Algorithms for neighborhood searches: The Voronoi diagram approach

Course in Computational Geometry

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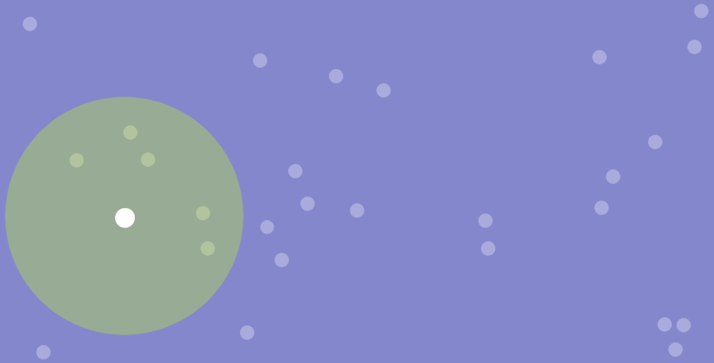
Abstract

In this presentetion I consider the neighborhood selection problem which I started to study in my bachelor's thesis and in a previous work[1]. I briefly recap the main results which I have already studied, namely, I define the problem in a precise way and I show a straightforward solution, then I review the common algorithmic approaches toghether with complexity analisies and I show the curse of dimensionality problem. Then I consider the Voronoi diagram approach to solve the neighborhood selection problem. First, I present the algorithm which shows how to properly use the data structure to implement an efficient solution, and second, I compare this method by the previous ones both with theoretical and experimental results.

[1] R. Borelli, A. Dovier, and F. Fogolari (2022). "Data Structures and Algorithms for k-th Nearest Neighbours Conformational Entropy Estimation". In: *Biophysica* 2.4, pp. 340–352. DOI: 10.3390/biophysica2040031.

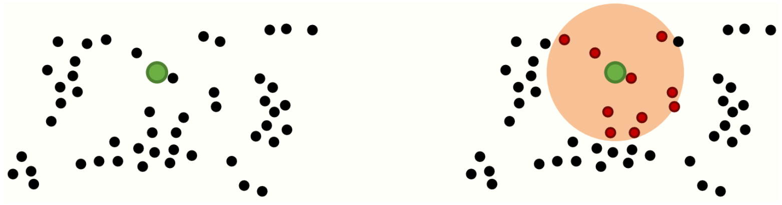
Contents



Problem overview

Problem formulation

- ALL-MNN: Given n point in a d dimensional space, find for each point p its m nearest neighbors



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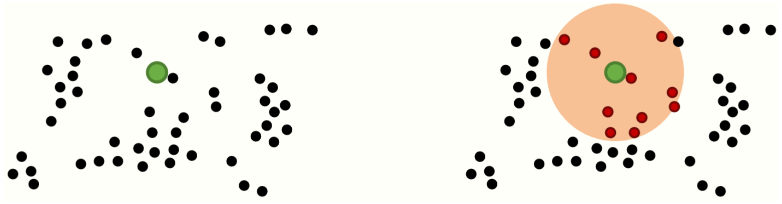

- The problem has a wide range of real applications
  - Conformational entropy estimation on biomolecular systems
  - Machine learning

Problem formulation

- I propose a very simple formulation (which I didn't found in the literature) based on integer linear programming
- It evidences the *optimization* nature of the problem
- It's usefull to define precisely the broblem
- It doesn't touch the geometry of the problem and it's very inefficient

Problem formulation

Le S the be the inpunt set $S = \vec{p_1}, \ldots, \vec{p_n}$ and let m be the number of neighbors $0 < m < n$

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$$x_{ij} = \begin{cases} 1 & \text{if } \vec{p_j} \in N_i \\ 0 & \text{otherwise} \end{cases} \qquad \forall i, j \in [n], i \neq j \tag{1}$$

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The integer programming model is now the following

$$\min \sum_{i \in [n]} \sum_{j \in [n] \setminus \{i\}} (x_{ij} dist(\vec{p_i}, \vec{p_j})) \tag{2}$$

subject to:

$$\sum_{j \in [n] \setminus \{i\}} x_{ij} = m \qquad \forall i \in [n] \tag{3}$$

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$$\Omega(nd) + \Omega(nmd) \tag{4}$$

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- I can improve the lower bound by a reduction through ELEMENT-UNIQUENESS:

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- Steps 3 and 4 take linear time
- Solving the ELEMENT-UNIQUENESS takes $\Omega(n \log n)$ time
- Solving the ALL-1NN problem in $o(n \log n)$ implies a contraddiction

Lower bound

Some details on the reduction:

- Note that Element-Uniqueness is a decision problem while the other 2 are functional problems. So we are referring to the more general definition of reduction between functional problems
- One (implicit) key assumption: the ALL-1NN takes as input a list (and not a set) of points. Otherwise the reduction doesn't make sense: a set always satisfies the uniqueness property
- In real world situations S is always a set
- By implementing the classical algorithms I observed that the code doesn't change much if we allow or not S to be a list
- To be precise I should also prove that $\text{ALL-1NN}_{\text{lists}} \preceq \text{ALL-1NN}_{\text{sets}}$

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    1. For each point $p$ in $S$, compute the vector $\vec{d_p}$ which contains the distances between $p$ and all the other points
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- Ordering (which takes $\Theta(n \log n)$) is not really necessary. After computing $\vec{d_p}$ we could just select (in linerar time) the m-th smallest distance
- So in the general case we have an algorithm which always takes linear space and $O(dn^2)$ time
- ... which of course is unaceptable

Classical approaches and results

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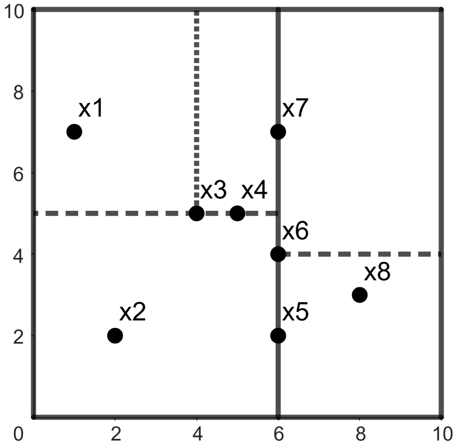
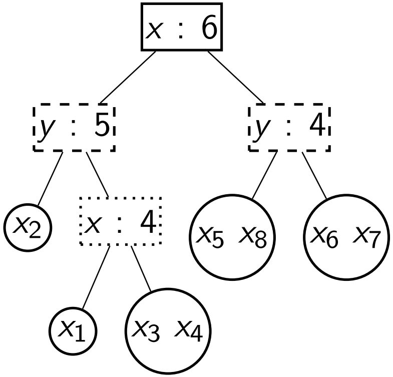
- **Querying:** Given a point $p \in S$ we visit the data structure (possibly a small part of it) in order to find the m nearest neighbors of p.

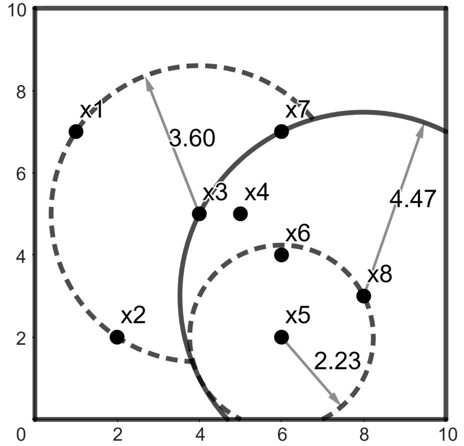
Classical approaches and results: The K-D Tree

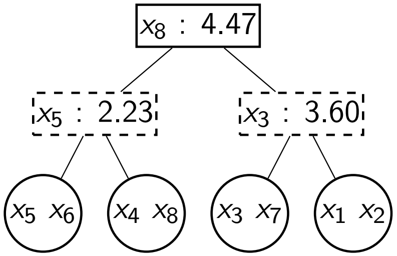




- Each internal node corresponds to a binary test which involves the projection operation
- At each node the set of points is split into two almost-balanced sets

Classical approaches and results: The VP Tree



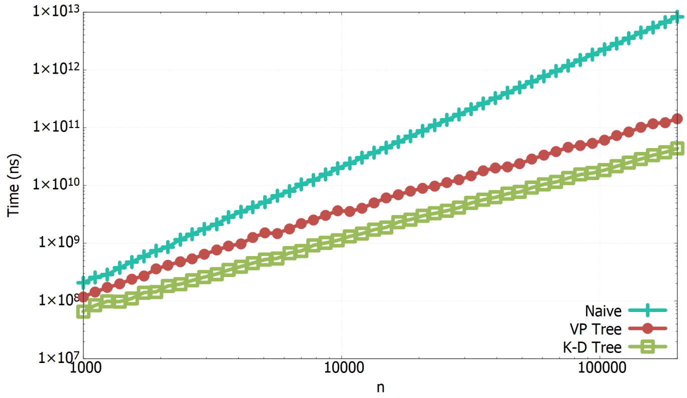


- Similar idea to K-D Trees but more general
- Each internal node is no more associated with a projection but only involves the dicotomy far/near with respect to the vantage point

Classical approaches and results: Costs

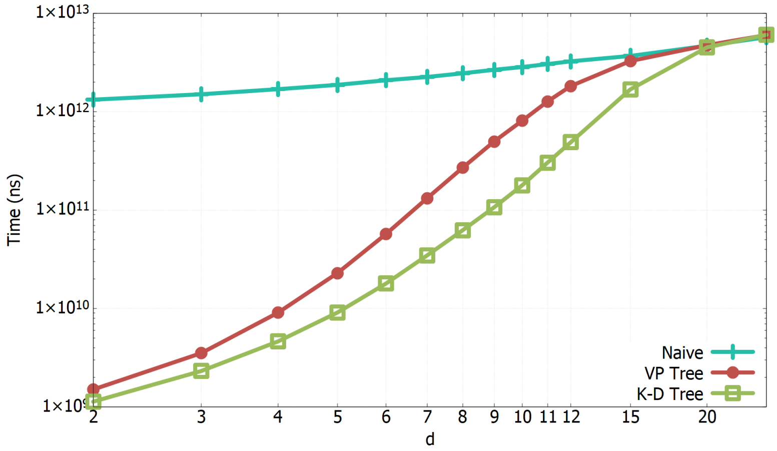
- The preprocessing steps is in some sense *easy* and takes $\Theta(n \log n)$ time
- The query should take $\Theta(\log n)$ time, but with currently-avalaible methods this happens only in the avarage case
- We get the worst case when d is sufficiently large. In such case the query algorithm takes linear time (we essentialy visit the entire tree structure) and the entire ALL-MNN algorithm degenretes to an exhaustive search which takes quadratic time
- This problem is known in the literature as **curse of dimensionality** and we currently don't know if the problem admits an optimal solution when the number of dimension increases

Classical approaches and results: Comparison



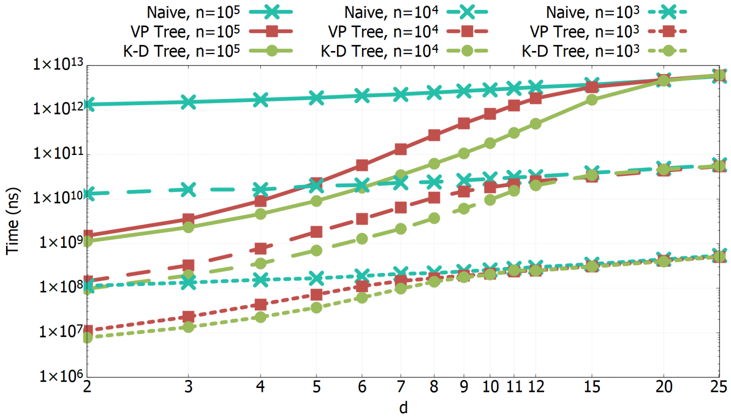
- Whith $d = 6$ dimensions and $m = 20$ VP Tree and the K-D tree performances are the same expect for a multiplicative constant
- Recall: In double logarithmic scale different lines inclinations means different polinomials

Classical approaches and results: Curse of dimensionality



- While working with $n = 100000$ points and $m = 20$ neighbors per point, advantages of tree-based methods are completely lost at $d = 20$

Classical approaches and results: Curse of dimensionality



- We observed that *curse of dimensionality* tends to attenuate when we increase n
- We also observed that the tree-based approaches degenerate in an exhaustive search when $d \in \Omega(\log n)$

The Voronoi diagram approach

The Voronoi diagram

Optimal solution to ALL-1NN in 2d

The *k*-th order Voronoi diagram

Optimal solution to ALL-MNN in 2d

Comparison

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Conclusion

Concluding remarks

Bibliography I

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