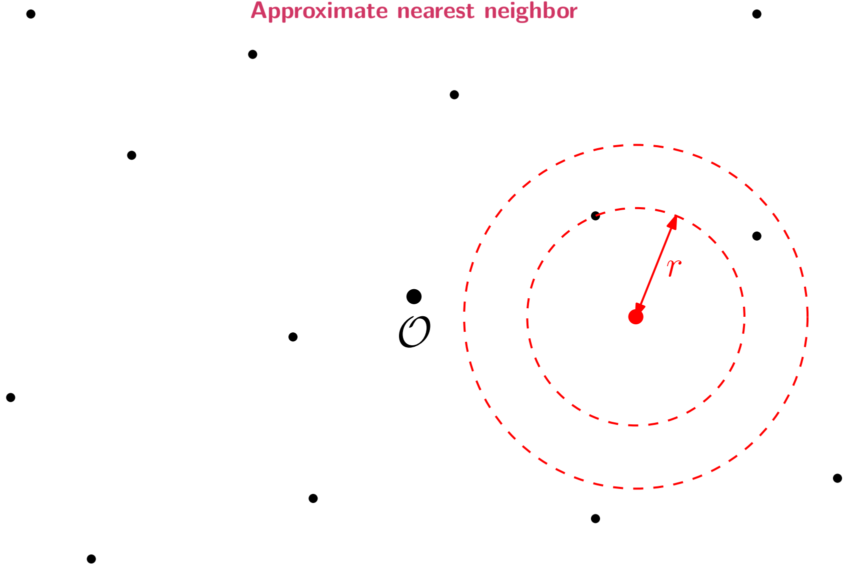
Nearest neighbor searching

Distance guarantee



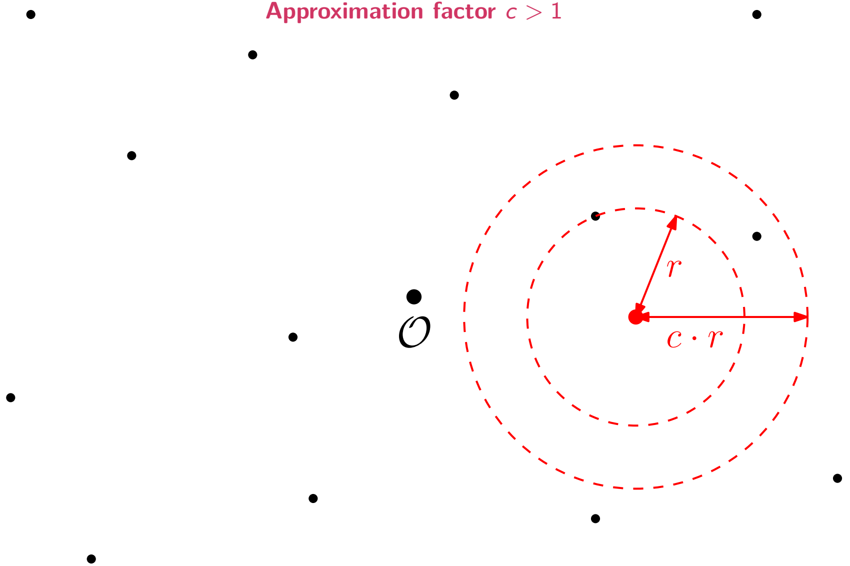
Nearest neighbor searching

Approximate nearest neighbor



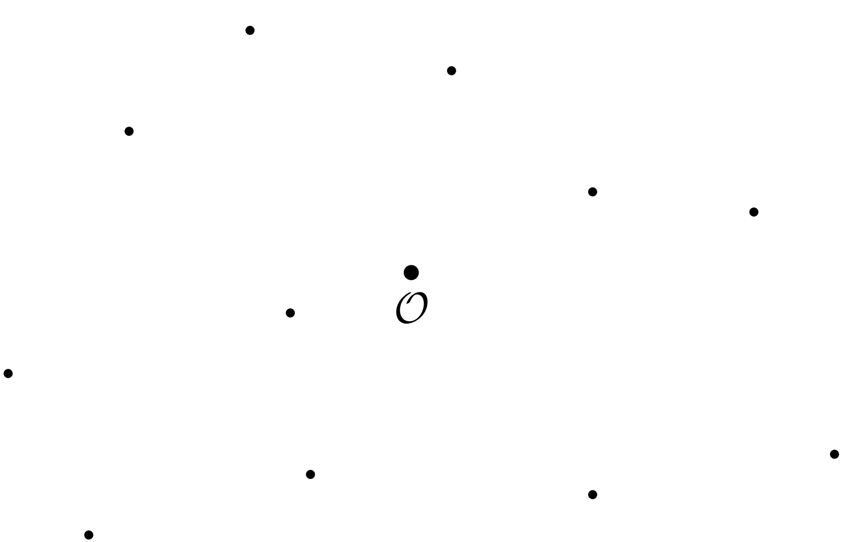
Nearest neighbor searching

Approximation factor $c > 1$



Nearest neighbor searching

Example: Precompute Voronoi cells



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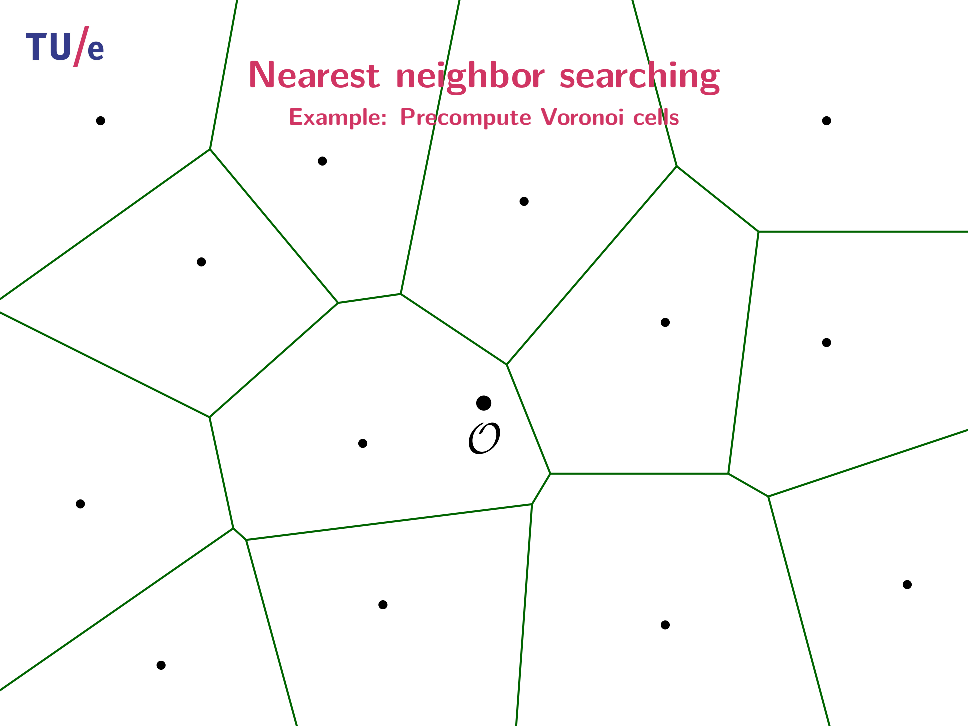
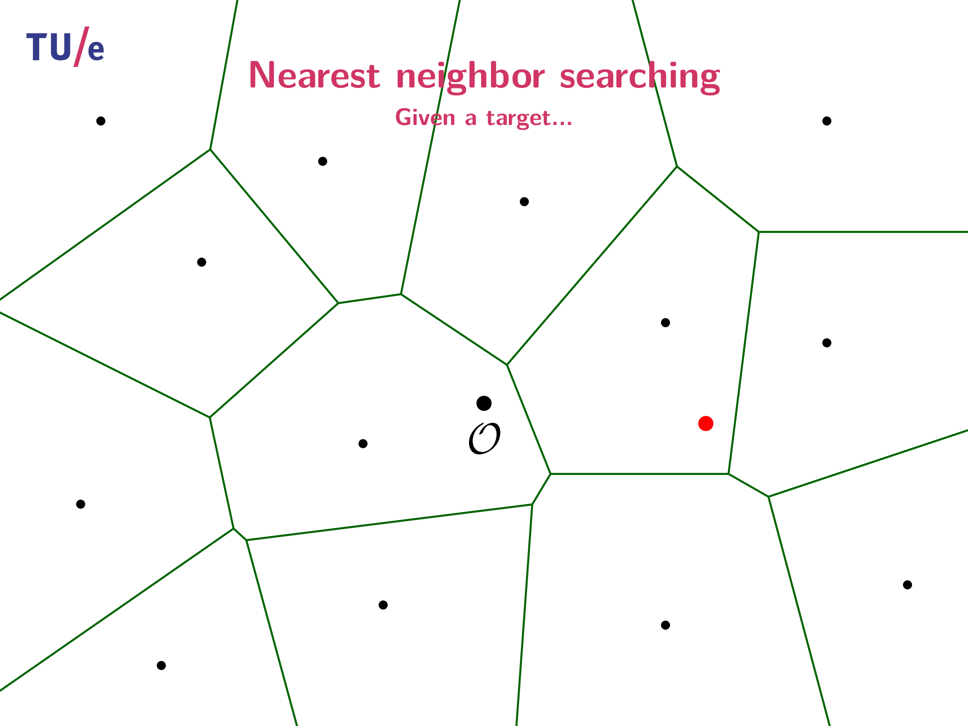


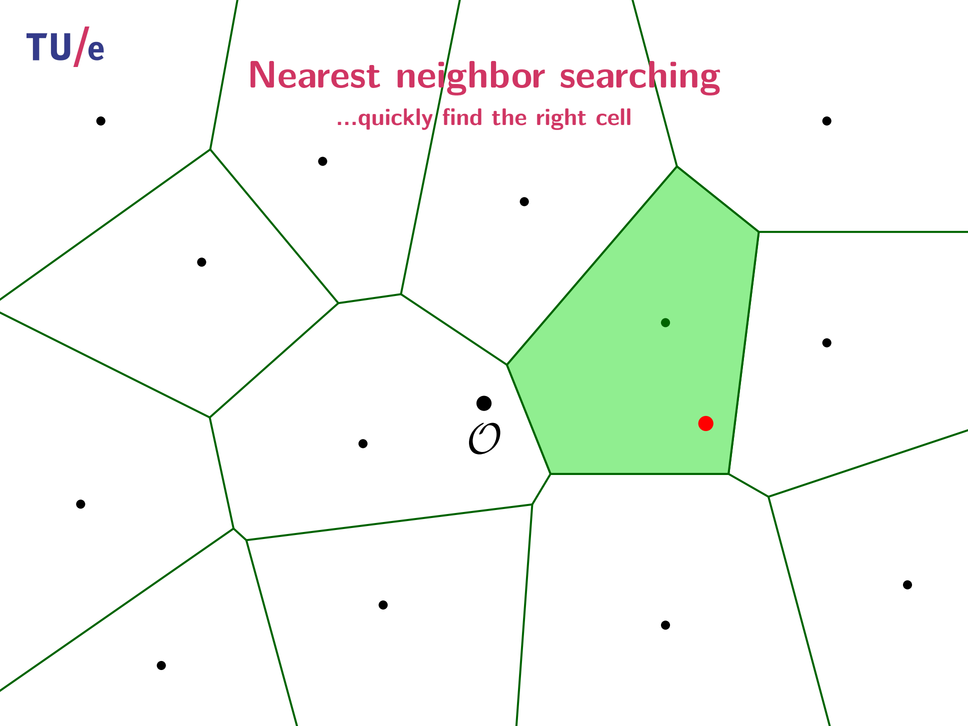
Nearest neighbor searching

Given a target...



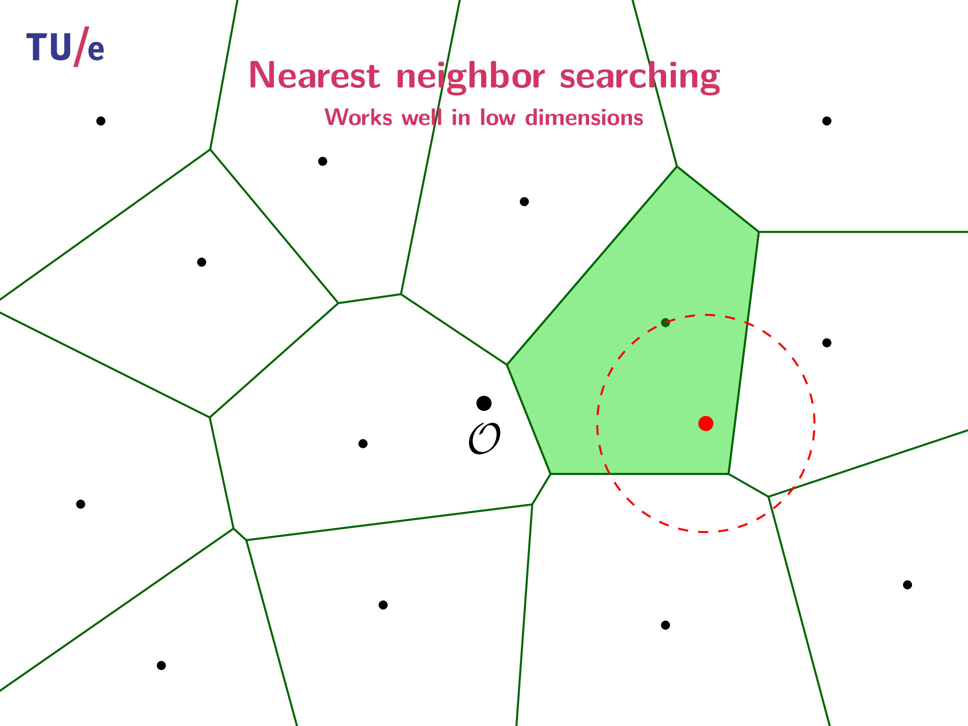
Nearest neighbor searching

...quickly find the right cell



Nearest neighbor searching

Works well in low dimensions



Nearest neighbor searching

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  - Smaller n? $\implies$ Use JLT to reduce d

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  - Angular NNS in $\mathbb{R}^d$ equivalent to Eucl. NNS on the sphere
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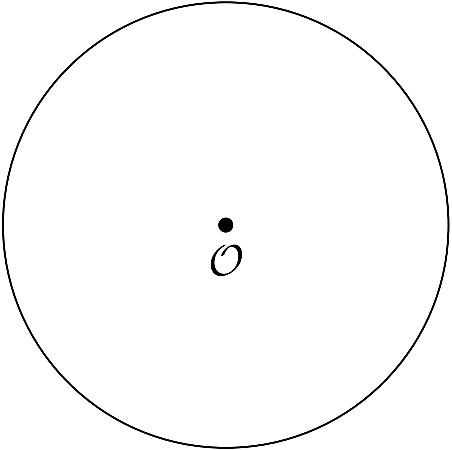
- "Random" case: $c \cdot r = \sqrt{2}$
  - Random unit vectors are usually approximately orthogonal
- Goal: Query time $O(n^\rho)$ with $\rho < 1$

Nearest neighbor searching

“Random” instances



Nearest neighbor searching

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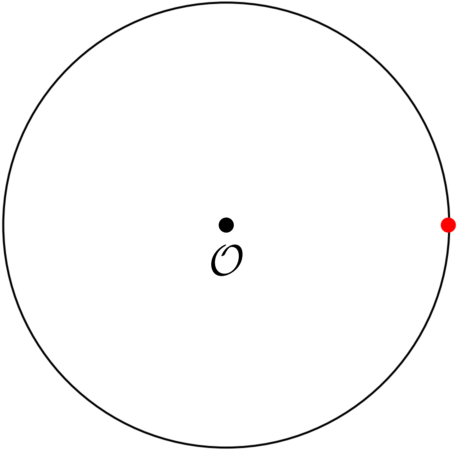

Nearest neighbor searching

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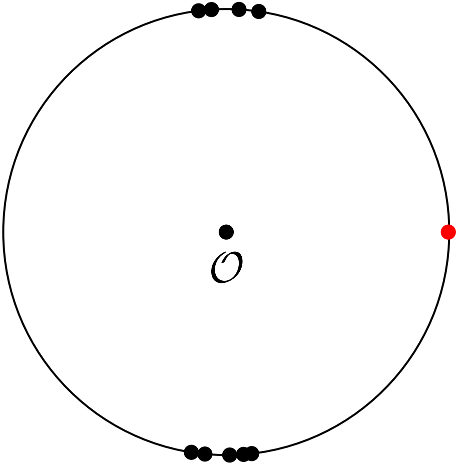

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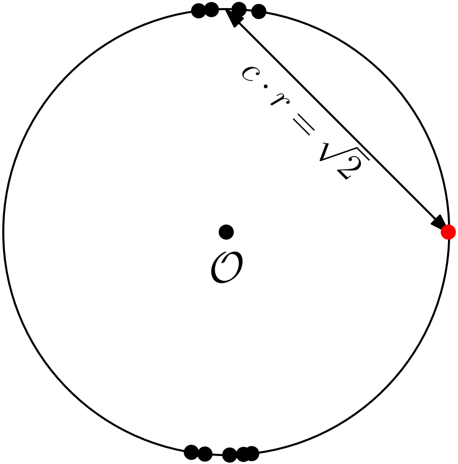

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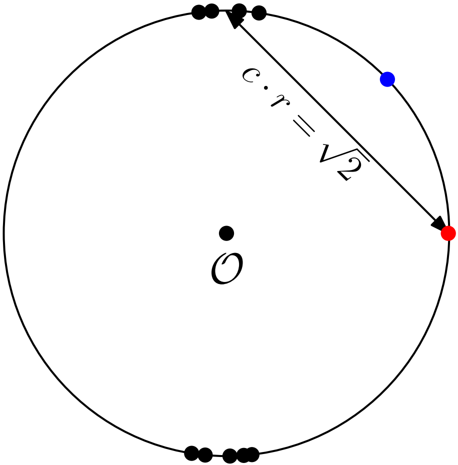

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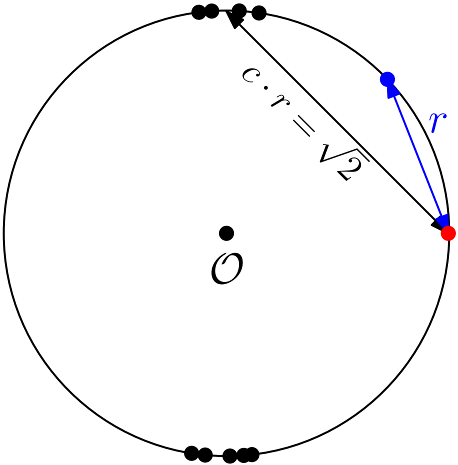

Locality-sensitive hashing

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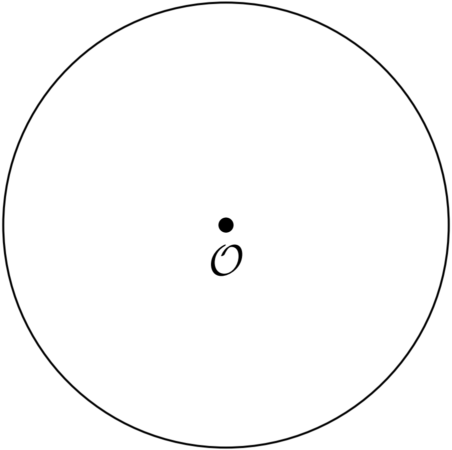
- Precomputation: Store hash tables of vectors per region
  - For each region, store contained vectors from data set
  - Rerandomization: Many partitions to increase success probability
- Query: Check hash tables for collisions
  - Compute target's region for each hash table
  - Check corresponding buckets for potential nearest neighbors
  - Reduces search space before doing a linear search

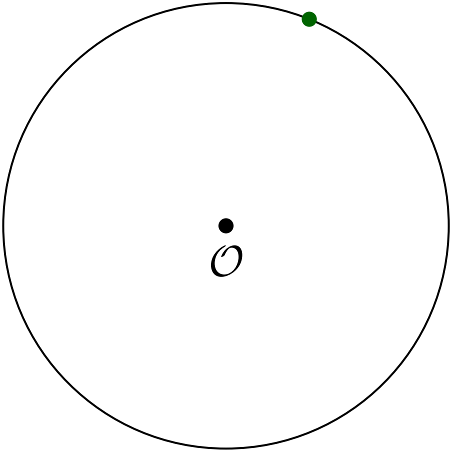
Hyperplane LSH

[Charikar, STOC'02]



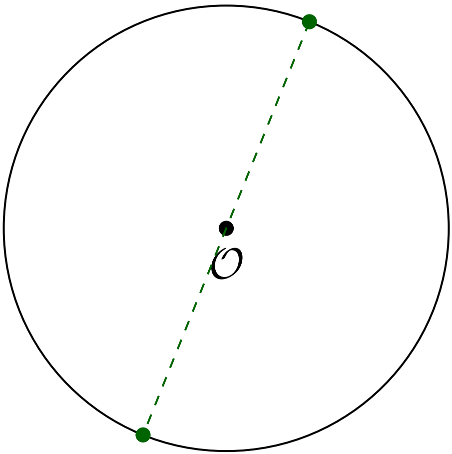
Hyperplane LSH

Random point



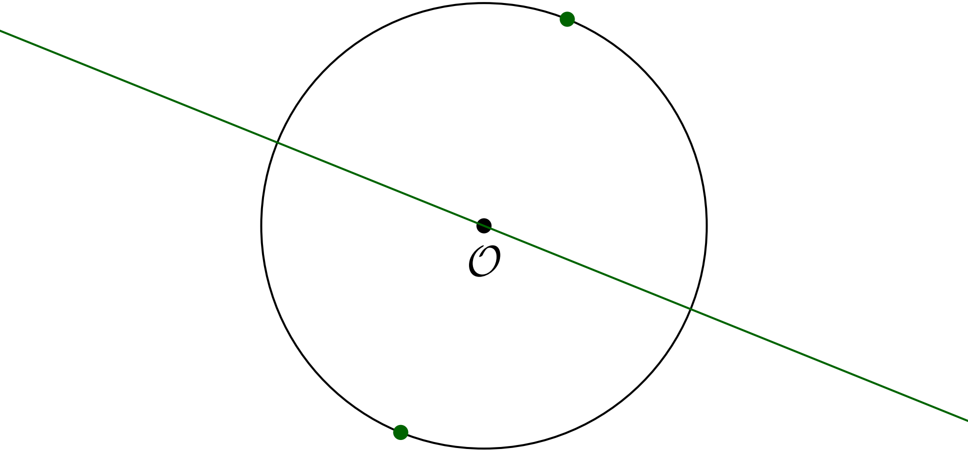
Hyperplane LSH

Opposite point



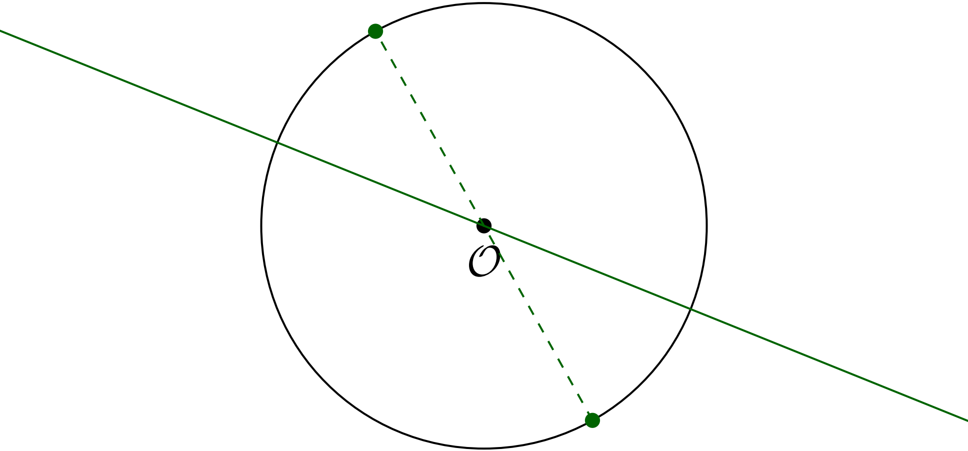
Hyperplane LSH

Two Voronoi cells



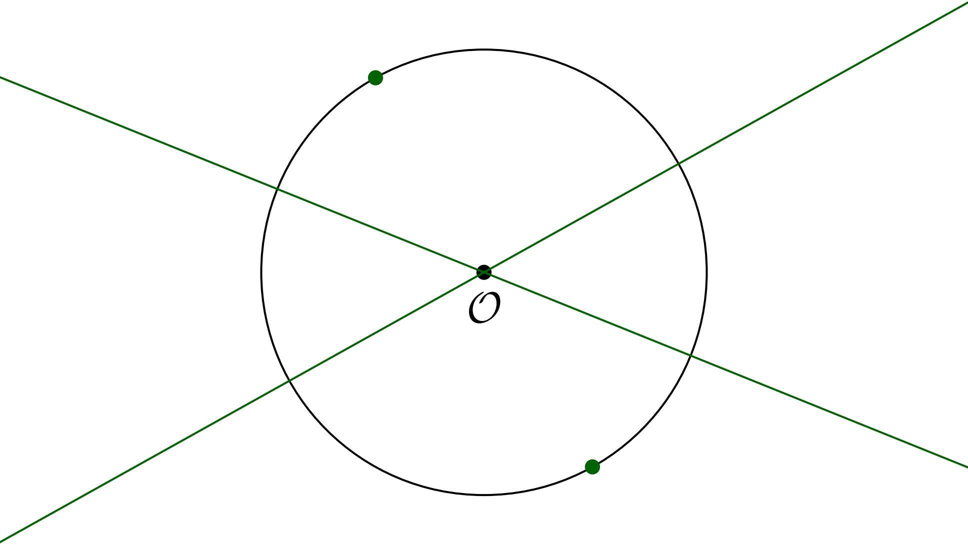
Hyperplane LSH

Another pair of points



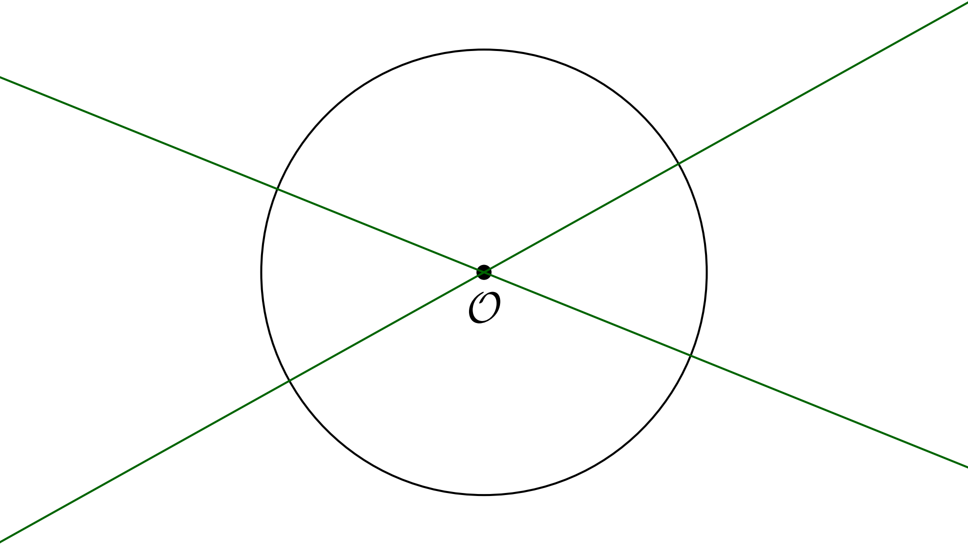
Hyperplane LSH

Another hyperplane



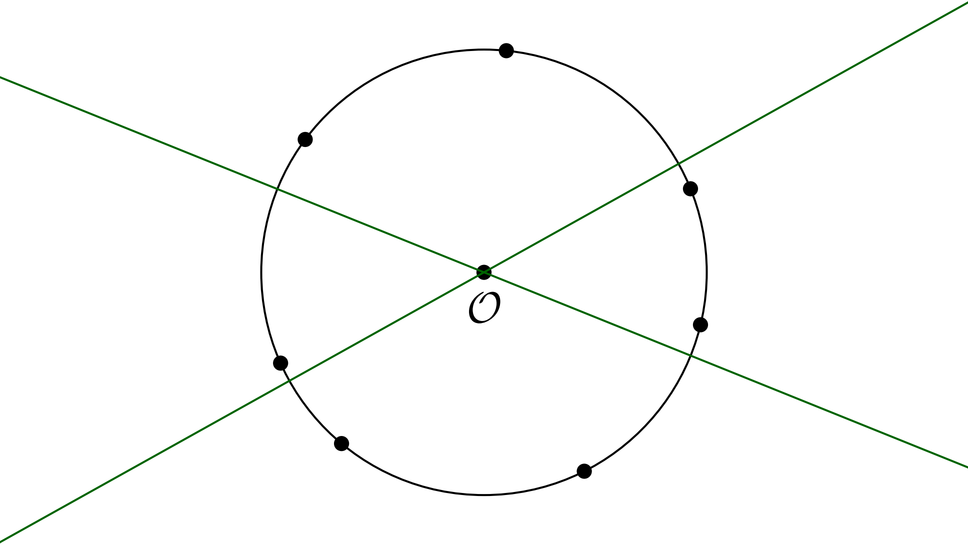
Hyperplane LSH

Defines partition



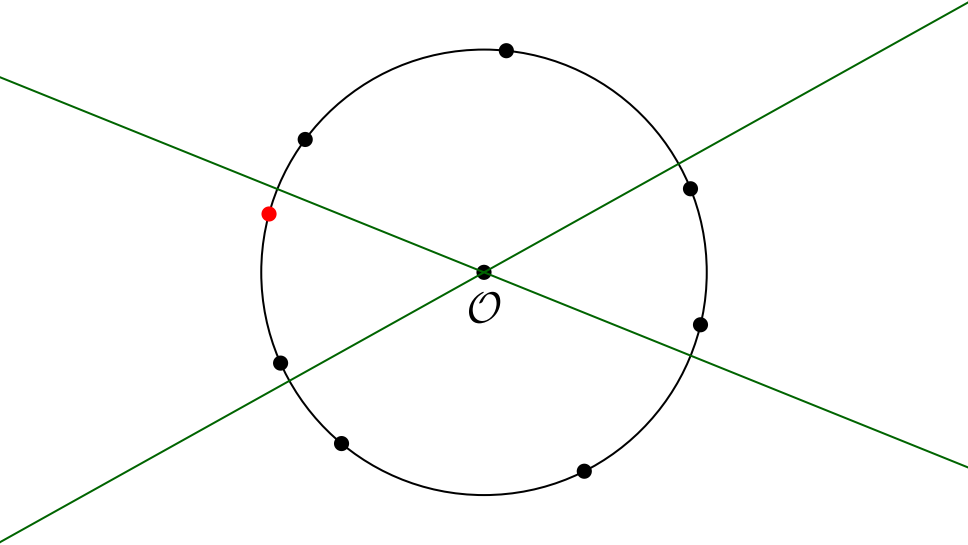
Hyperplane LSH

Preprocessing



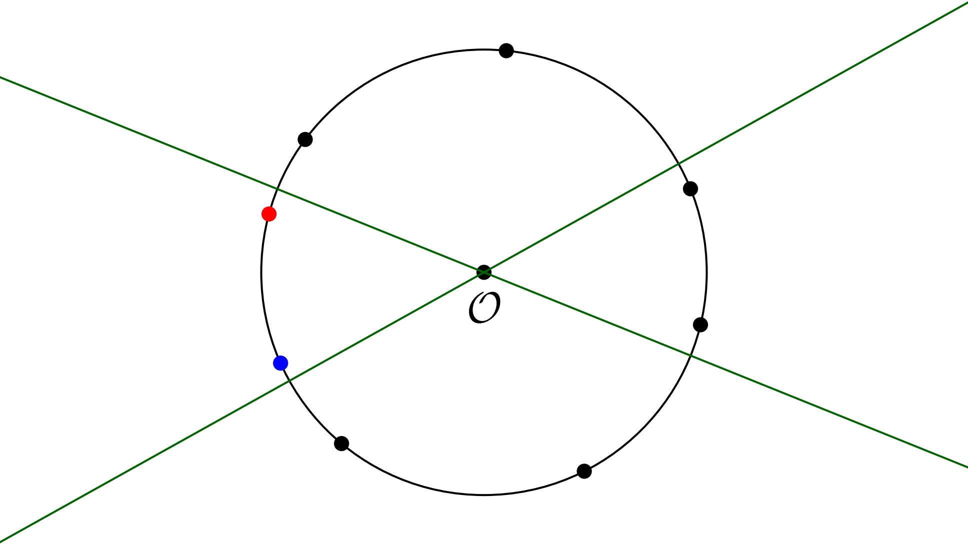
Hyperplane LSH

Query



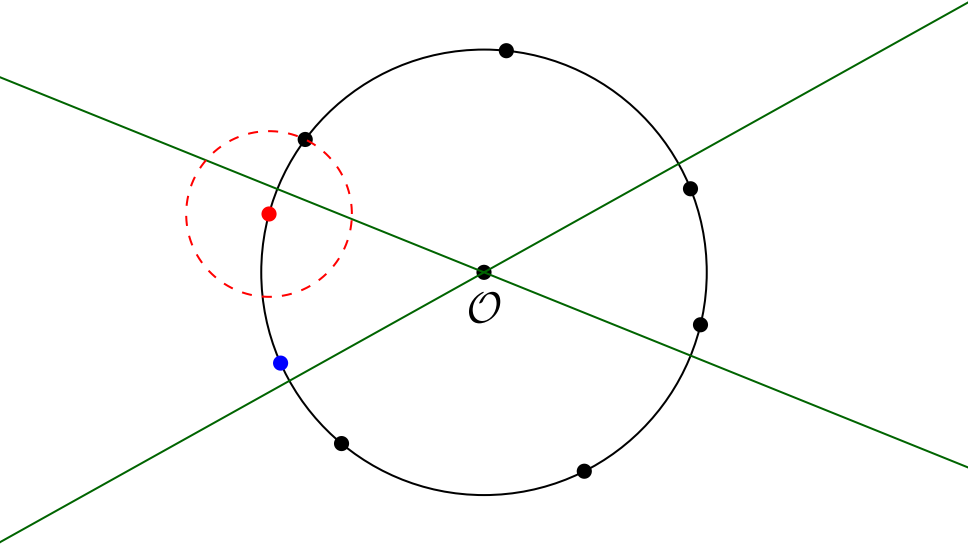
Hyperplane LSH

Collisions



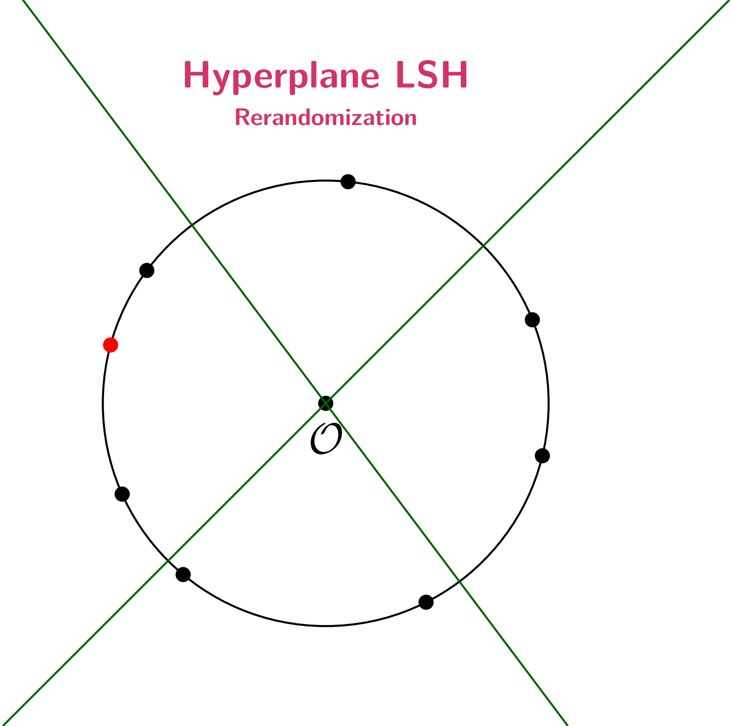
Hyperplane LSH

Failure



Hyperplane LSH

Rerandomization



Hyperplane LSH

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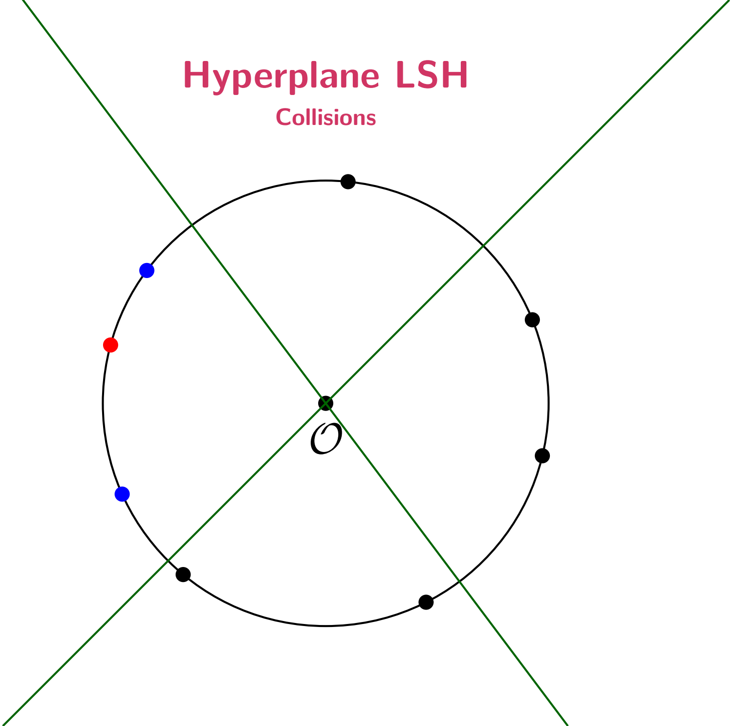
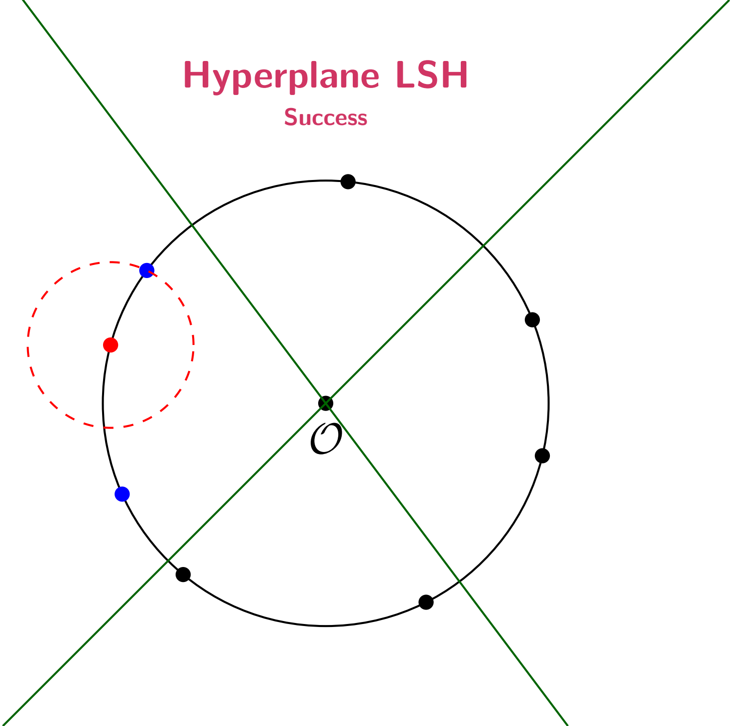


TU/e

Hyperplane LSH

Success



Hyperplane LSH

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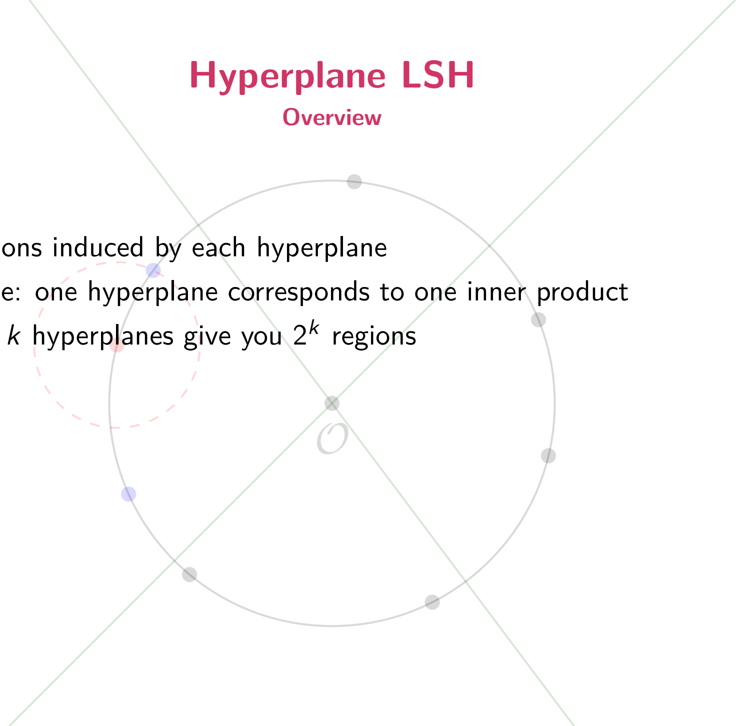
- 2 regions induced by each hyperplane
- Simple: one hyperplane corresponds to one inner product
- Fast: k hyperplanes give you 2^k regions



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$$\rho = \frac{\sqrt{2}}{\pi \ln 2} \cdot \frac{1}{c} \left(1 + o_{d,c}(1)\right).$$

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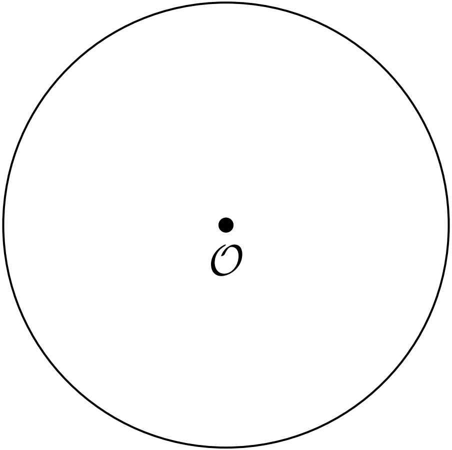
Efficient but suboptimal as $\rho \propto \frac{1}{c^2}$ is achievable

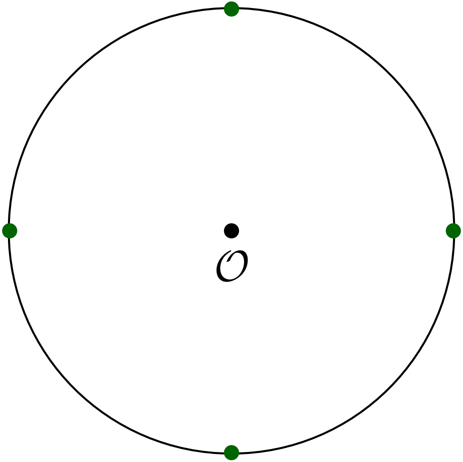
Cross-Polytope LSH

[Terasawa–Tanaka, WADS'07]
[Andoni et al., NIPS'15]



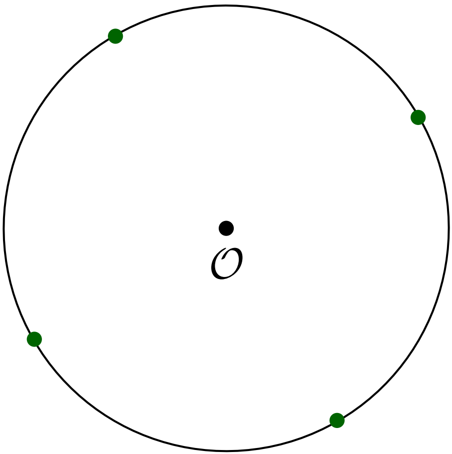
Cross-Polytope LSH

Vertices of cross-polytope (simplex)



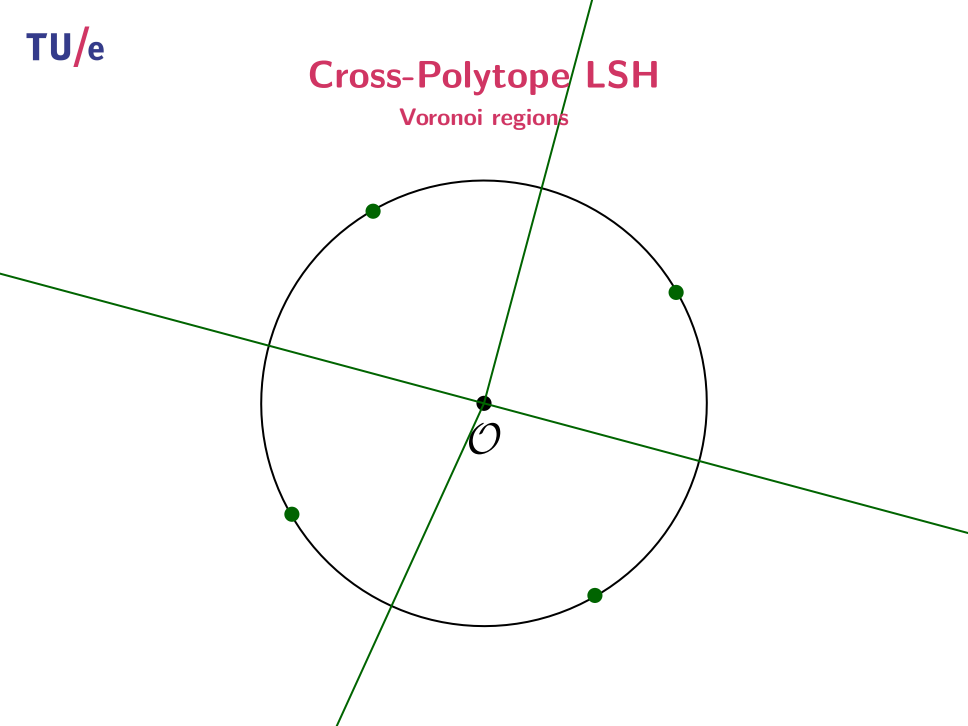
Cross-Polytope LSH

Random rotation



Cross-Polytope LSH

Voronoi regions



Cross-Polytope LSH

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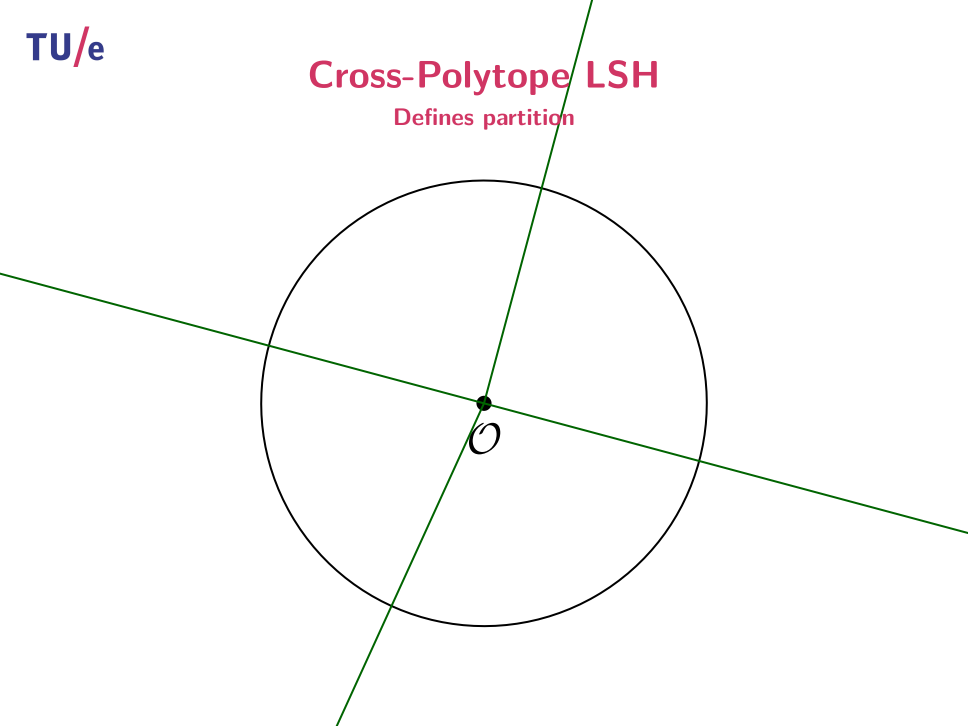

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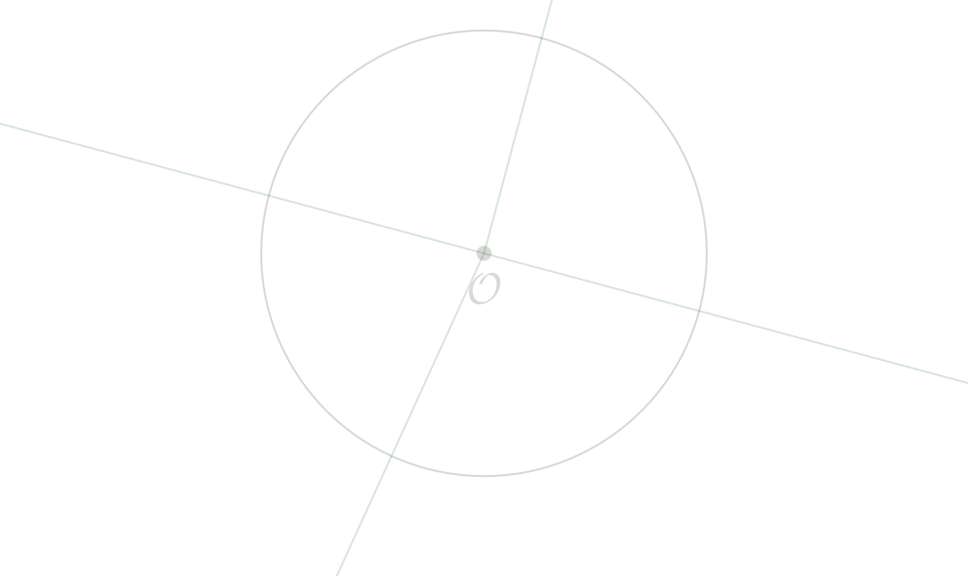

Cross-Polytope LSH

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- $2d$ regions in d dimensions
- Advantage: regions same size and more symmetric

For "random" settings, query time $O(n^{\rho})$ with

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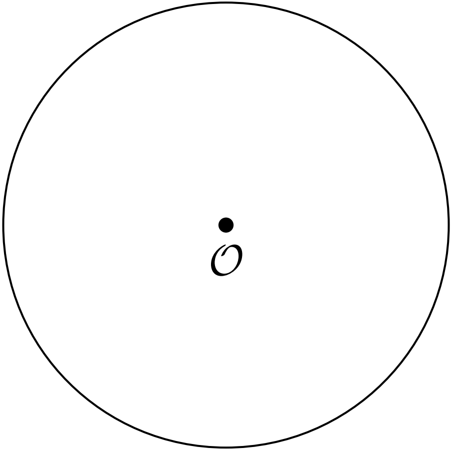
Essentially optimal for large c and $n = 2^{o(d)}$ [Dub’10, AR’15]

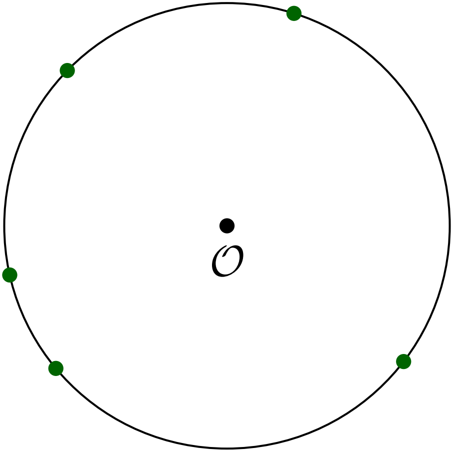
Spherical/Voronoi LSH

[Andoni et al., SODA'14]
[Andoni–Razenshteyn, STOC'15]



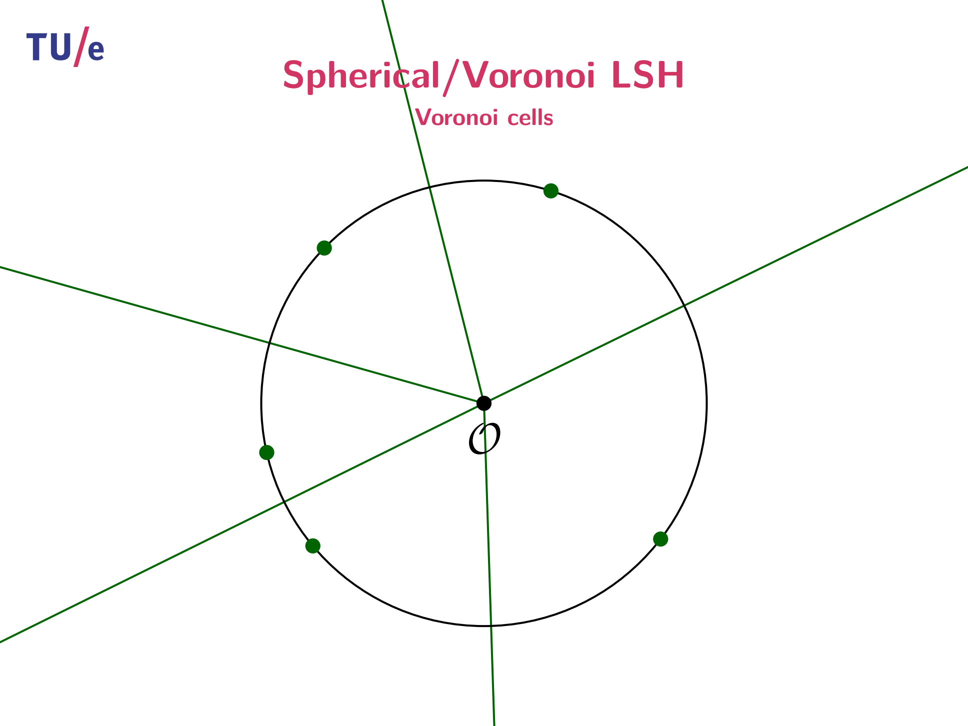
Spherical/Voronoi LSH

Random points



Spherical/Voronoi LSH

Voronoi cells



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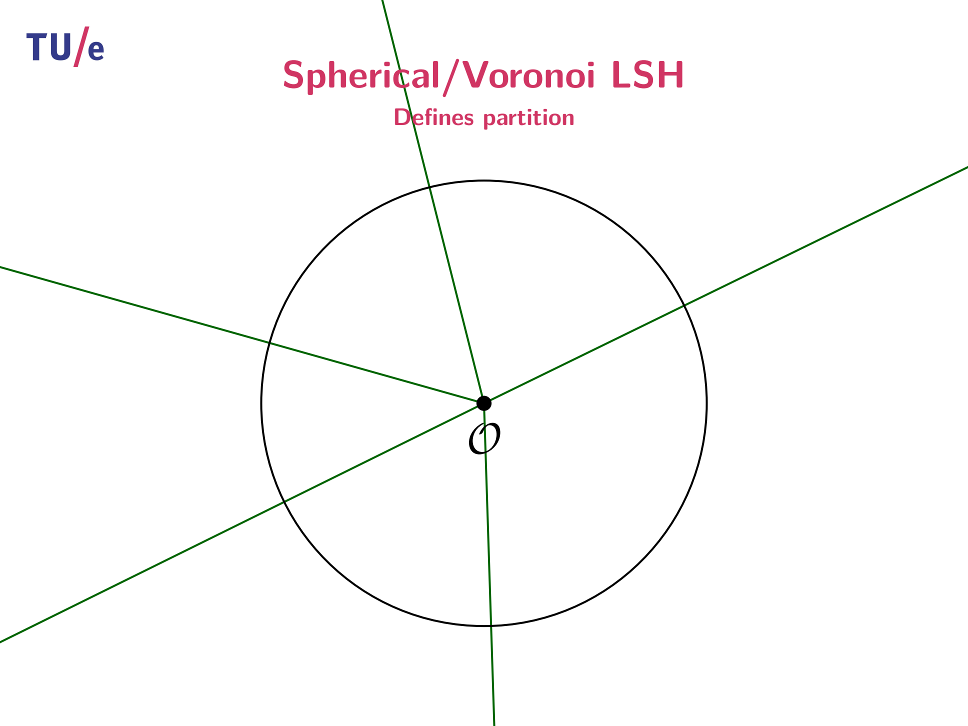

Spherical/Voronoi LSH

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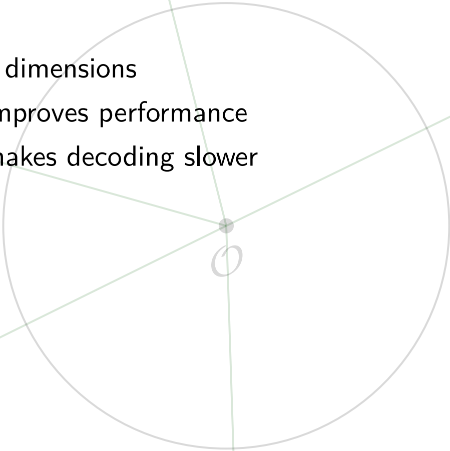
$2^{O(\sqrt{d})}$ points in d dimensions

- More points improves performance
- More points makes decoding slower



TU/e

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LSH overview

- Hyperplane LSH: 2 Voronoi cells
  - Efficient decoding
  - Suboptimal for large d, c
- Cross-Polytope LSH: $2d$ Voronoi cells
  - Reasonably efficient decoding
  - Optimal for large c and $n = 2^{o(d)}$
- Spherical/Voronoi LSH: $2^{O(\sqrt{d})}$ Voronoi cells
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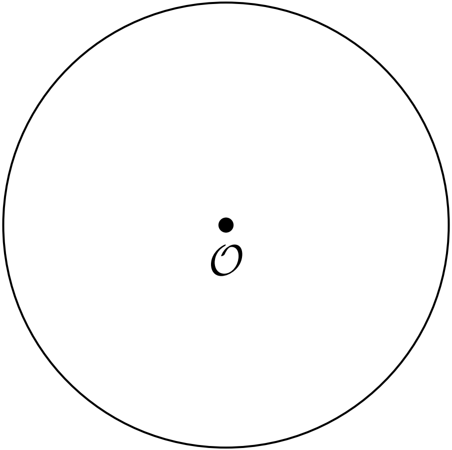
1. Can we use even more Voronoi cells?
2. Can decoding be made faster?
3. What about $n = 2^{\Omega(d)}$?

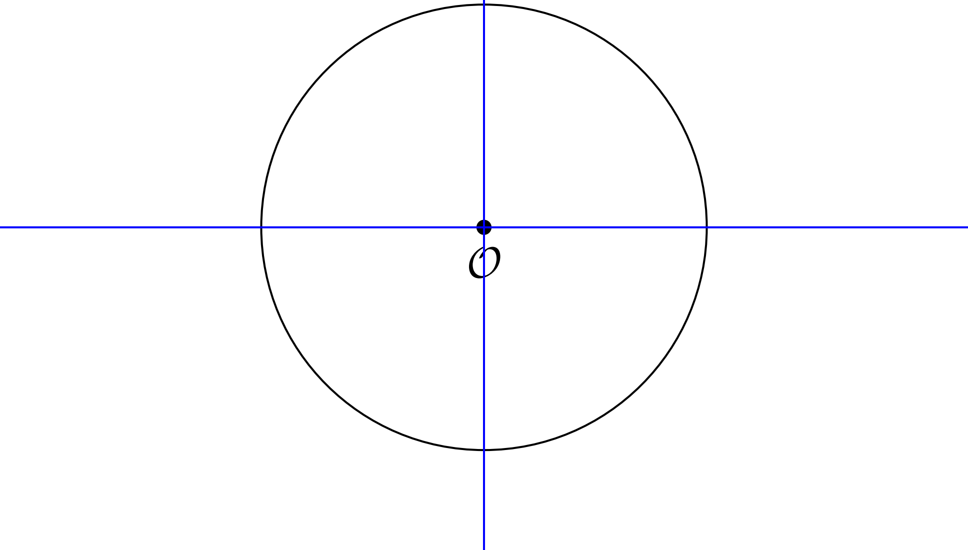
Structured filters

Overview



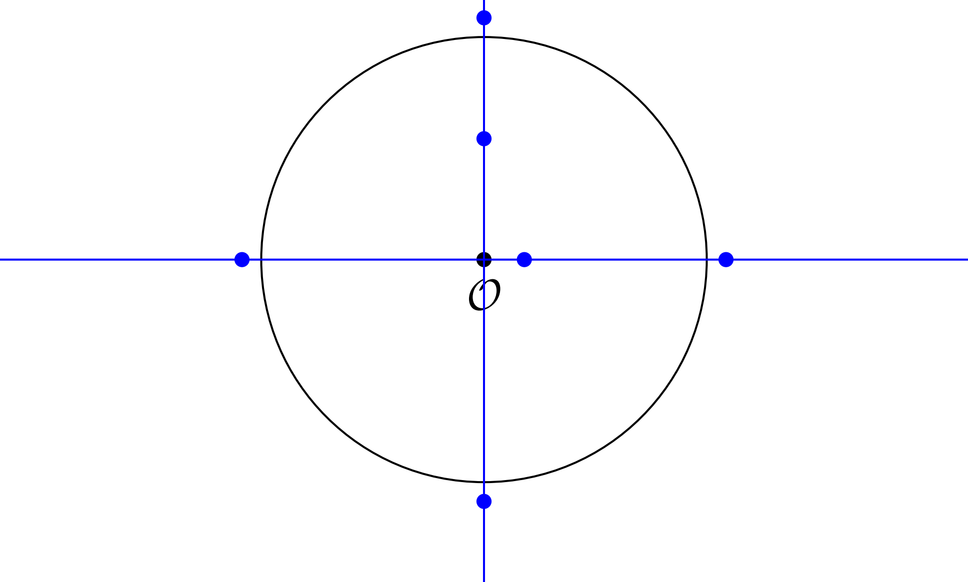
Structured filters

Partition dimensions into blocks



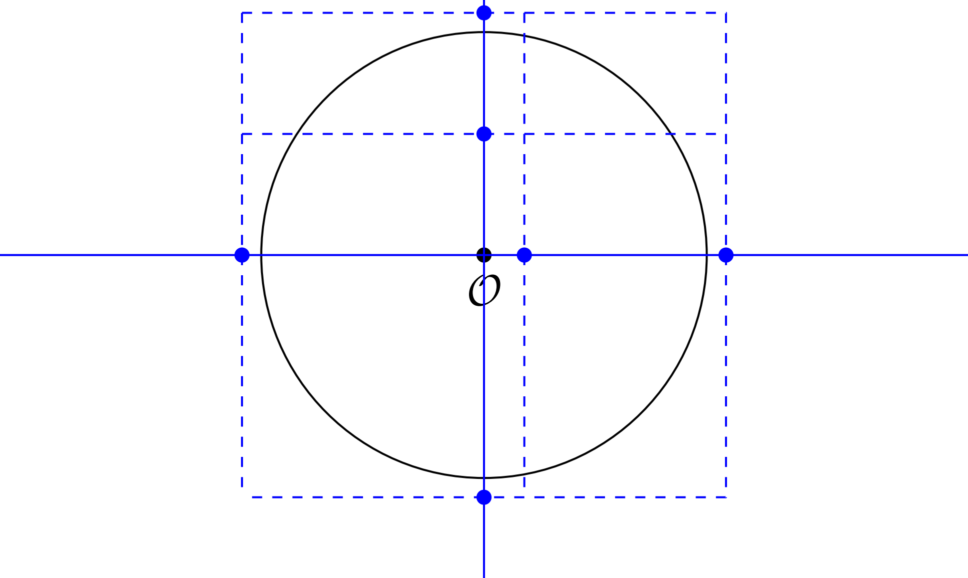
Structured filters

Random subcodes



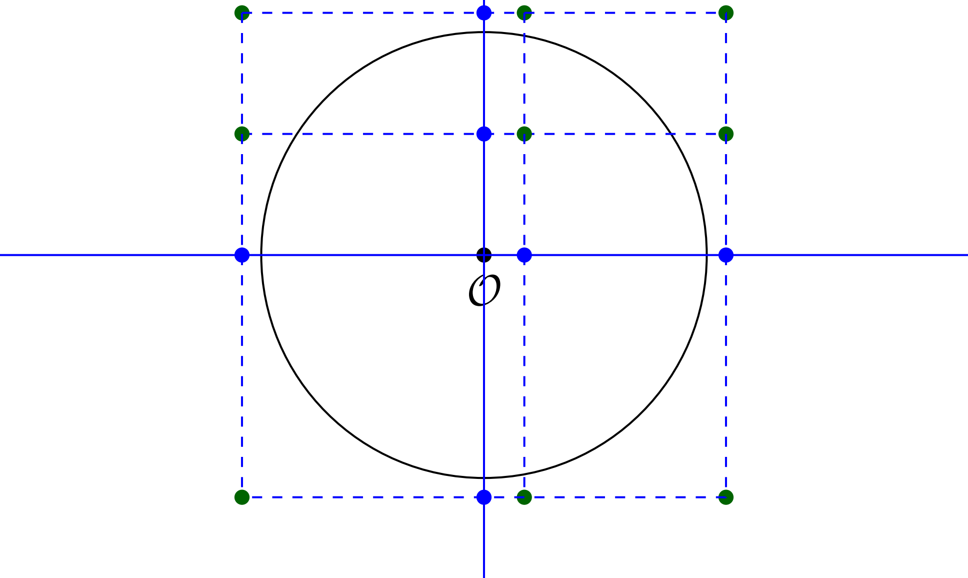
Structured filters

Construct concatenated code



Structured filters

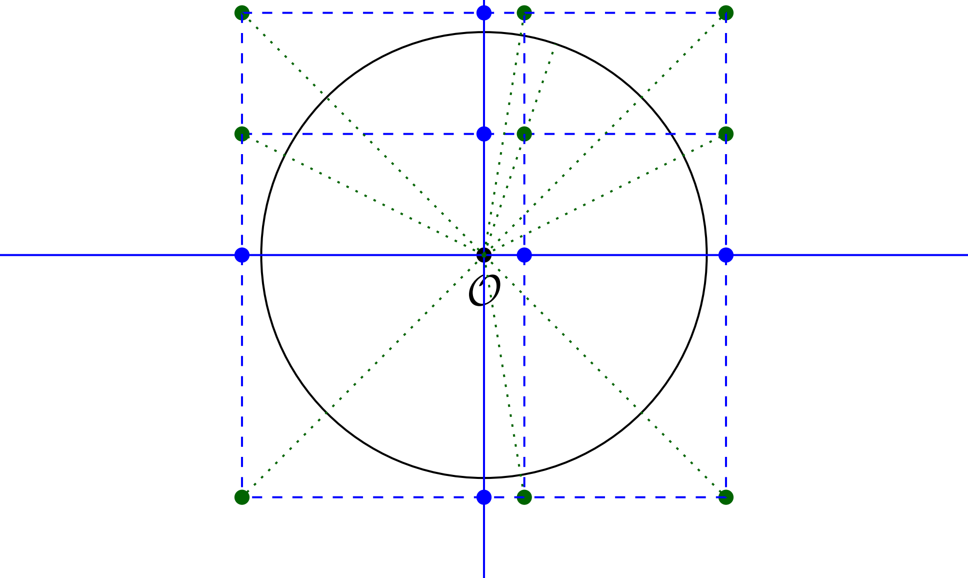
Construct concatenated code



TU/e

Structured filters

Normalize (only for example)



Structured filters

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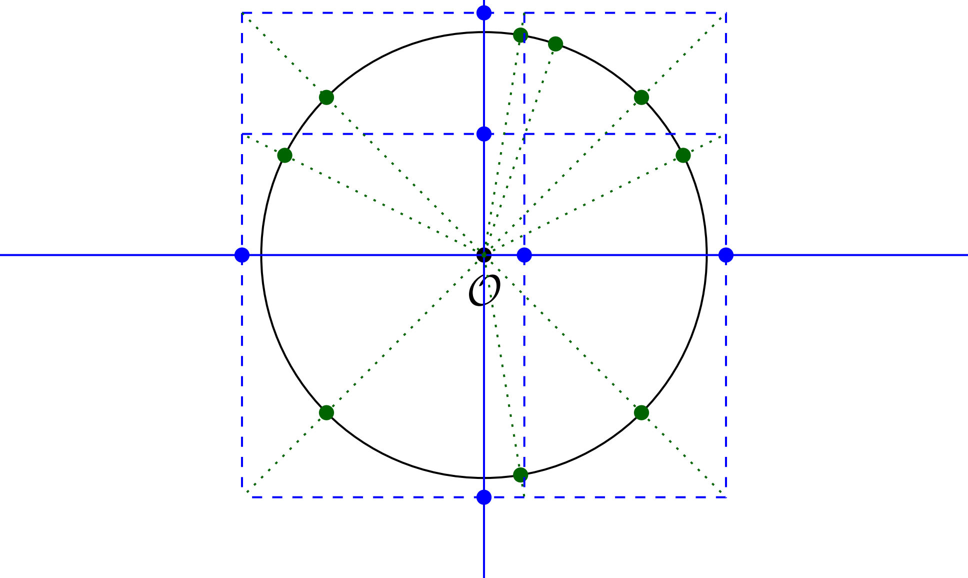

Structured filters

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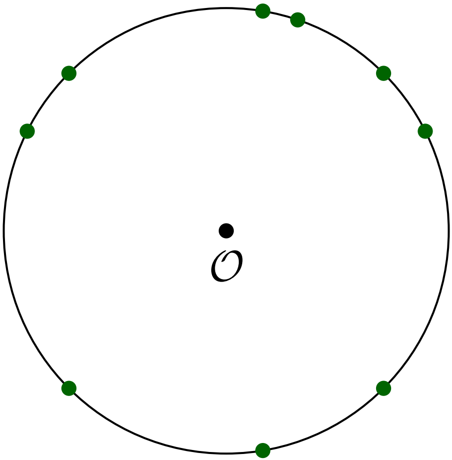
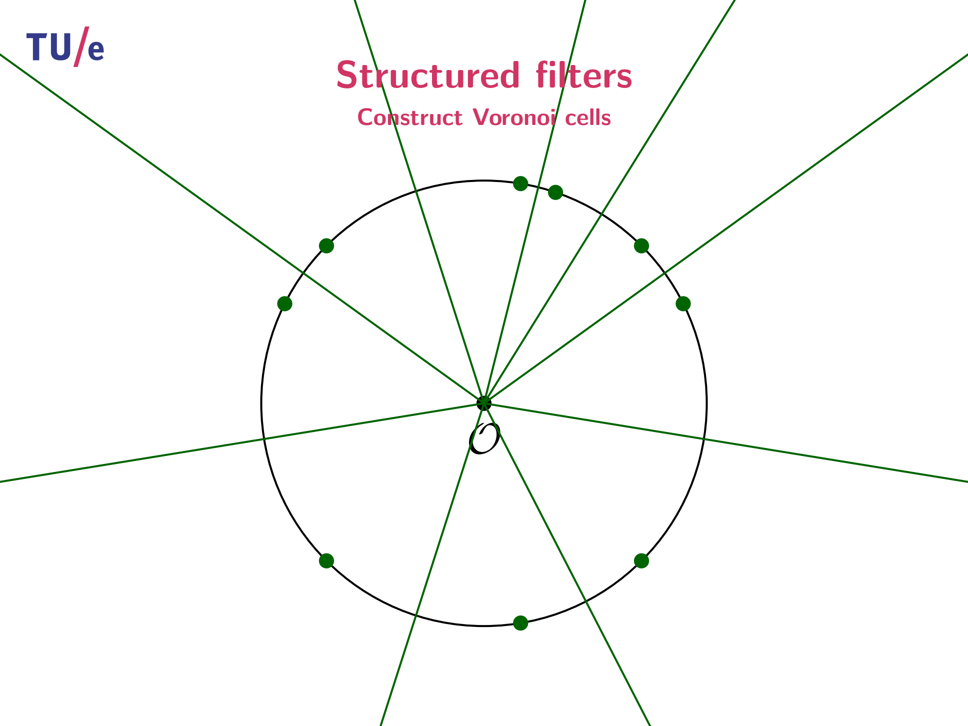


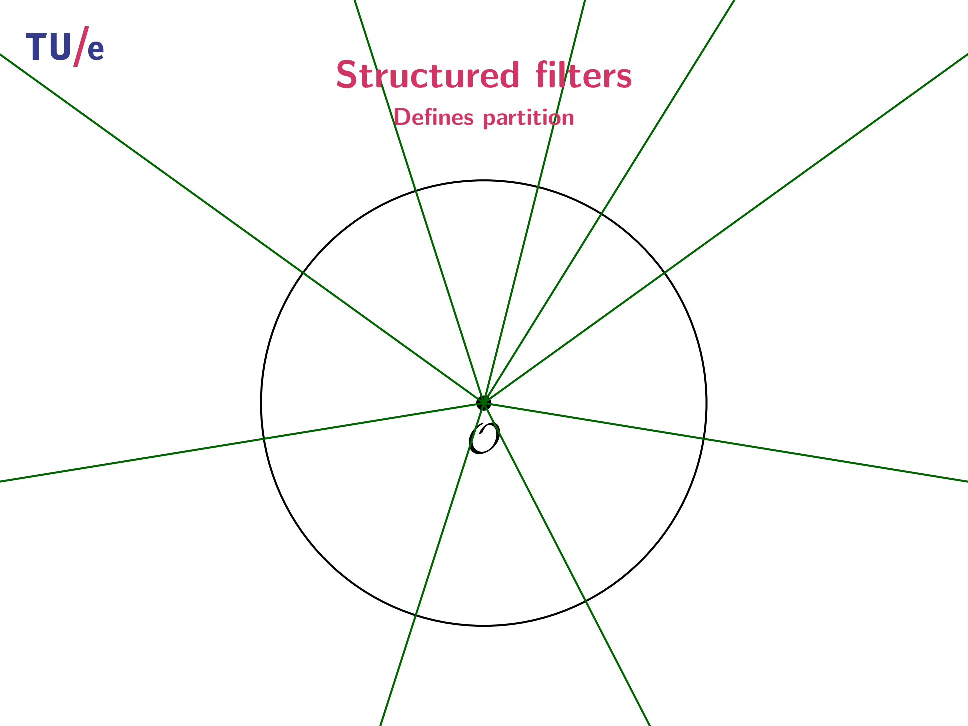
Structured filters

Construct Voronoi cells



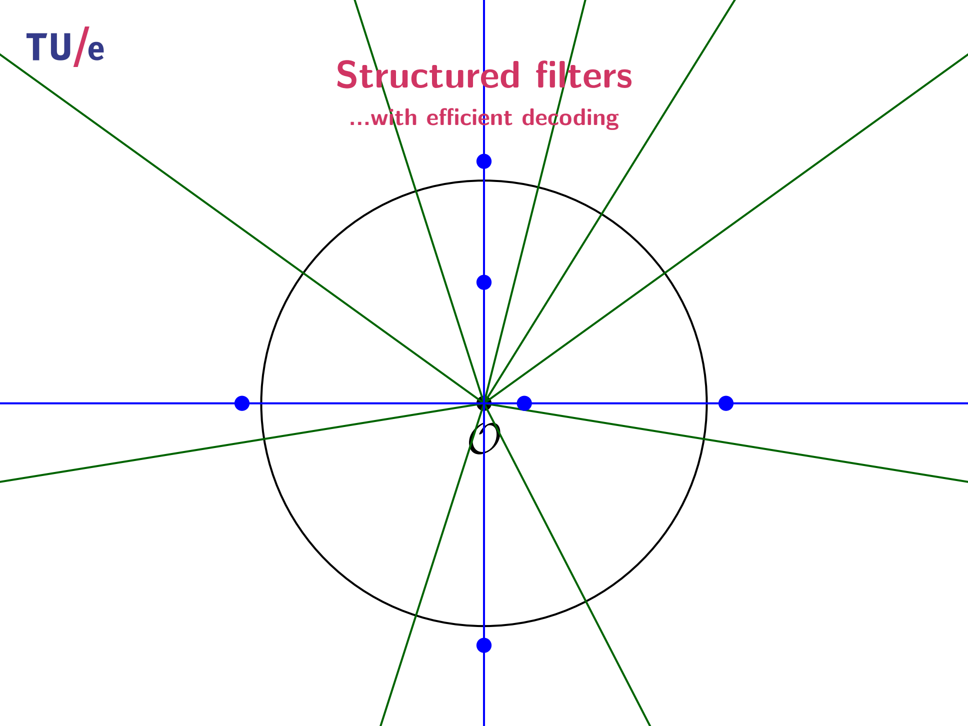
Structured filters

Defines partition



Structured filters

...with efficient decoding

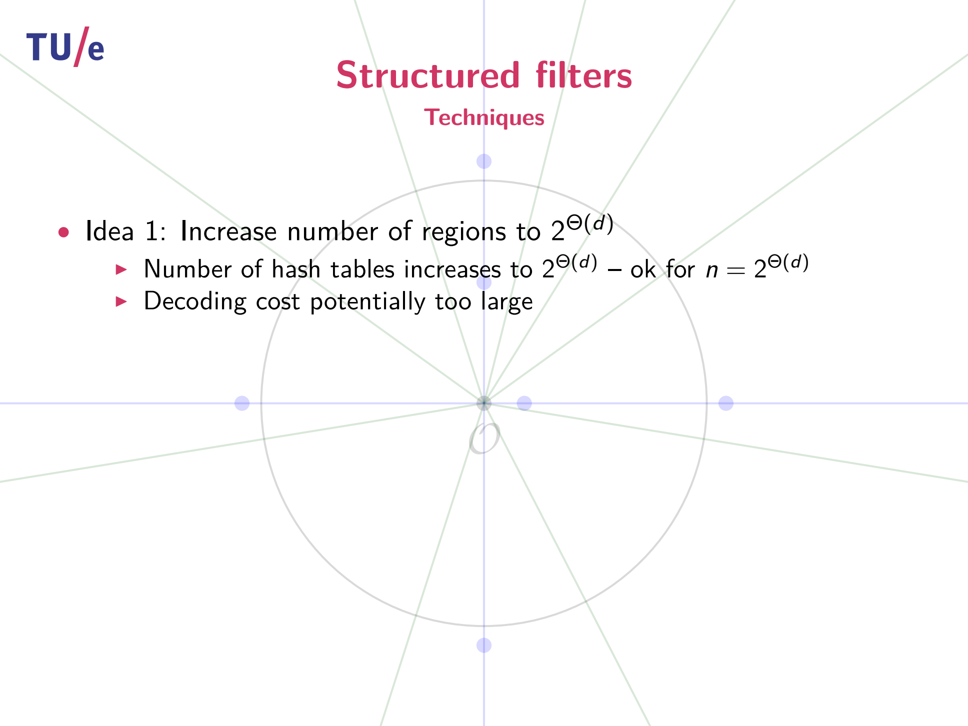


TU/e

Structured filters

Techniques

- Idea 1: Increase number of regions to $2^{\Theta(d)}$
  - Number of hash tables increases to $2^{\Theta(d)}$ – ok for $n = 2^{\Theta(d)}$
  - Decoding cost potentially too large



Structured filters

Techniques

- Idea 1: Increase number of regions to $2^{\Theta(d)}$
  - Number of hash tables increases to $2^{\Theta(d)}$ – ok for $n = 2^{\Theta(d)}$
  - Decoding cost potentially too large
- Idea 2: Use structured codes for random regions
  - Spherical/Voronoi LSH with dependent random points
  - Concatenated code of $\log d$ low-dim. spherical codes
  - Allows for efficient list-decoding

Structured filters

Techniques

- Idea 1: Increase number of regions to $2^{\Theta(d)}$
  - Number of hash tables increases to $2^{\Theta(d)}$ – ok for $n = 2^{\Theta(d)}$
  - Decoding cost potentially too large
- Idea 2: Use structured codes for random regions
  - Spherical/Voronoi LSH with dependent random points
  - Concatenated code of $\log d$ low-dim. spherical codes
  - Allows for efficient list-decoding
- Idea 3: Replace partitions with filters
  - Relaxation: filters need not partition the space
  - Simplified analysis
  - Might not be needed to achieve improvement

Structured filters

Results

For random sparse settings ($n = 2^{o(d)}$), query time $O(n^{\rho})$ with

$$\rho = \frac{1}{2c^2 - 1}\Big(1 + o_d(1)\Big).$$

Structured filters

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For random dense settings ($n = 2^{\kappa d}$ with small κ), we obtain

$$\rho = \frac{1 - \kappa}{2c^2 - 1}\Big(1 + o_{d,\kappa}(1)\Big).$$

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Structured filters

Results

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For random dense settings ($n = 2^{\kappa d}$ with small κ), we obtain

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For random dense settings ($n = 2^{\kappa d}$ with large κ), we obtain

$$\rho = \frac{-1}{2\kappa}\log\left(1 - \frac{1}{2c^2 - 1}\right)\Big(1 + o_d(1)\Big).$$

Asymmetric nearest neighbors

Previous results: symmetric NNS

- Query time: $O(n^{\rho})$
- Update time: $O(n^{\rho})$
- Preprocessing time: $O(n^{1+\rho})$
- Space complexity: $O(n^{1+\rho})$

Asymmetric nearest neighbors

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- Update time: $O(n^{\rho})$
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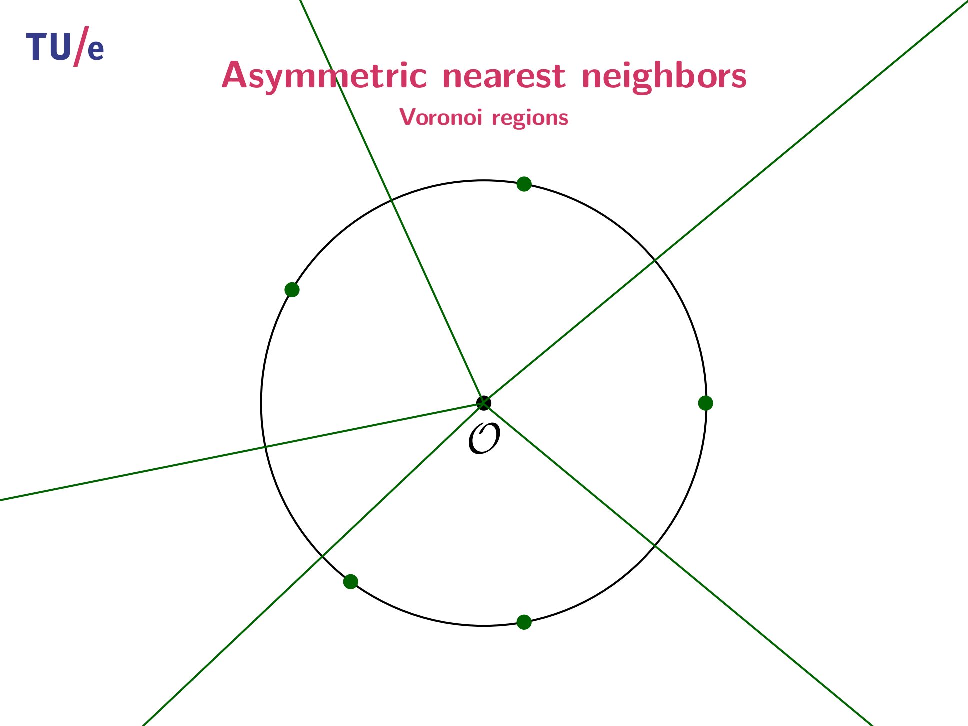
Can we get a tradeoff between these costs?

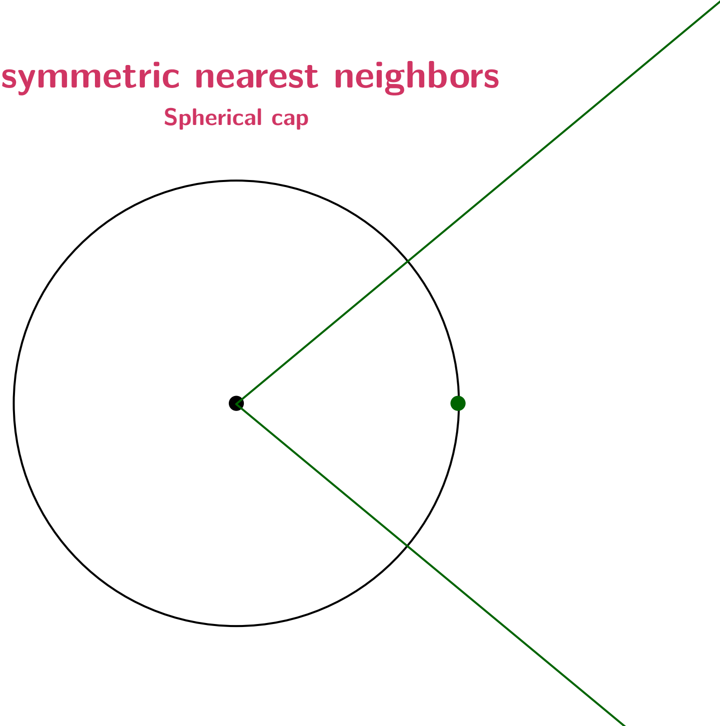
Asymmetric nearest neighbors

Voronoi regions



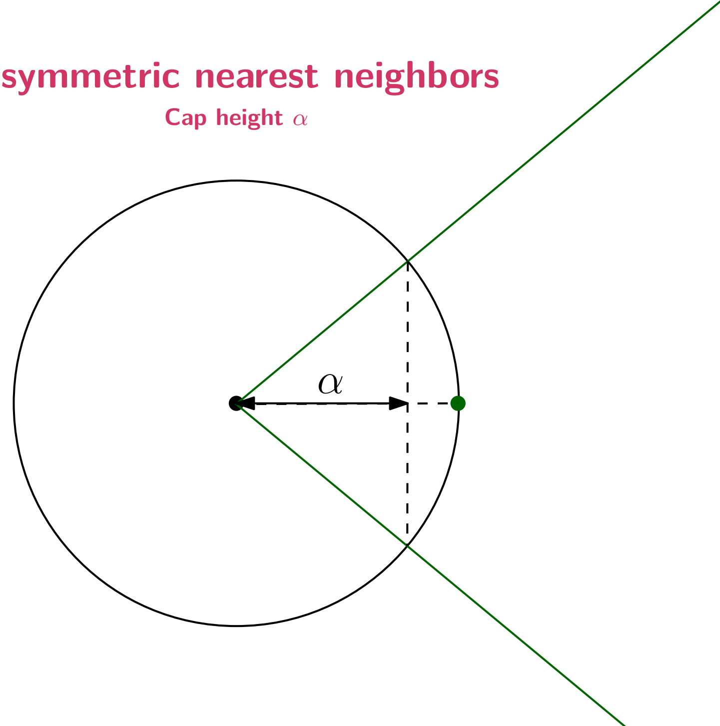
Asymmetric nearest neighbors

Spherical cap



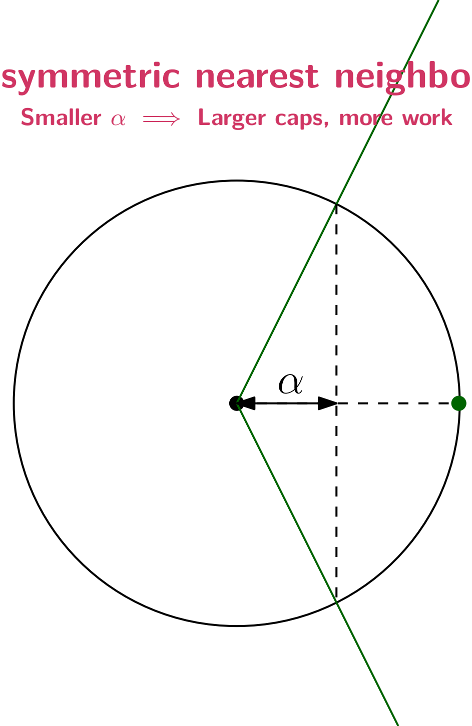
Asymmetric nearest neighbors

Cap height α



Asymmetric nearest neighbors

Smaller $\alpha \implies$ Larger caps, more work



Asymmetric nearest neighbors

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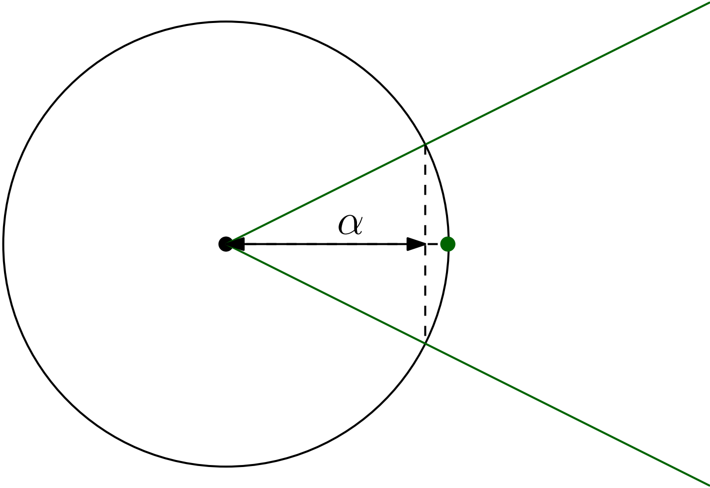
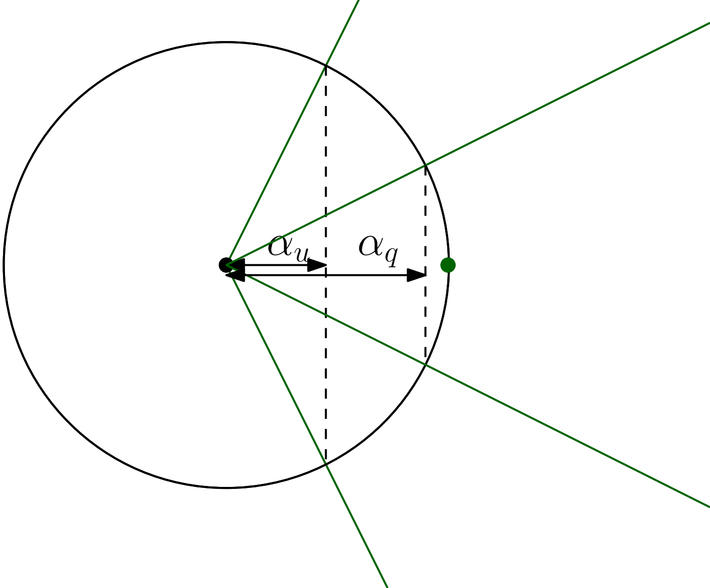


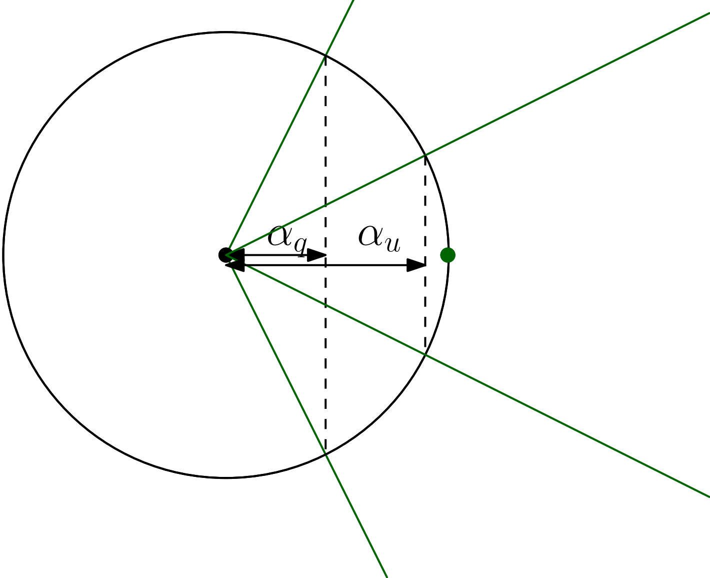
Asymmetric nearest neighbors

$\alpha_q > \alpha_u \implies$ **Faster queries, slower updates**



Asymmetric nearest neighbors

$\alpha_{\mathrm{q}} < \alpha_{\mathrm{u}} \implies$ **Slower queries, faster updates**



Asymmetric nearest neighbors

Results

	General expressions
Minimize space $(\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = \cos\theta)$	$\rho_{\mathrm{q}} = (2c^2 - 1)/c^4$ $\rho_{\mathrm{u}} = 0$
Balance costs $(\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = 1)$	$\rho_{\mathrm{q}} = 1/(2c^2 - 1)$ $\rho_{\mathrm{u}} = 1/(2c^2 - 1)$
Minimize time $(\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = 1/\cos\theta)$	$\rho_{\mathrm{q}} = 0$ $\rho_{\mathrm{u}} = (2c^2 - 1)/(c^2 - 1)^2$

Query time $O(n^{\rho_{\mathrm{q}}})$, update time $O(n^{\rho_{\mathrm{u}}})$, preprocessing time $O(n^{1+\rho_{\mathrm{u}}})$, space complexity $O(n^{1+\rho_{\mathrm{u}}})$

Asymmetric nearest neighbors

Results

	General expressions	Small $c = 1 + \varepsilon$
Minimize space	$\rho_{\mathrm{q}} = (2c^2 - 1)/c^4$	$\rho_{\mathrm{q}} = 1 - 4\varepsilon^2 + O(\varepsilon^3)$
$(\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = \cos\theta)$	$\rho_{\mathrm{u}} = 0$	$\rho_{\mathrm{u}} = 0$
Balance costs	$\rho_{\mathrm{q}} = 1/(2c^2 - 1)$	$\rho_{\mathrm{q}} = 1 - 4\varepsilon + O(\varepsilon^2)$
$(\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = 1)$	$\rho_{\mathrm{u}} = 1/(2c^2 - 1)$	$\rho_{\mathrm{u}} = 1 - 4\varepsilon + O(\varepsilon^2)$
Minimize time	$\rho_{\mathrm{q}} = 0$	$\rho_{\mathrm{q}} = 0$
$(\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = 1/\cos\theta)$	$\rho_{\mathrm{u}} = (2c^2 - 1)/(c^2 - 1)^2$	$\rho_{\mathrm{u}} = 1/(4\varepsilon^2) + O(1/\varepsilon)$

Query time $O(n^{\rho_{\mathrm{q}}})$, update time $O(n^{\rho_{\mathrm{u}}})$, preprocessing time $O(n^{1+\rho_{\mathrm{u}}})$, space complexity $O(n^{1+\rho_{\mathrm{u}}})$

Asymmetric nearest neighbors

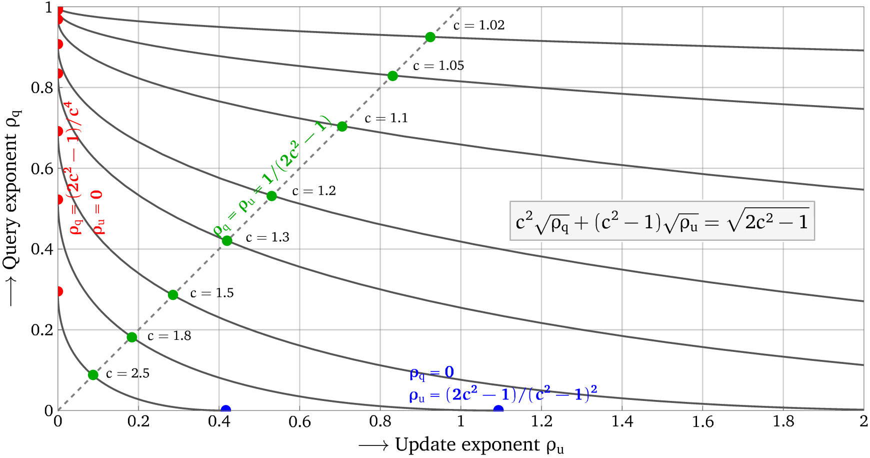
Results

	General expressions	Large $c \to \infty$
Minimize space ($\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = \cos\theta$)	$\rho_{\mathrm{q}} = (2c^2 - 1)/c^4$ $\rho_{\mathrm{u}} = 0$	$\rho_{\mathrm{q}} = 2/c^2 + O(1/c^4)$ $\rho_{\mathrm{u}} = 0$
Balance costs ($\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = 1$)	$\rho_{\mathrm{q}} = 1/(2c^2 - 1)$ $\rho_{\mathrm{u}} = 1/(2c^2 - 1)$	$\rho_{\mathrm{q}} = 1/(2c^2) + O(1/c^4)$ $\rho_{\mathrm{u}} = 1/(2c^2) + O(1/c^4)$
Minimize time ($\alpha_{\mathrm{q}}/\alpha_{\mathrm{u}} = 1/\cos\theta$)	$\rho_{\mathrm{q}} = 0$ $\rho_{\mathrm{u}} = (2c^2 - 1)/(c^2 - 1)^2$	$\rho_{\mathrm{q}} = 0$ $\rho_{\mathrm{u}} = 2/c^2 + O(1/c^4)$

Query time $O(n^{\rho_{\mathrm{q}}})$, update time $O(n^{\rho_{\mathrm{u}}})$, preprocessing time $O(n^{1+\rho_{\mathrm{u}}})$, space complexity $O(n^{1+\rho_{\mathrm{u}}})$

Asymmetric nearest neighbors

Tradeoffs



Conclusions

Main result: Allow using more regions with list-decodable codes

- For $n = 2^{o(d)}$, non-asymptotic improvement
- For $n = 2^{\Theta(d)}$, asymptotic improvement
- Corollary: Lower bounds for $n = 2^{o(d)}$ do not hold for $n = 2^{\Theta(d)}$
- Improved tradeoffs between query and update complexities

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Open problems

- Tradeoff for $n = 2^{o(d)}$ optimal?
- Lower bounds for $n = 2^{\Theta(d)}$?
- Apply similar ideas to other norms?
- Practicality?

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Questions?