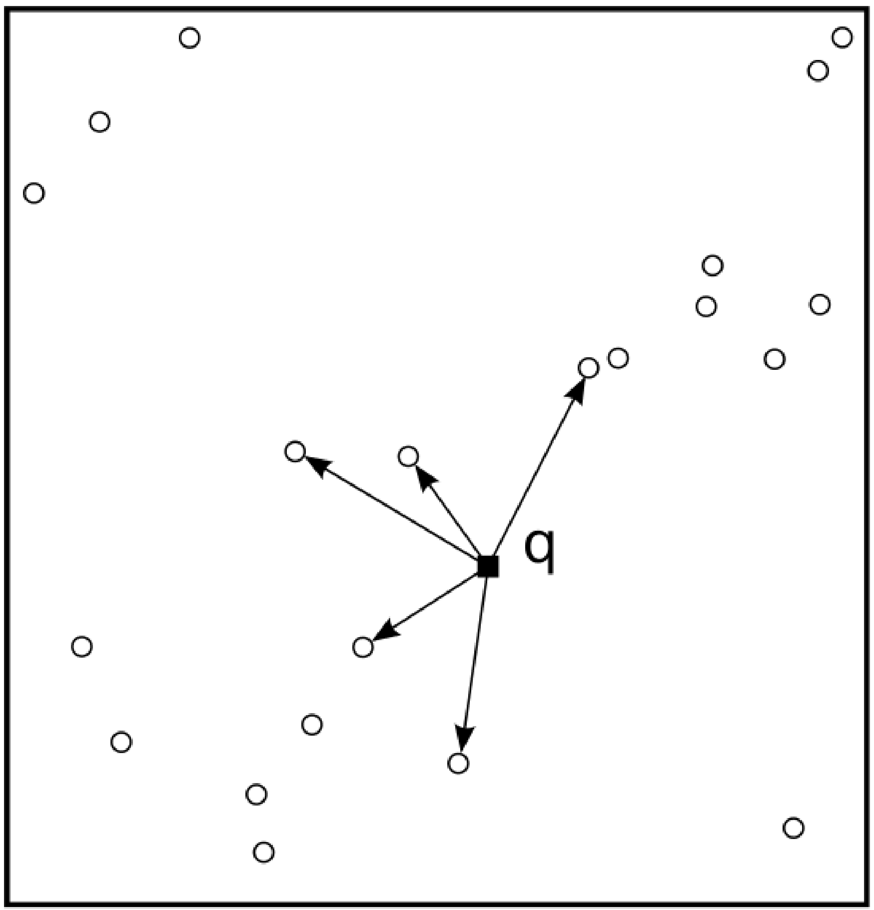
Fast nearest neighbor searches in high dimensions

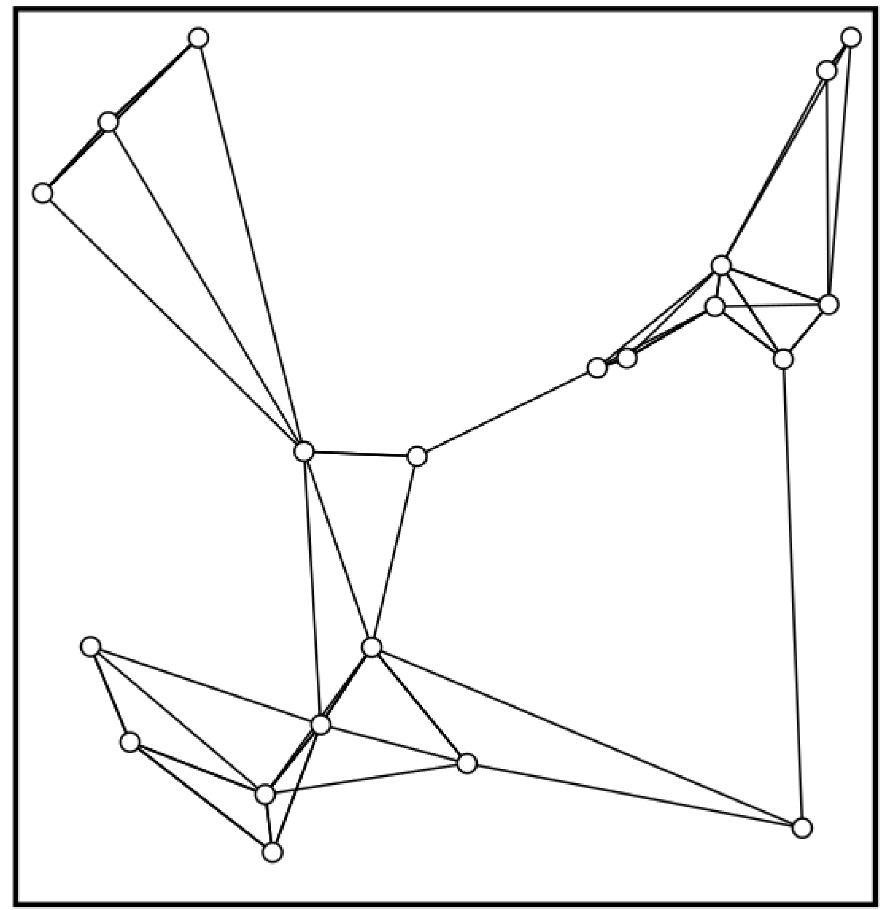
Sami Sieranoja

Nearest neighbor problems

k-nearest neighbors, $k = 5$



k nearest neighbors graph ($k = 3$)



Notation: k = number of neighbors, not clusters (k-means).

Contents

- (exact) Nearest neighbor search in low dimensions
- What makes higher dimensions (D>20) difficult
- (approximate) High dimensional *k* nearest neighbor graph construction

Introduction

In clustering, KNN graph:

- Has been used in agglomerative clustering[1].
- Has potential to speed up k-means (open question).

[1] P. Fränti, O. Virmajoki and V. Hautamäki, "Fast agglomerative clustering using a k-nearest neighbor graph", IEEE Trans. on Pattern Analysis and Machine Intelligence, 28 (11), 1875-1881, November 2006.

Brute force search

K Nearest neighbor search:

- Brute force O(N) method calculates distances from query point *q* to all points.
- Faster (exact) log(N) methods exist, but only for low dimensional data

*k*NN graph construction:

- Brute force $O(N^2)$ method calculates between all pairs of points.
- Faster (exact) N*log(N) methods exist, but only for low dimensional data

Nearest neighbor search in low dimensions: kd-tree

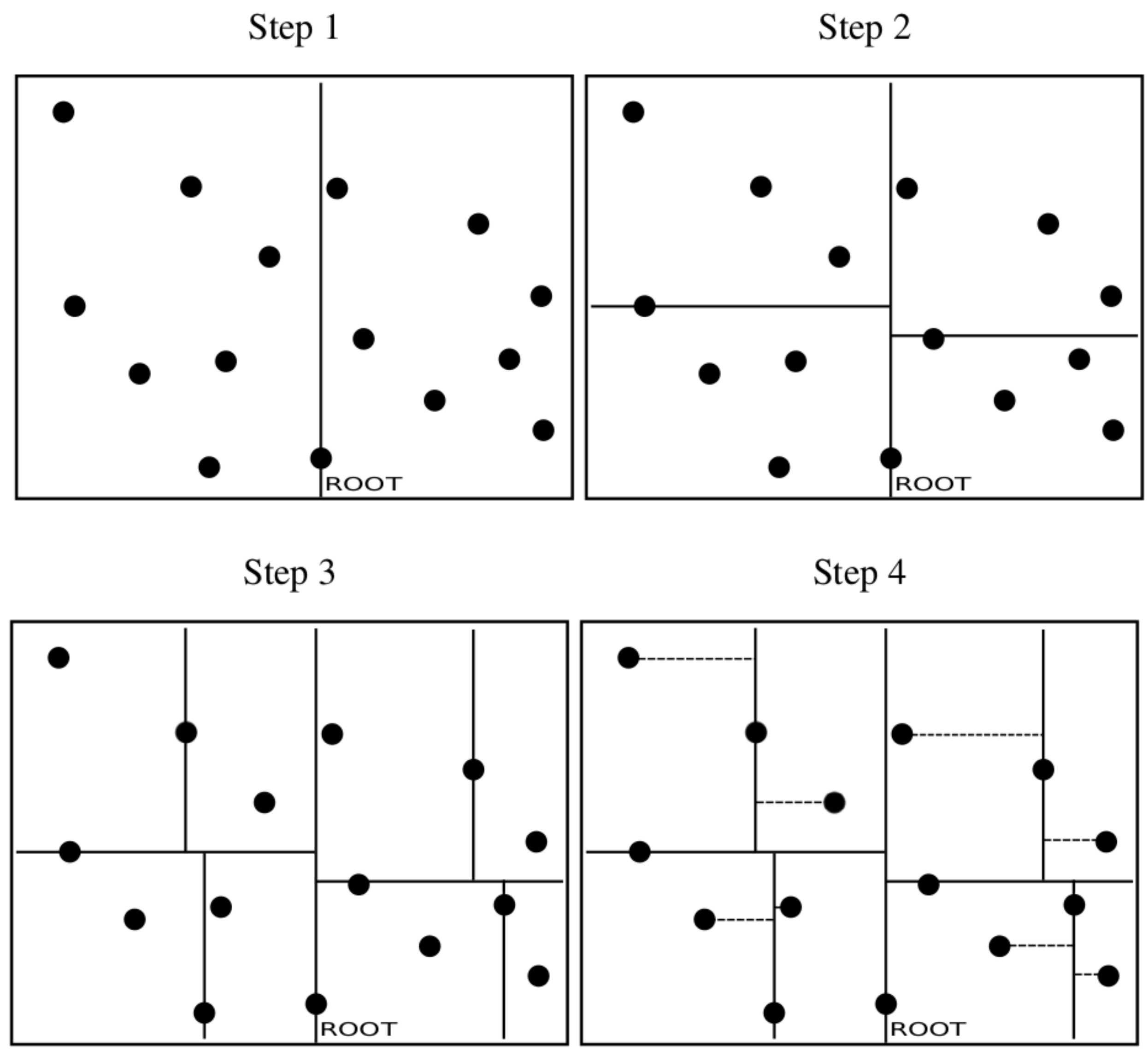
D=2 dimensional dataset with N=14 points (black circles)

1) Take first dimension
2) Divide points into two halves according to median
3) Continue step 2 recursively for next dimension

Number of recursions: log(N)
log(N=14) = 3.8
Tree contruction: O(N*log(N))

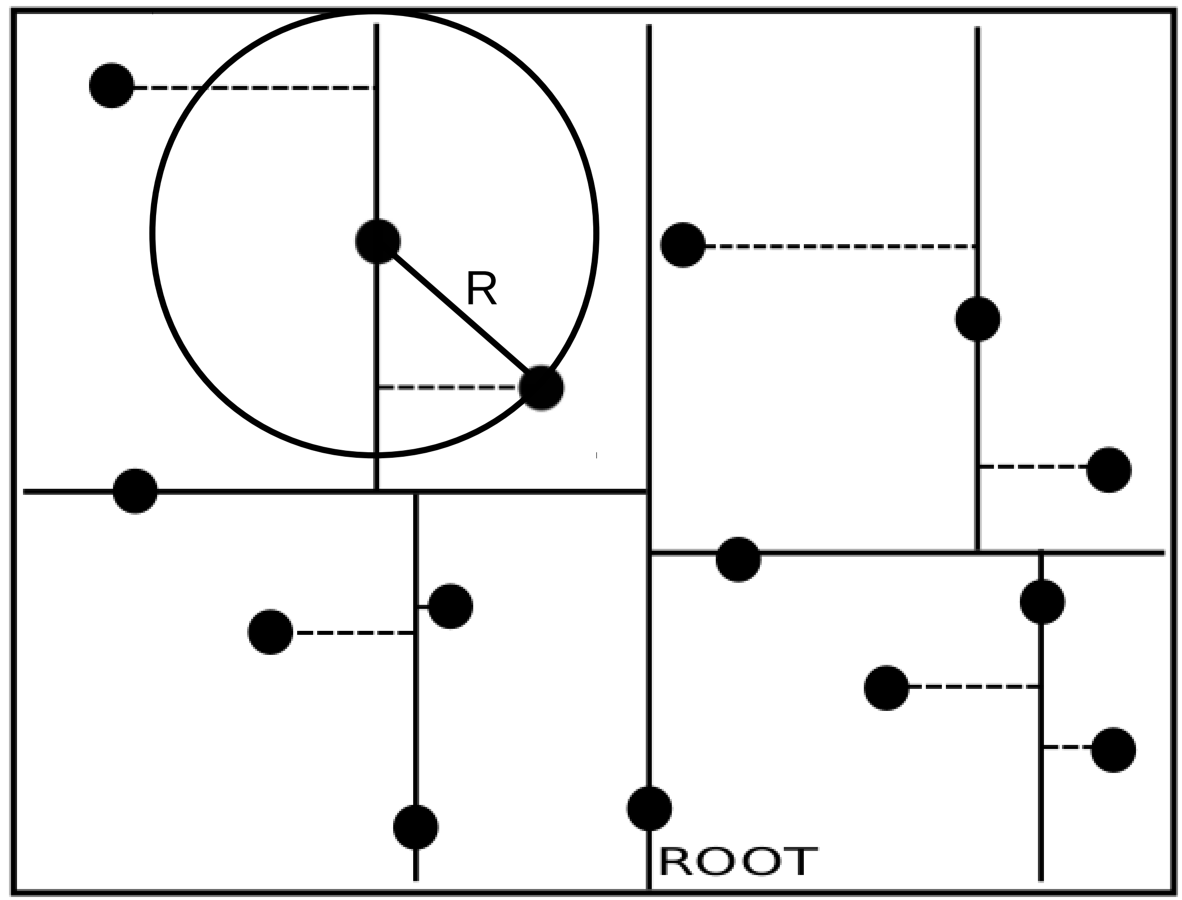
K-nearest neighbor search using tree: O(log(N))

K-nn graph: O(N*log(N))



Nearest neighbor search using kd-tree

If nearest neighbor ball is within bounding rectangle
AND
Have checked all points within that rectangle
=>
Results are exact



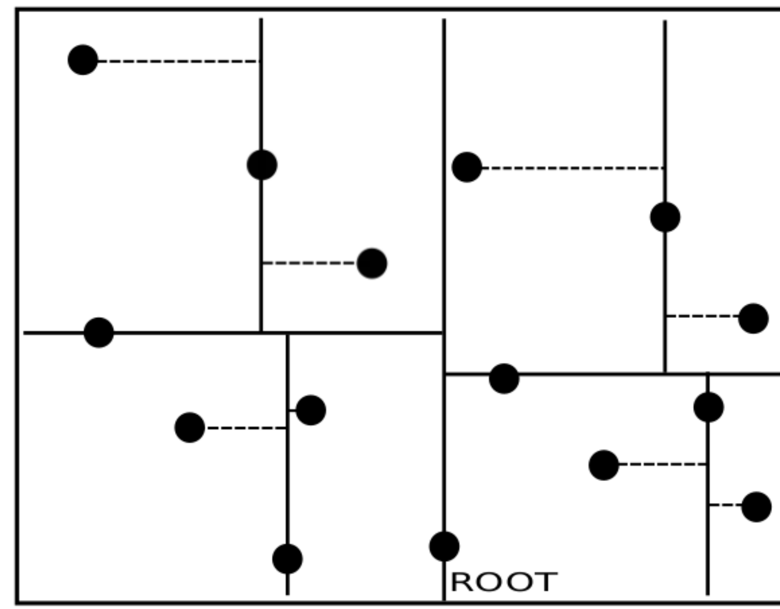
What makes higher dimensions difficult?
(Why kd-trees fail)

Recursive subdivision in high dimensions

For large D, leaf nodes are reached before handling all dimensions.

- Number of recursions to construct tree: log(N)
- What if D > log(N) ? →
- Only a log(N)/D portion of data is used to construct the tree.
- D=1000, N=1,000,000. log(N) = 20
- log(N)/D = 2%.

4 steps to construct:

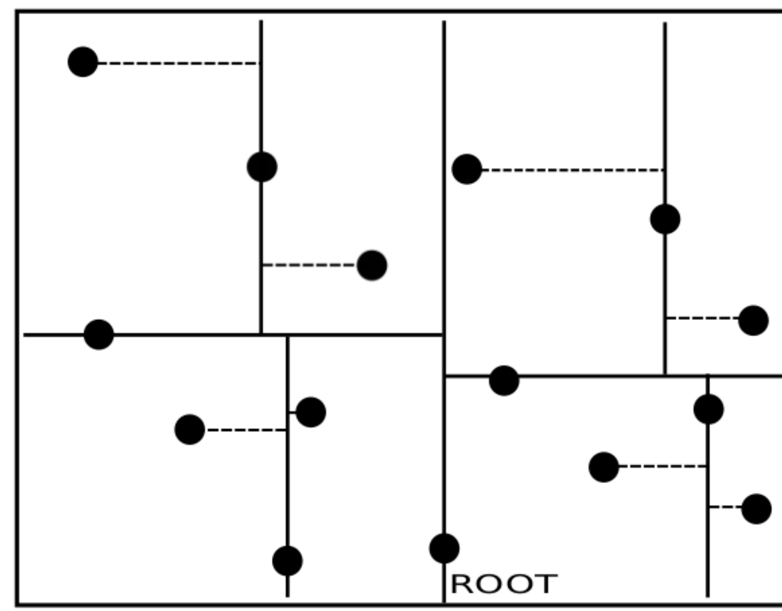


Recursive subdivision in high dimensions

Fast methods are possible for large enough data sets

- For log(N)/D >= 1, data set size of $N=2^D$ needed.
- D=20 ⇒ N=1,048,576
- D=1000 ⇒ $N = 2^{1000} = 10^{301}$

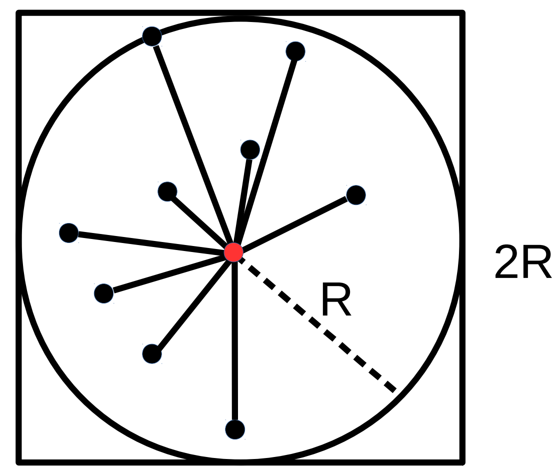
4 steps to construct:



Searching the bounding rectangle

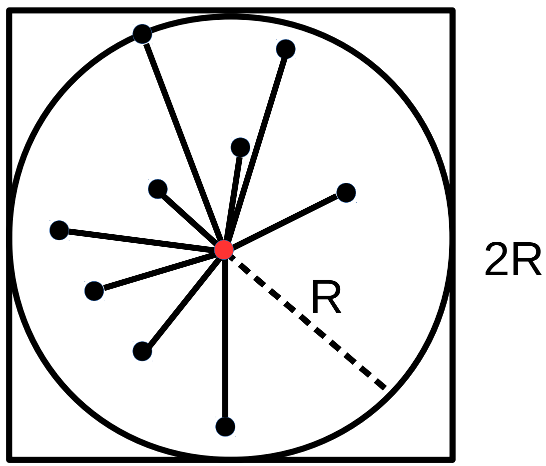
- Works because rectangle is usually not much larger than the circle
- Best case: square with side length 2R
- 2D: If 10 points inside circle, how many expected to be inside rectangle?
- 3D?

K=9 nearest neighbor sphere/cube:



Estimating number of expected points using volume

K=9 nearest neighbor sphere/cube:



Assume R=0.5.

Size of rectangle: $V=(2R)^2=1$
Size of cube: $V=(2R)^3=1$
Size of D-dimensional hypercube: $V=(2R)^D=1$

Volume of 2D rectangle: $V=\pi R^2$

Volume of 3D sphere: $\frac{4}{3}\pi R^3$

Volume of D-dimensional Hypersphere: $$V=R^D\frac{\pi^{(D/2)}}{\Gamma(D/2+1)}$$

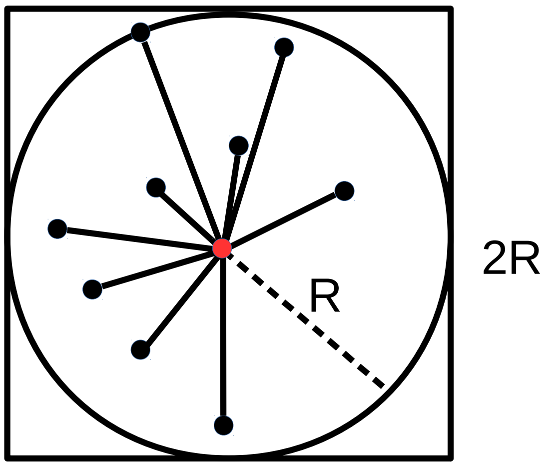
Volumes of the sphere and cube correspond to the number of expected points in that area, assuming points are uniformly distributed.

Volume of unit diameter hypersphere vs. hypercube

For D=2, if ten points within sphere, 10/0.79 = 13 points expected to be within rectangle

D	Volume(Sphere)/ Volume(Cube)	Expected N(points) in hypercube
2	79%	13
3	52%	19
5	16%	62
10	0.25%	5000
100	1.9e-68 %	5.3e+68

K=9 nearest neighbor sphere/cube:



$D \rightarrow \inf \Rightarrow$ Volume(Hypersphere)/Volume(Hypercube) $\rightarrow 0$

KNN graph for high dimensional data

- For high dimensional data (D>20, Euclidean space), no known exact method exists, faster than brute force $O(N^2)$.
- Approximate methods exist that produce > 90% accurate graph in just 1% time of the brute force method.

Existing methods

Existing methods: KGRAPH[1], NNDES[2], Lanczos[3], LSH[4], LargeViz[5]

[2] Wei Dong. KGraph[software]. Available from http://www.kgraph.org/. 2014.

[3] W. Dong, C. Moses, and K. Li, “Efficient k-nearest neighbor graph construction for generic similarity measures,” in Proceedings of the 20th international conference on World wide web, p. 577–586, ACM, 2011.

[4] J. Chen, H.-r. Fang, and Y. Saad, “Fast approximate k NN graph construction for high dimensional data via recursive Lanczos bisection,” The Journal of Machine Learning Research, vol. 10, p. 1989–2012, 2009.

[5] Y.-M. Zhang, K. Huang, G. Geng, and C.-L. Liu, “Fast kNN Graph Construction with Locality Sensitive Hashing,” in Machine Learning and Knowledge Discovery in Databases, p. 660–674, Springer, 2013.

[6] J. Wang, J. Wang, G. Zeng, Z. Tu, R. Gan, and S. Li, “Scalable k-NN graph construction for visual descriptors,” in Computer Vision and Pattern Recognition (CVPR), 2012 IEEE Conference on, p. 1106–1113, IEEE, 2012.

Existing methods

Algorithm	Graph initialization	Graph refinement	General
KGRAPH	Random graph	Neighborhood propagation	Yes
NNDES	Random graph	Neighborhood propagation	Yes
Lanczos	Divide & Conquer	Neighborhood propagation	No
LSH	Hashing	Neighborhood propagation	No
LargeViz	Divide & Conquer	Neighborhood propagation	No

Z-order neighborhood propagation(ZNP)

Two parts: (1) graph initialization (2) graph refinement.

Outline of algorithm:

1) Construct initial graph using one dimensional ordering called Z-order

2) Improve graph by using Neighborhood propagation.

(paper under review)

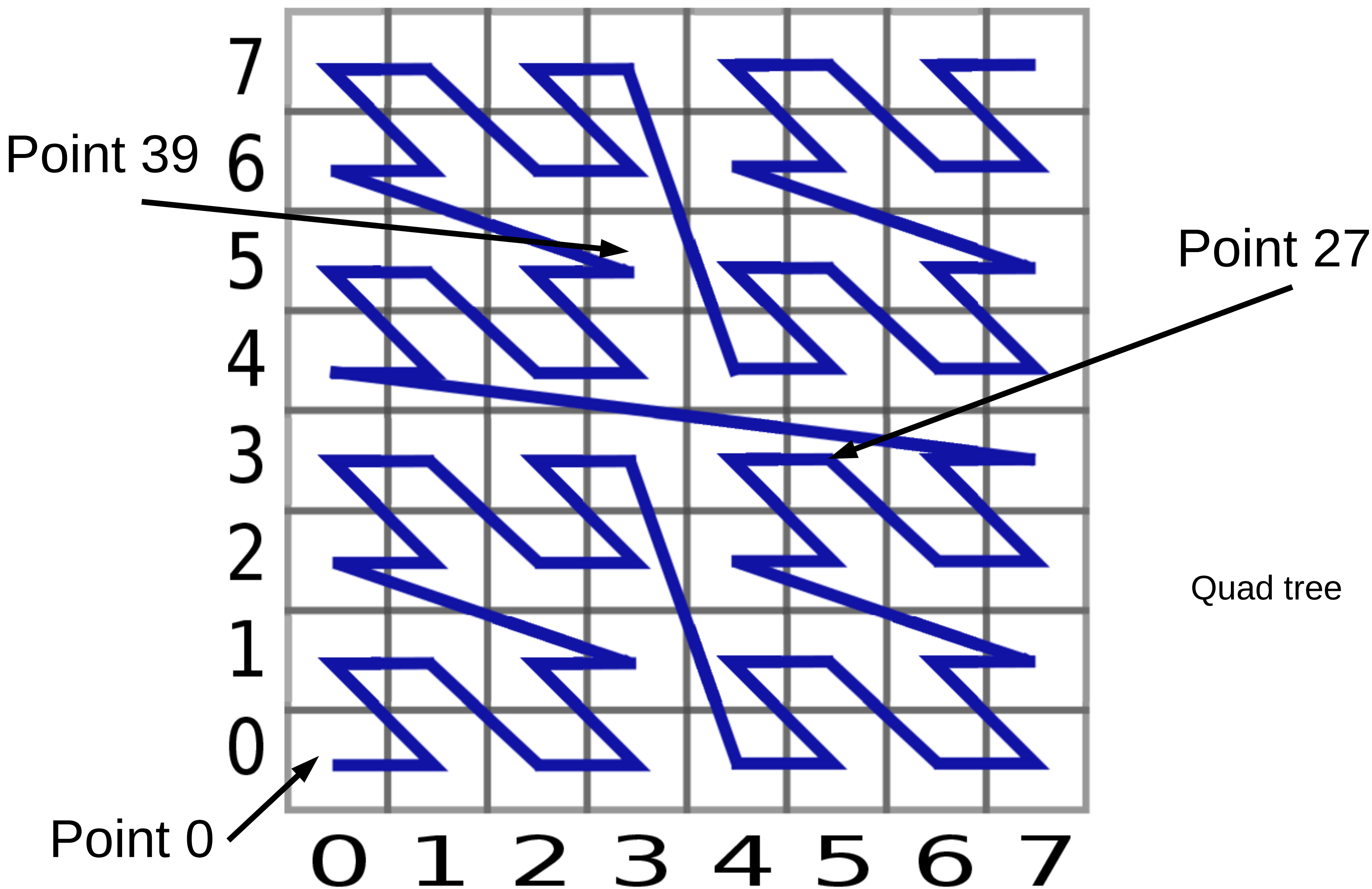
Z-values

$$
\begin{array}{r}
\text{interleaved bits} \downarrow \\
(3,5) = (\textcolor{red}{011}_2, \textcolor{blue}{101}_2) \rightarrow \textcolor{red}{0}\textcolor{blue}{1}\ \textcolor{red}{1}\textcolor{blue}{0}\ \textcolor{red}{1}\textcolor{blue}{1}_2 = 27 \\
\rightarrow \textcolor{blue}{1}\textcolor{red}{0}\ \textcolor{blue}{0}\textcolor{red}{1}\ \textcolor{blue}{1}\textcolor{red}{1}_2 = 39
\end{array}
$$

$\uparrow$ 2D vector $\qquad\qquad\qquad$ z-value $\uparrow$

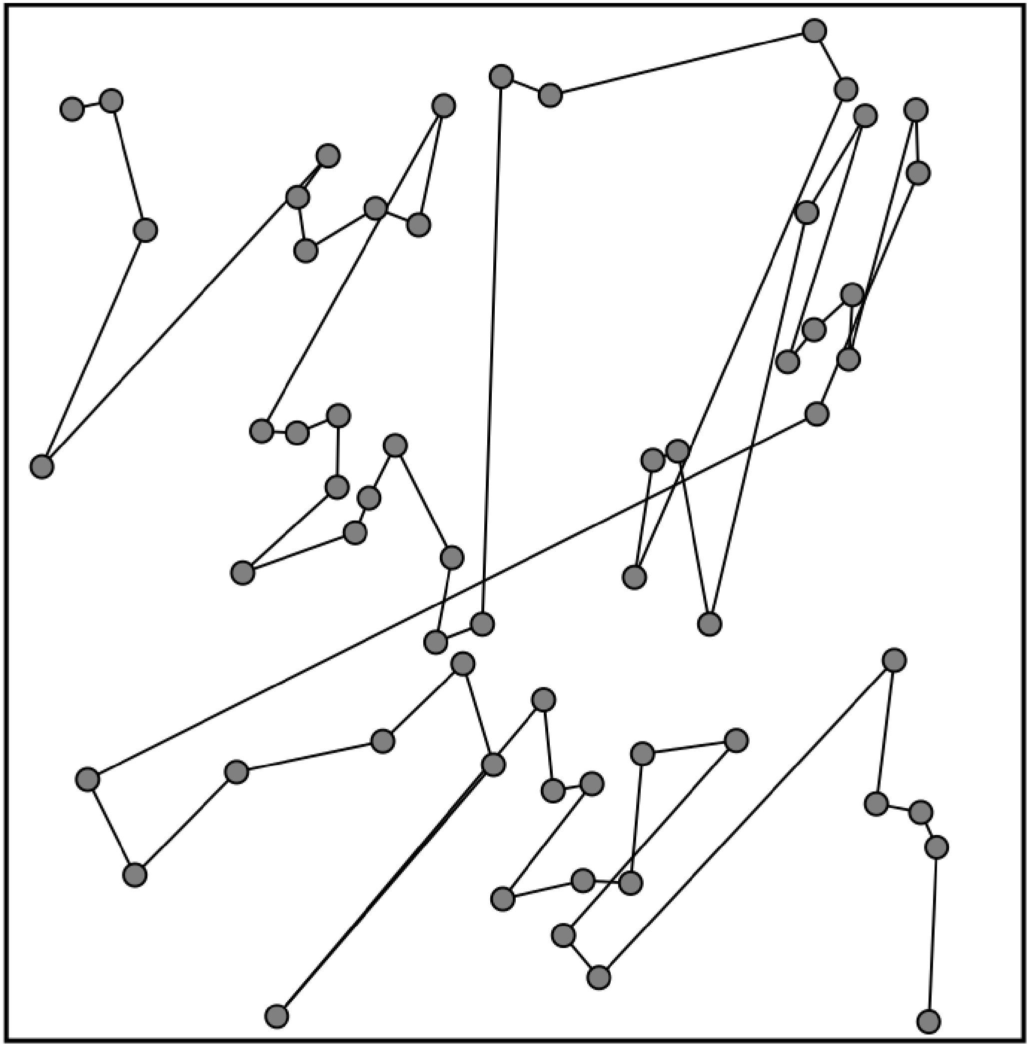
G. M. Morton, A computer oriented geodetic data base and a new technique in file sequencing. International Business Machines Company, 1966.

2D grid ordered by Z-values

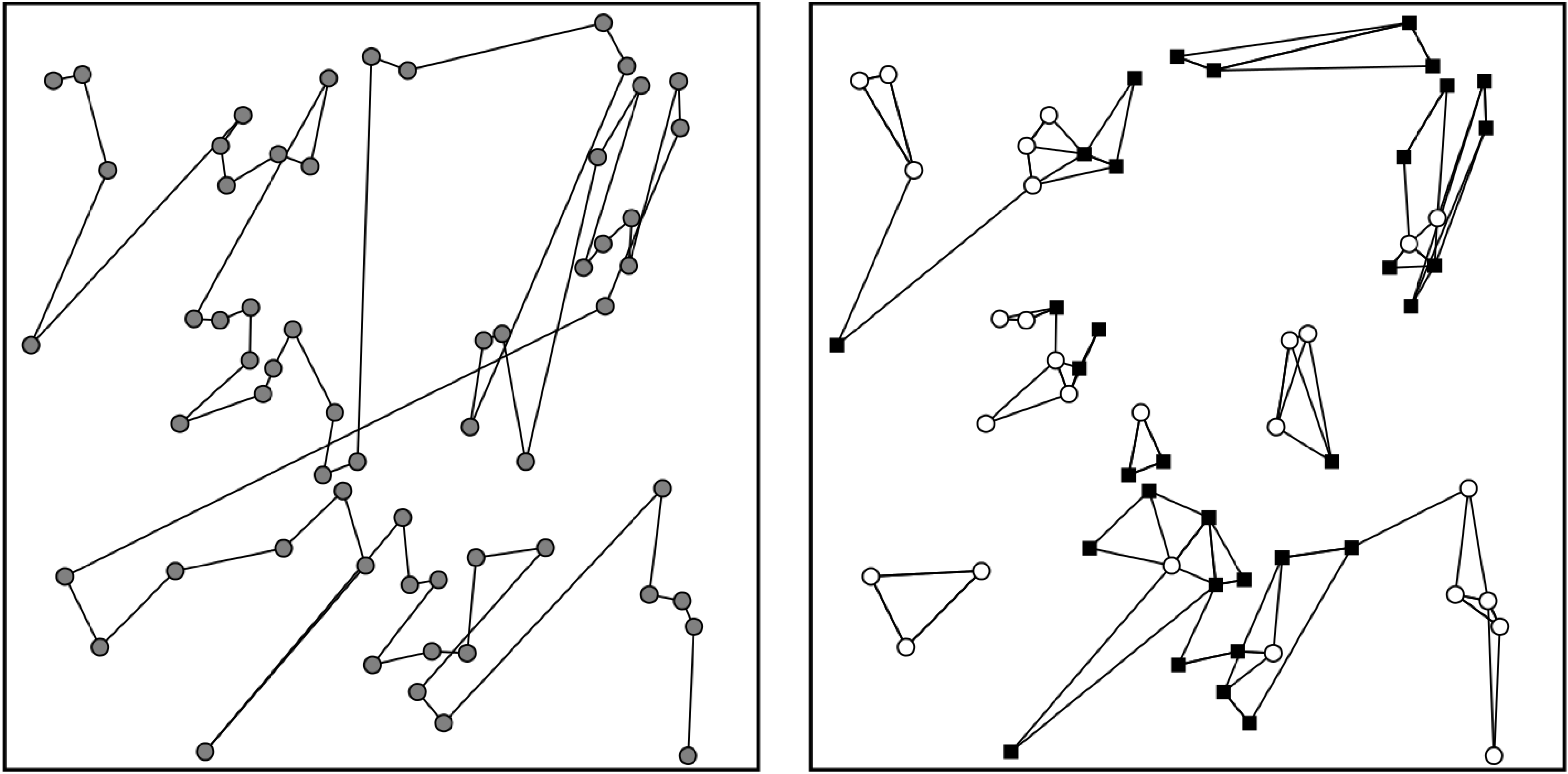


Quad tree

Points ordered by Z-values: *Z-order*



Sliding window search,
k=2-nn graph, window size W=3

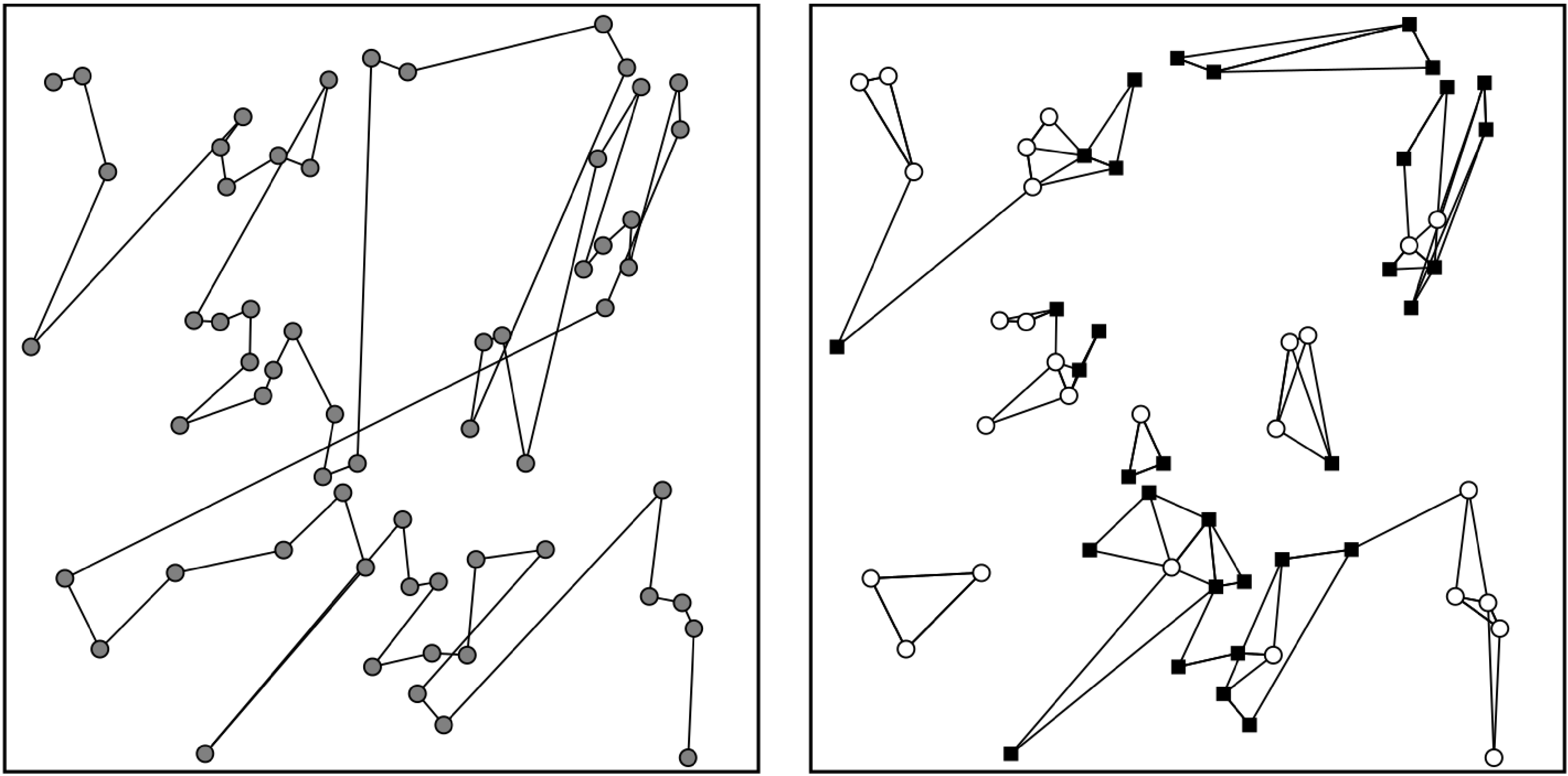


Constructing different Z-orders

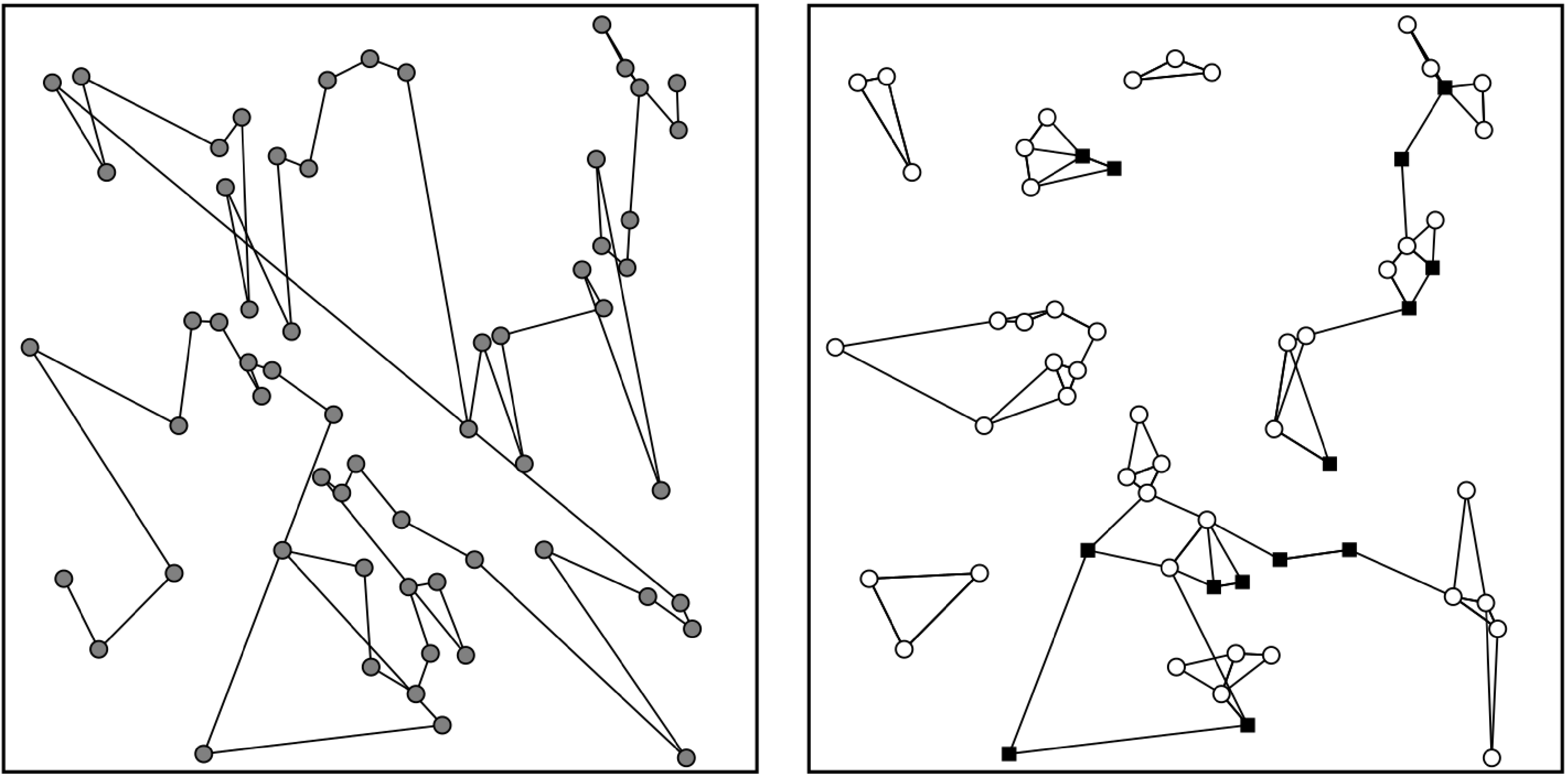
- Shift whole point set X by adding a random vector v to all points. $X' = X + v_{rand}$
- Rotate point set.
- 2D rotation: $v' = Rv$

$$R = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

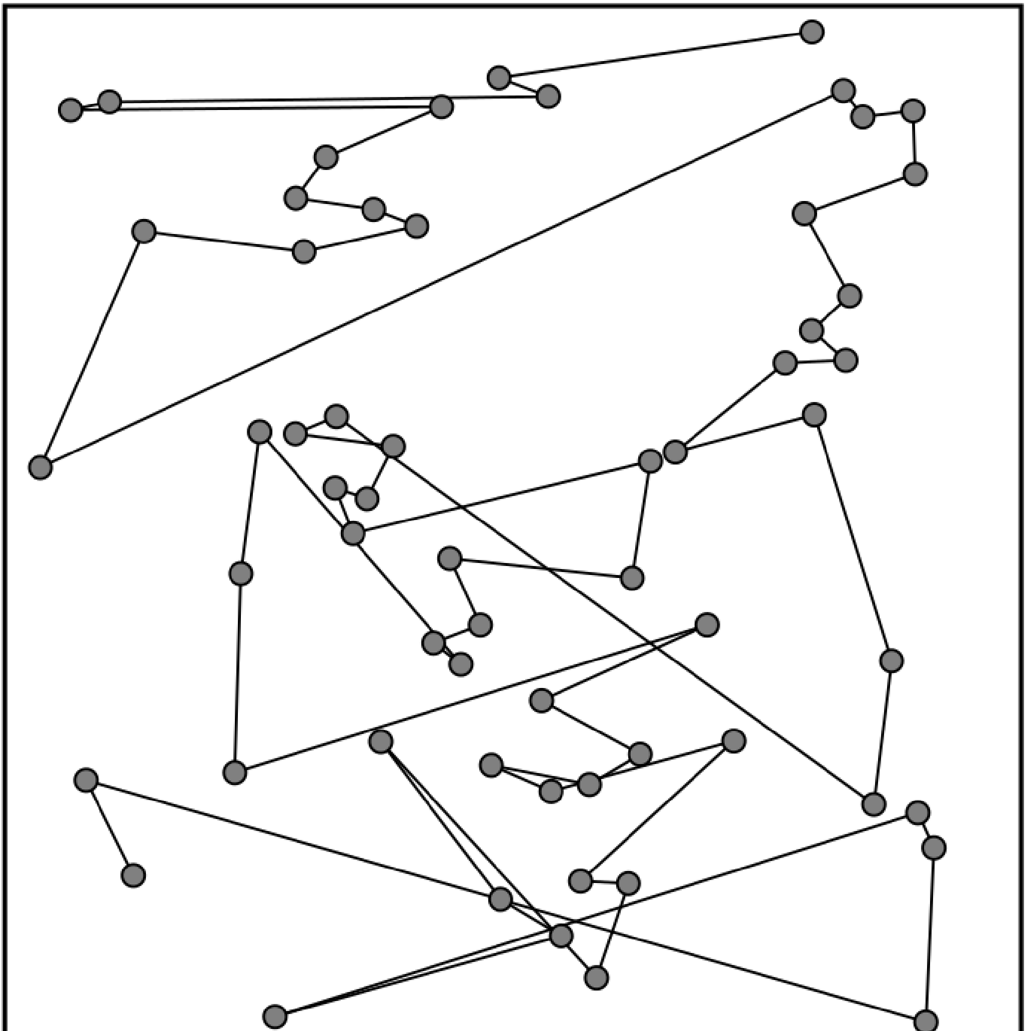
- D > 3: Random permutation of dimensions (Change the order of dimensions)

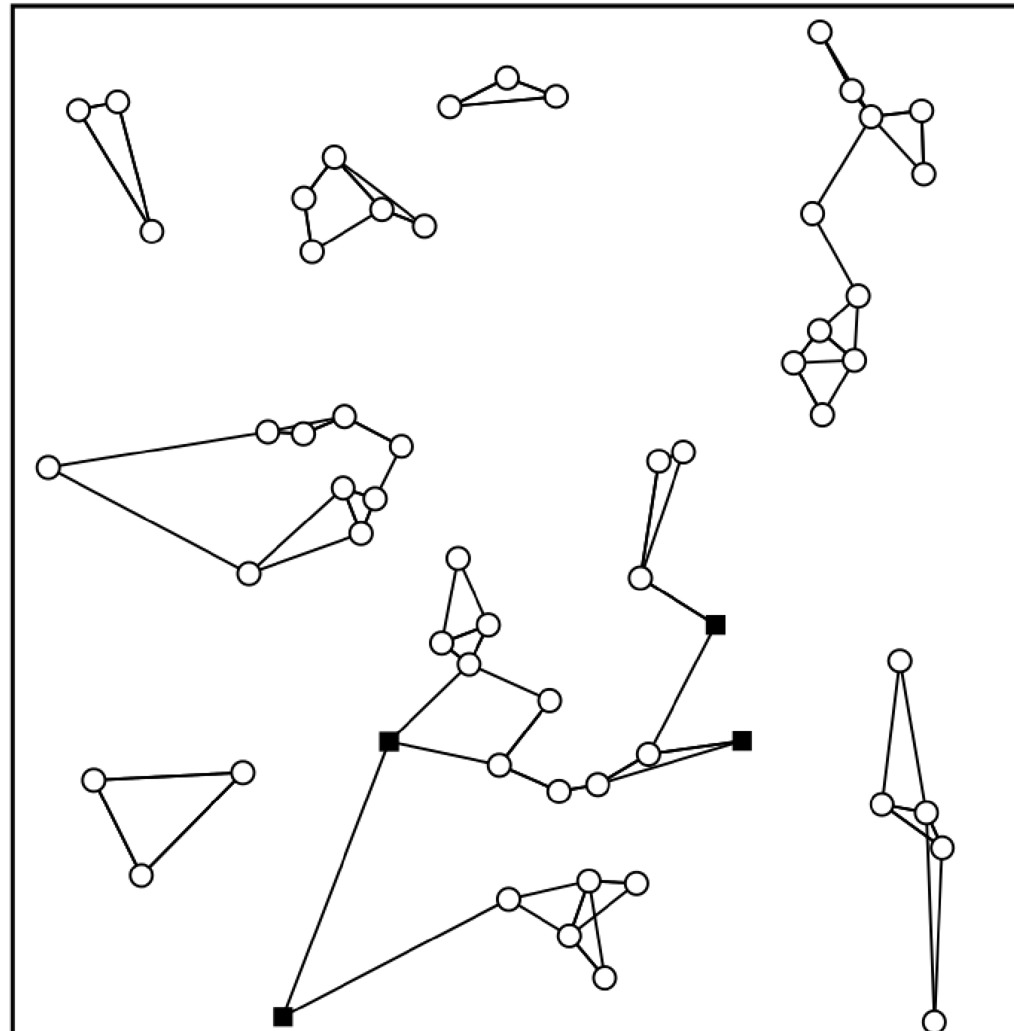


Different z-order by
(1) random shifting of point set
(2) rotation



Different z-order by
(1) random shifting of point set
(2) rotation





Reduce dimensionality, preserve neighbor connections

For high D, bit interleaving in results in very large integers. Therefore, if D > 32, reduce dimensionality to D_z=32 before z-value calculation.

- Divide each vector into subvectors with roughly equal sizes
- Map each subvector to one dimension by summing the elements
- Sums of subvectors form final vector

Example, from D=6 to D_z=3:

$$\boldsymbol{M} = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \quad \boldsymbol{M}' = shuffleColumns(\boldsymbol{M}) = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 \end{bmatrix} \quad \boldsymbol{v} = \begin{bmatrix} 5 \\ 4 \\ 7 \\ 0 \\ 3 \\ 2 \end{bmatrix}$$

$$\boldsymbol{M}' v = \begin{bmatrix} 3 \\ 7 \\ 11 \end{bmatrix}$$

Neighborhood propagation

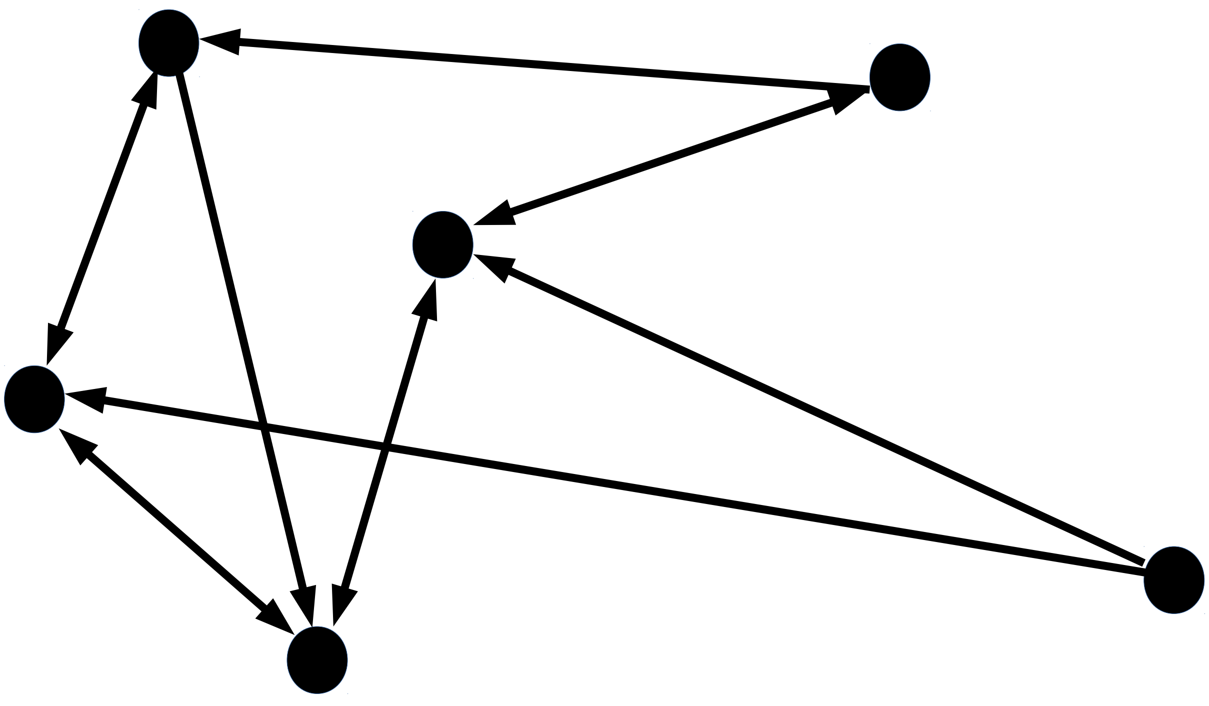
Used to improve graph. Different variants used in many methods[2-6]. Most extensively investigated in [3].

Pseudocode of algorithm:

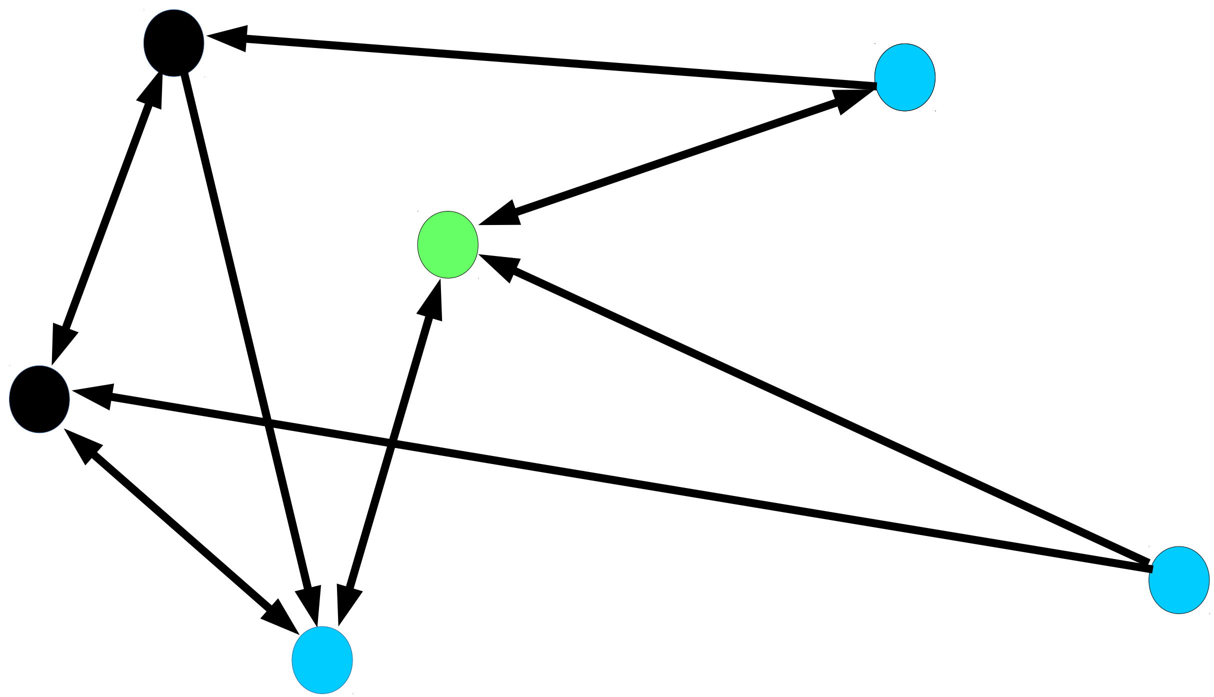
```
Do
    For each point x ∈ X:
        For each pair (y,z) in neighbors of x:
            // (Introduce neighbors:)
            Add edge (y,z) to G if it improves the graph
        end
    End
While G improved
```

[3] W. Dong, C. Moses, and K. Li, “Efficient k-nearest neighbor graph construction for generic similarity measures,” in Proceedings of the 20th international conference on World wide web, p. 577–586, ACM, 2011.

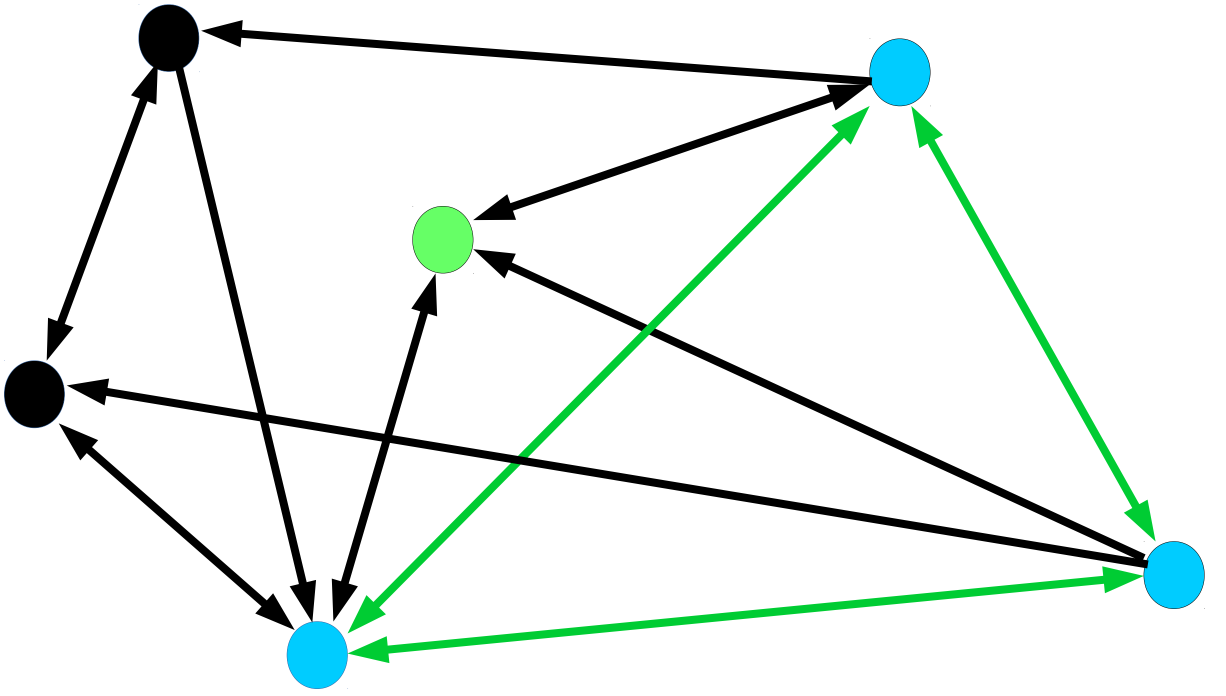
Neighborhood propagation (k=2)



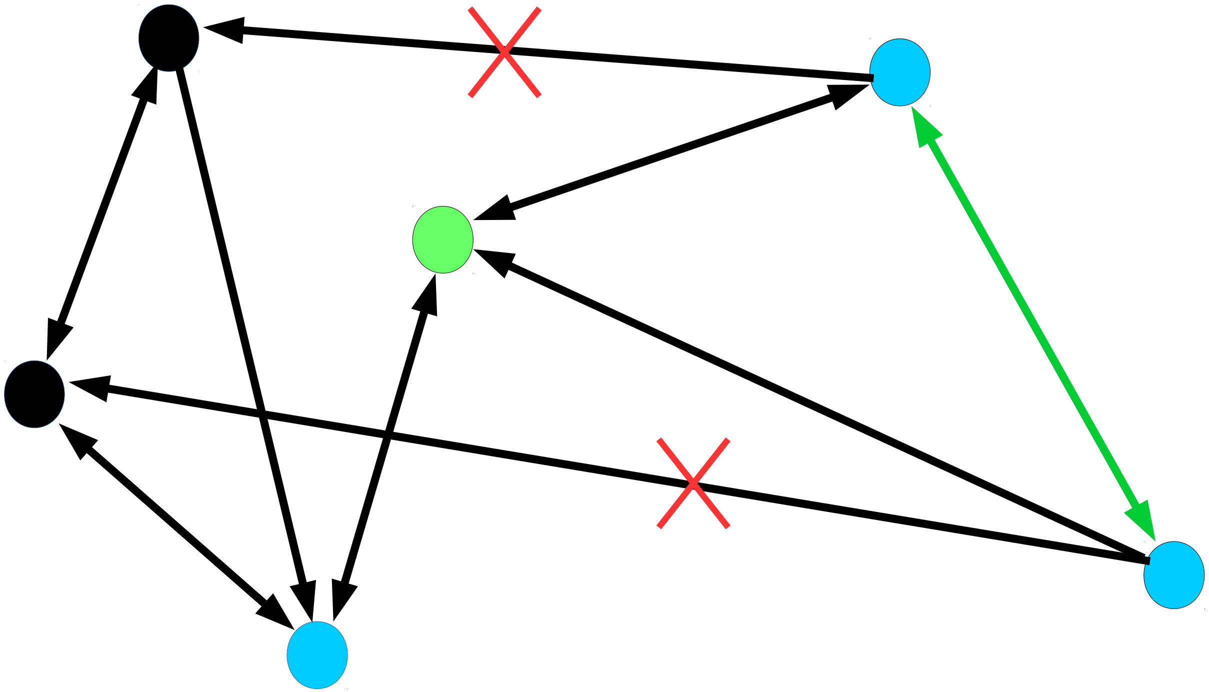
Select point's neighbors



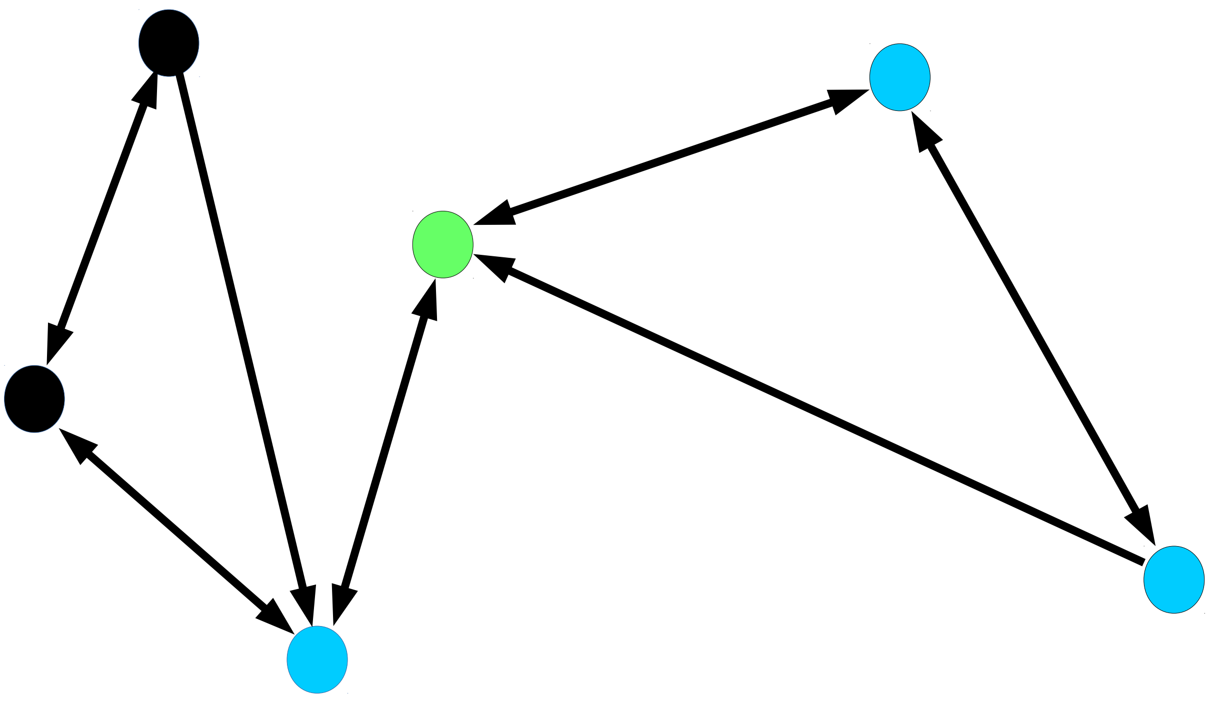
Introduce neighbors



Keep edges that improve graph



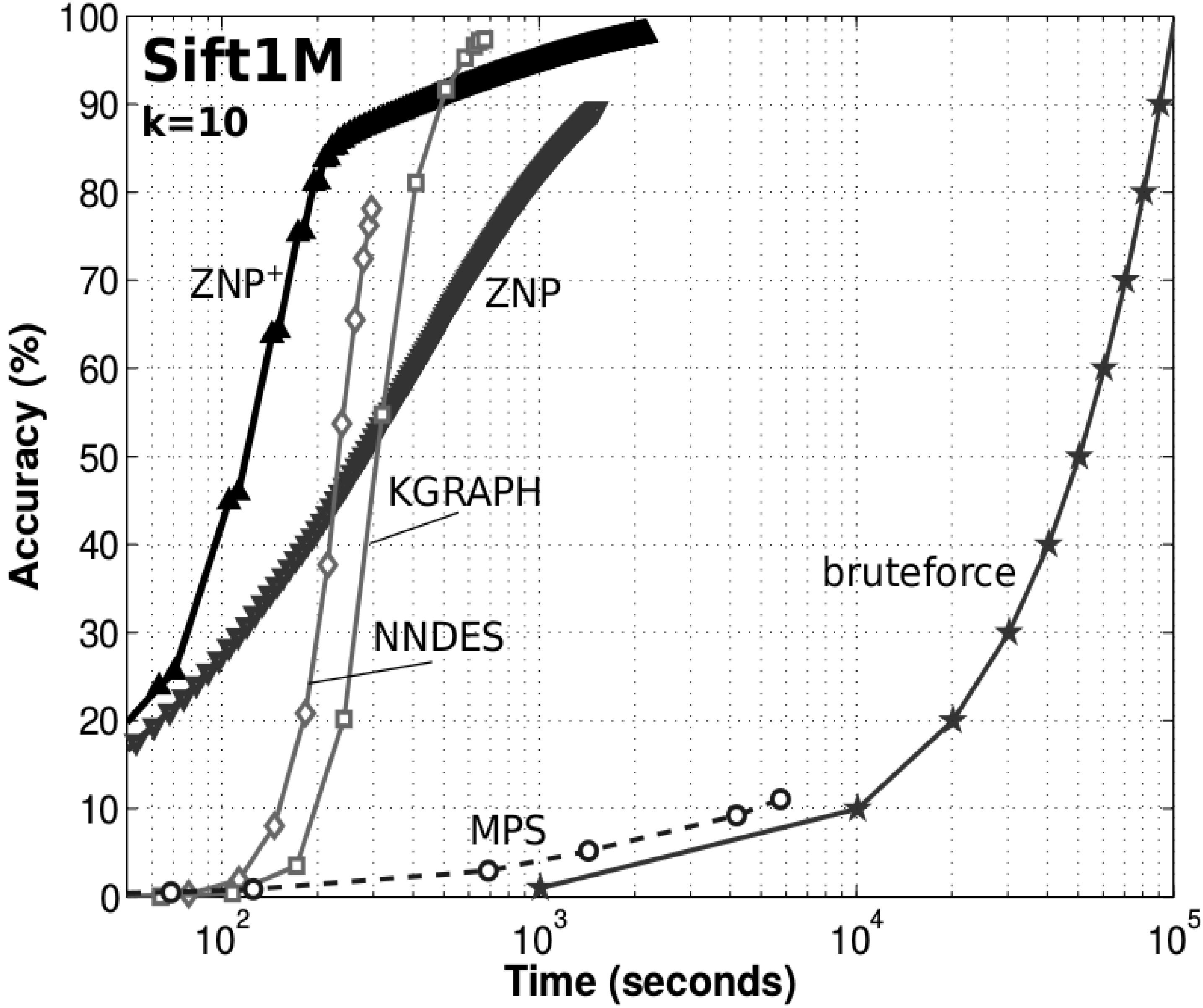
Result



Benchmarks: kNN graph construction (1/2)

Image features
D = 128
N = 1,000,000

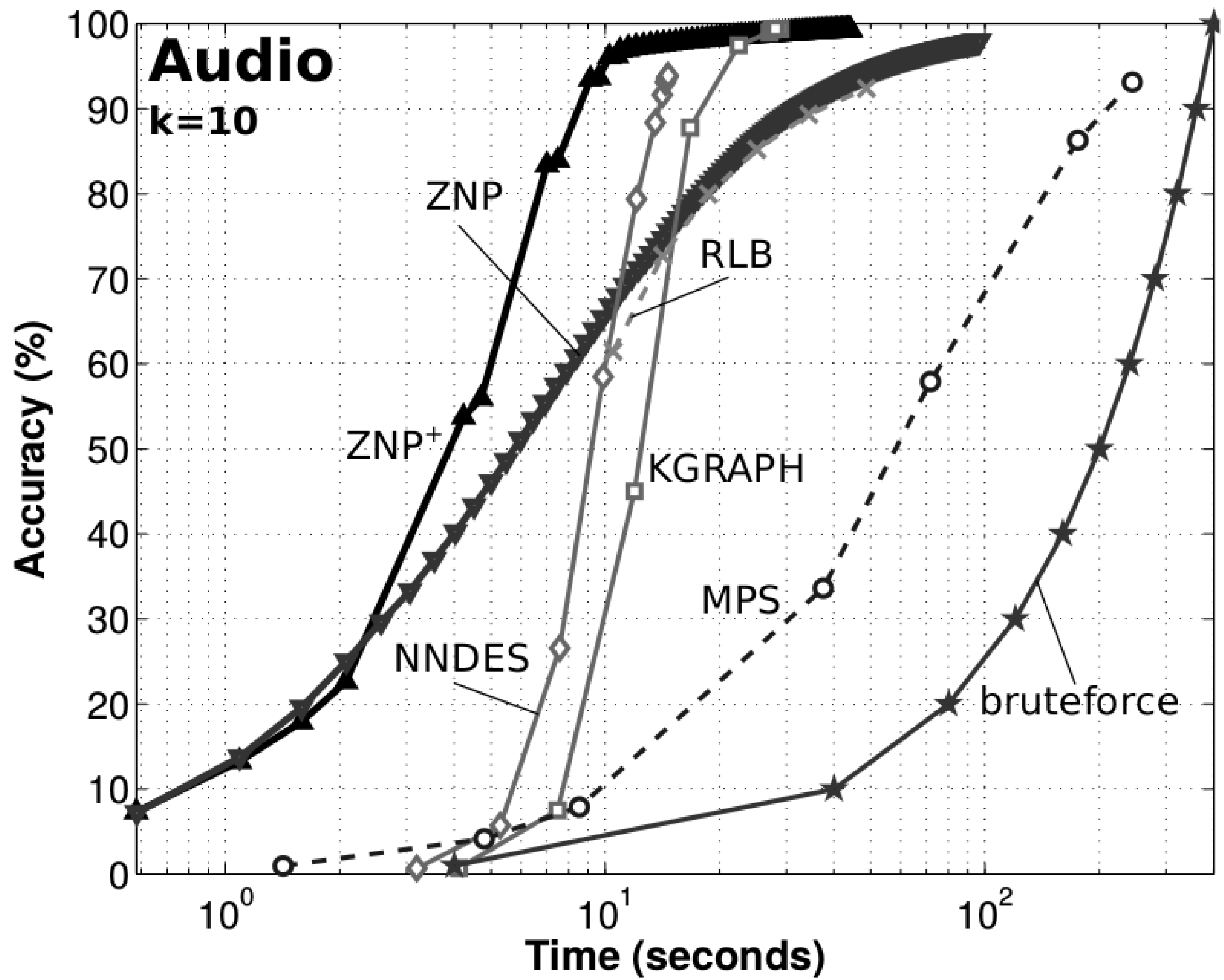
ZNP: Z-order search
ZNP+: Z-order search with neighborhood propagation



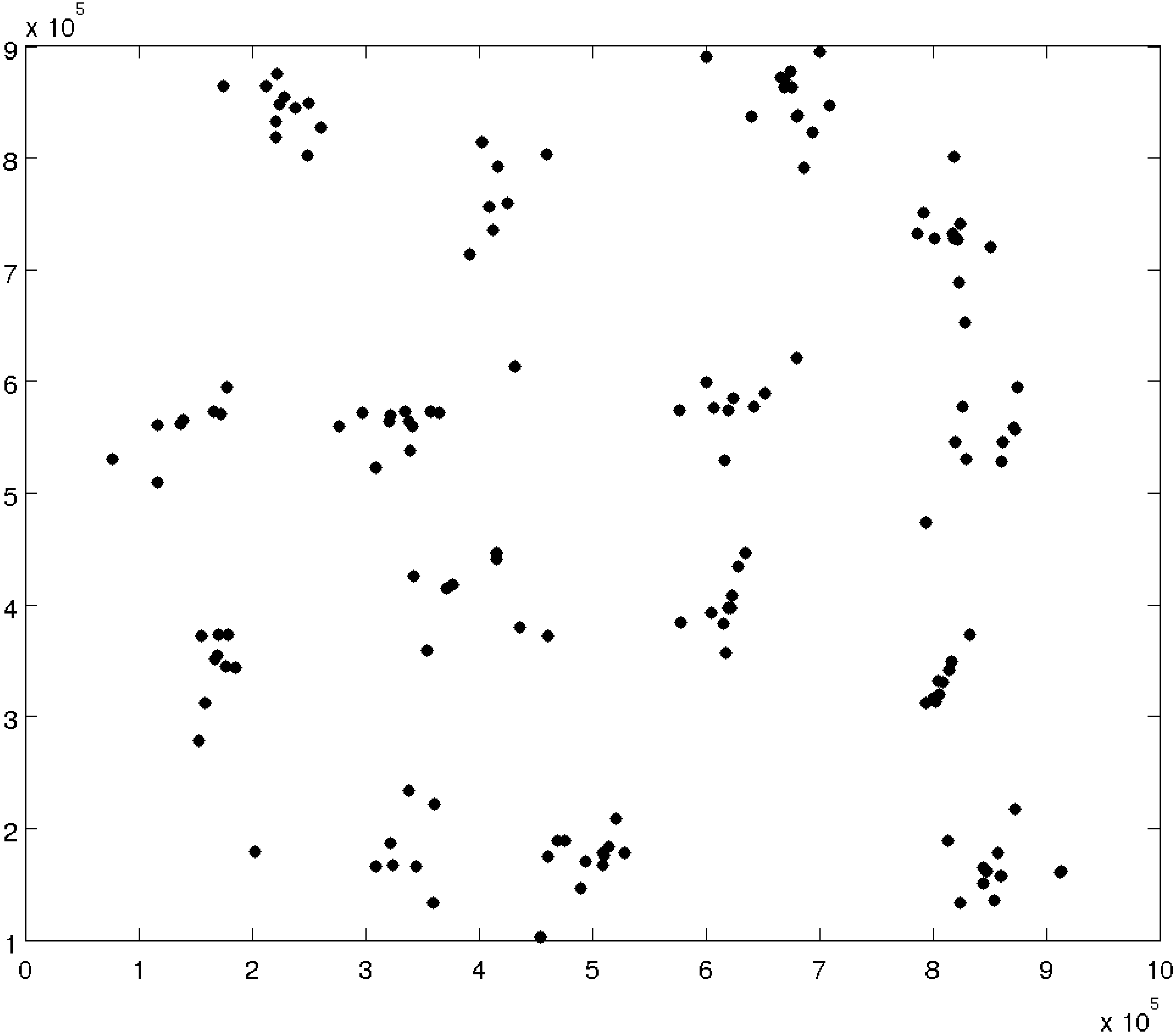
Benchmarks: kNN graph construction (2/2)

Audio features
D = 192
N = 54,387

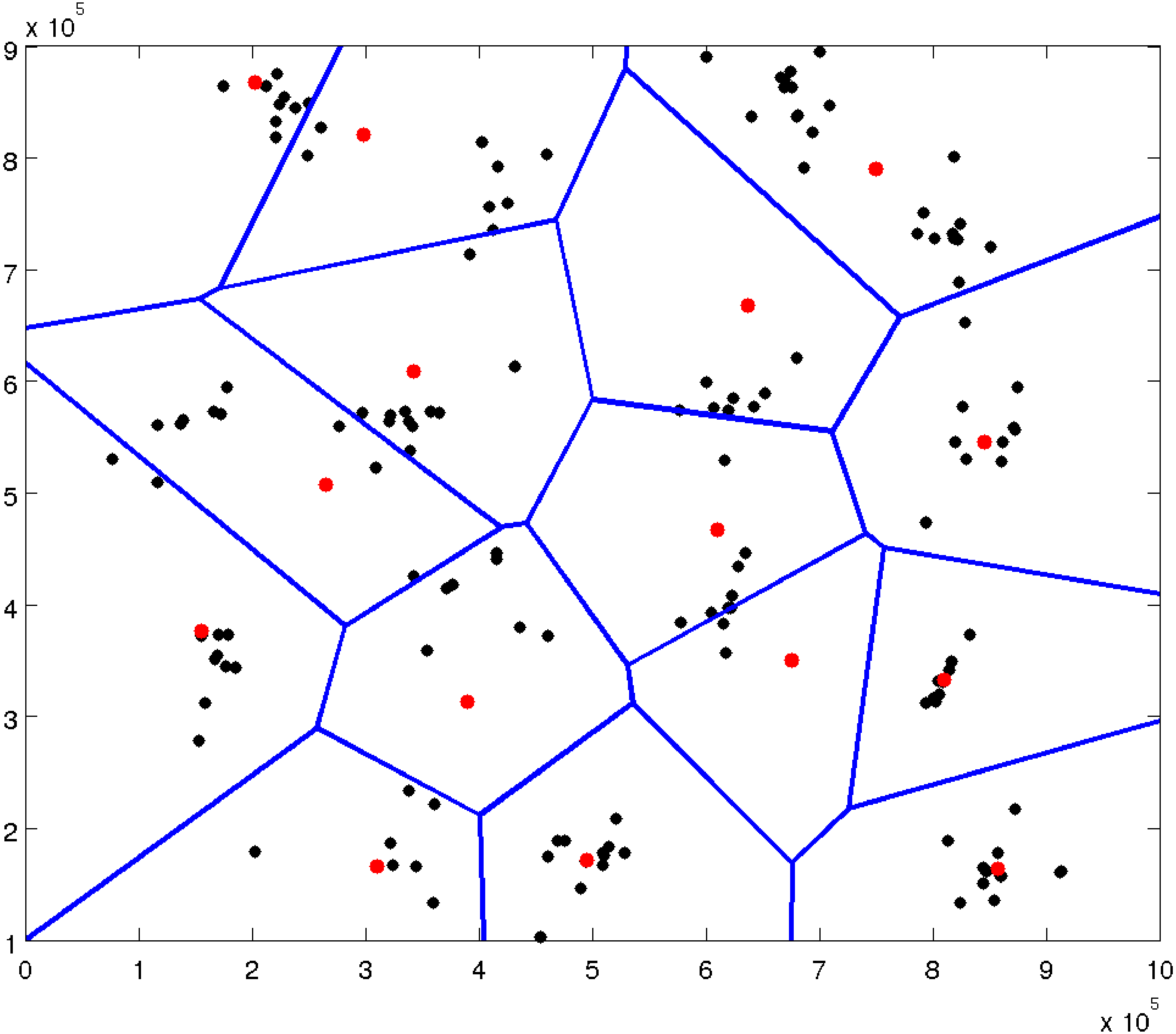
ZNP: Z-order search
ZNP+: Z-order search with neighborhood propagation



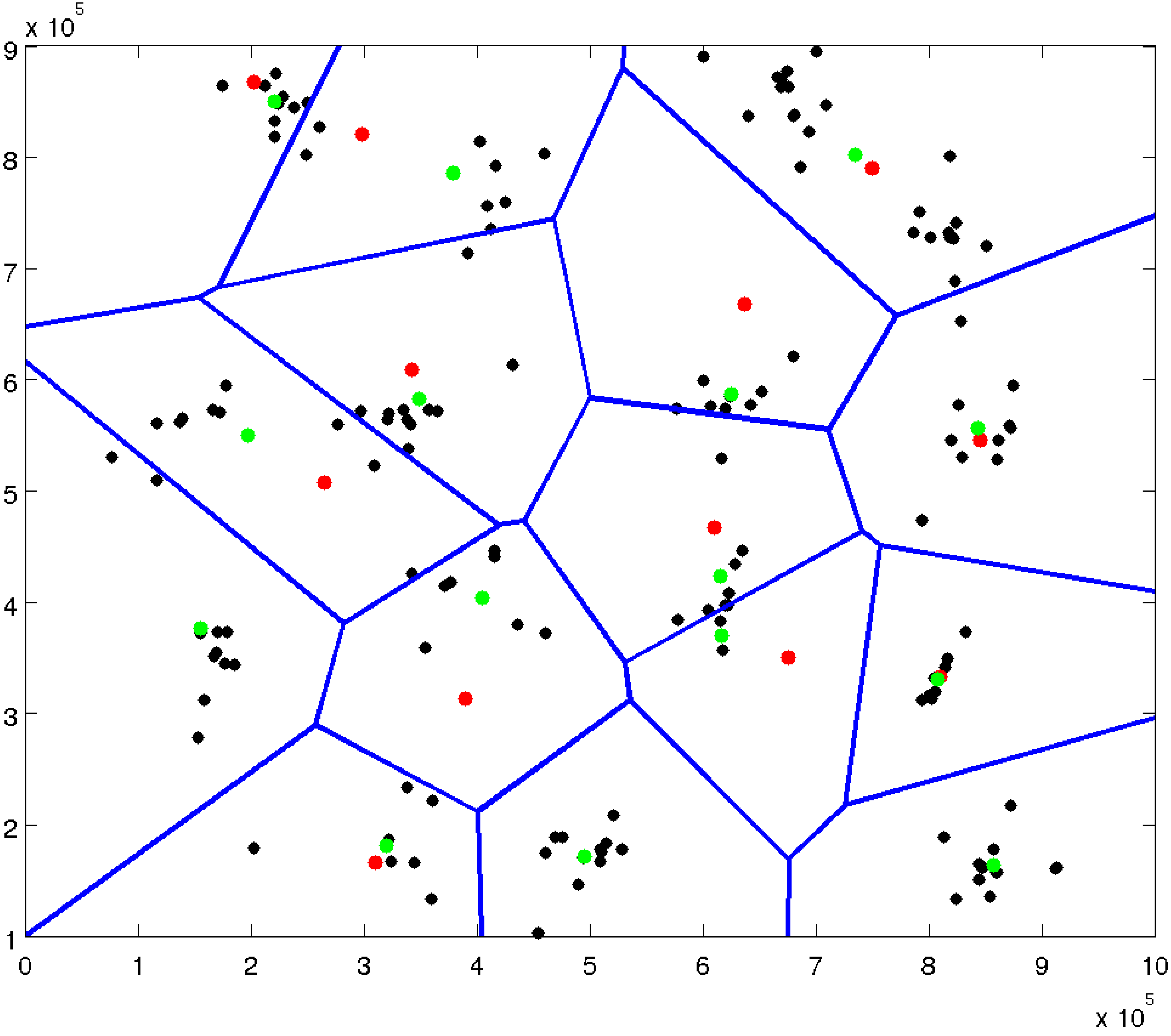
KNN graph to speed up k-means



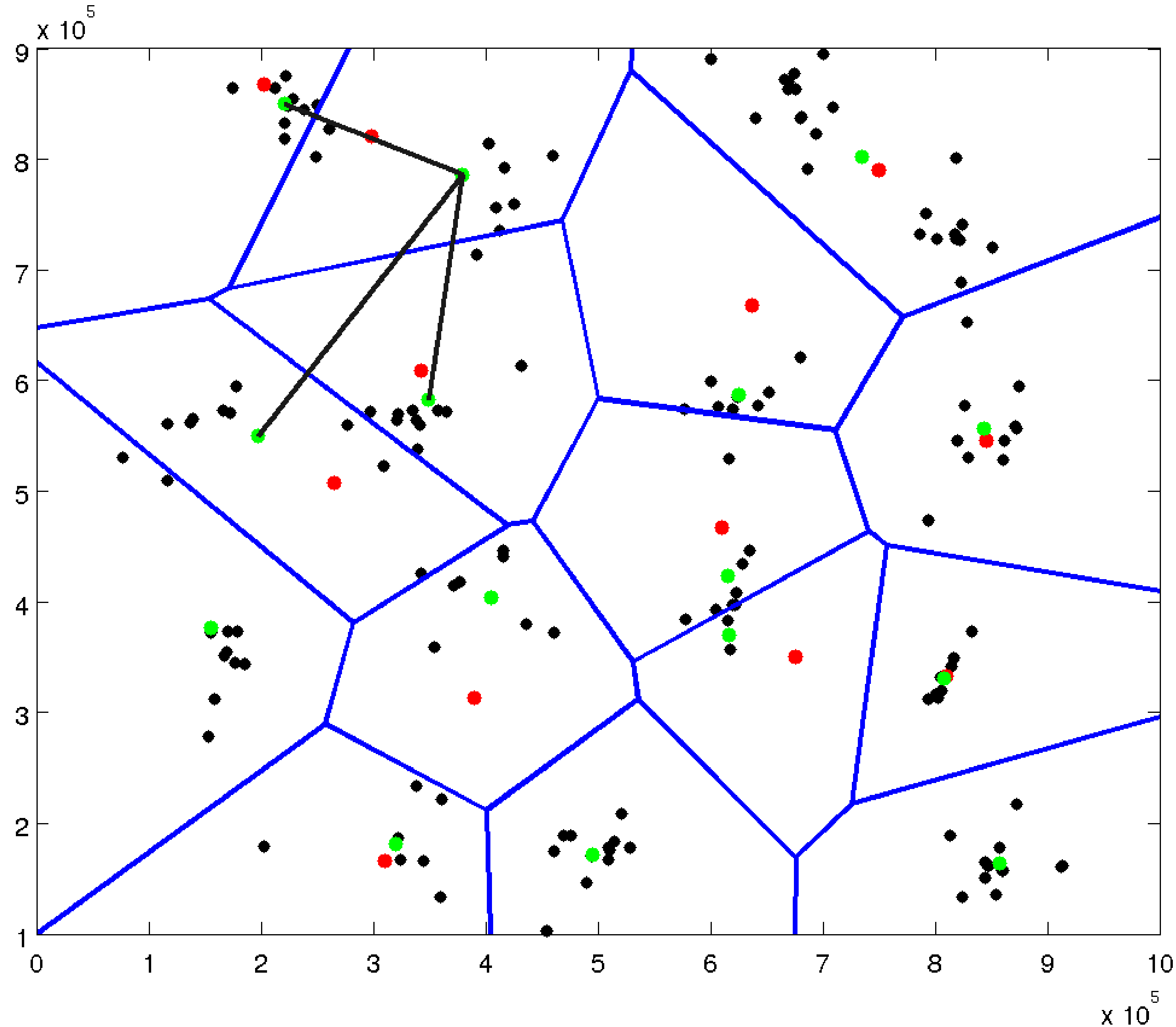
One iteration of k-means



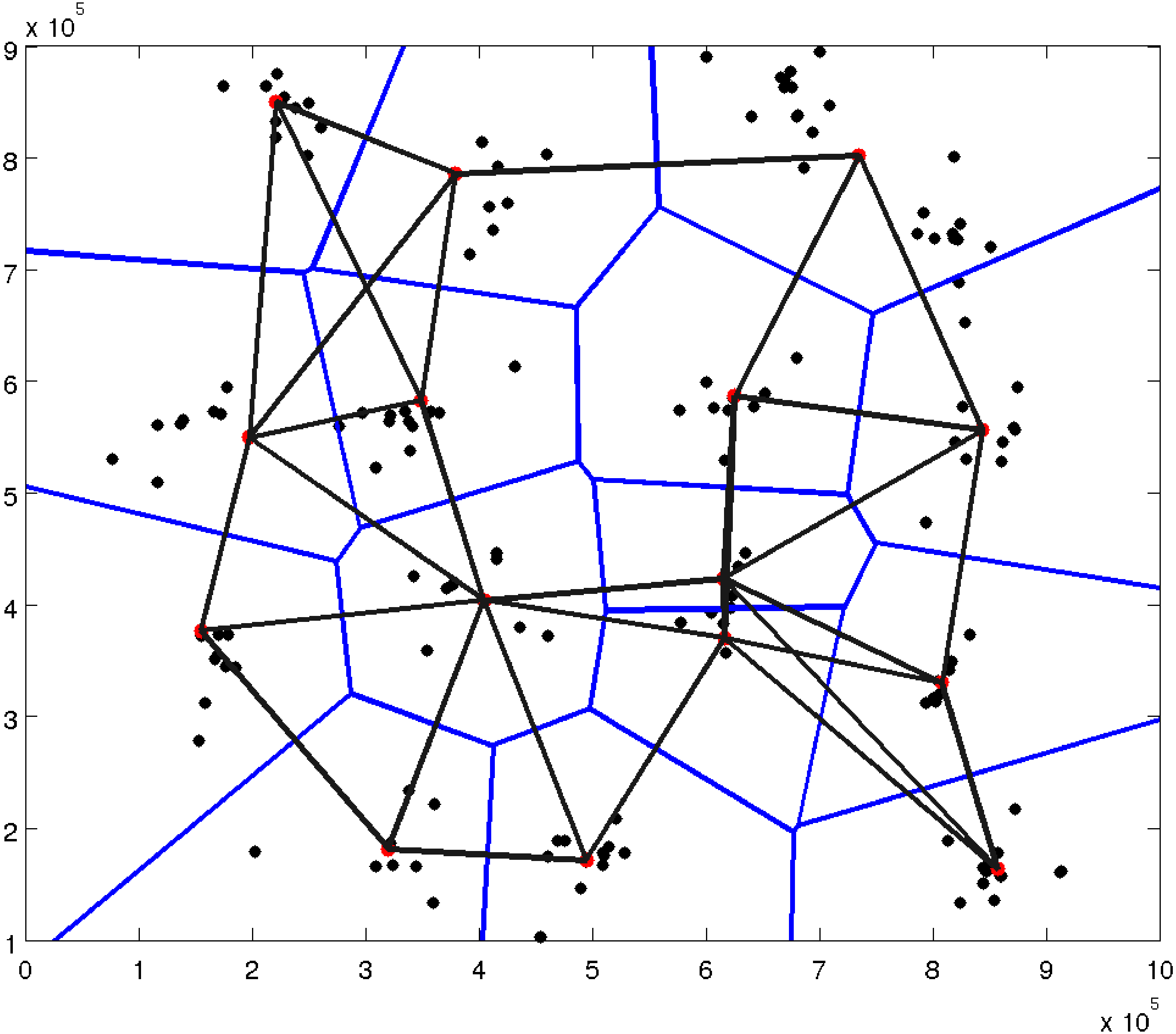
One iteration of k-means



One iteration of k-means



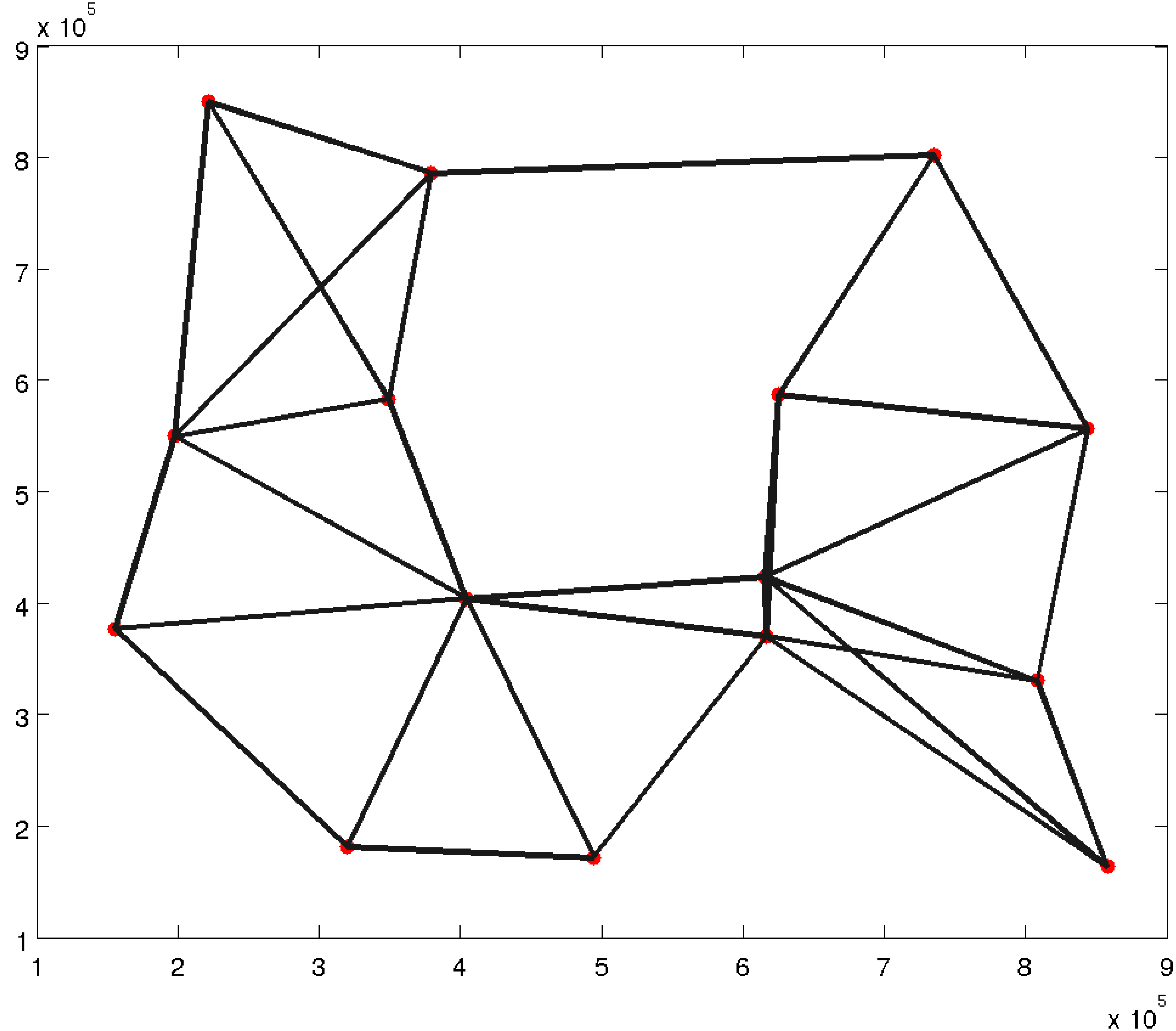
One iteration of k-means



KNN graph to speed up k-means

- K-means assignment step complexity: O(N*C)
- When using kNN graph, complexity of assignment is reduced to O(N*k)
- Graph construction with brute force: O(C^2)
- Total complexity with kNN graph: O(N*k +C^2)

Is O(N*k +C^2) faster than O(N*C)?


x 10^5
9
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9
x 10^5