Fast K-Means with Accurate Bounds

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Given data $(x_i)_{i=1}^N \in (\mathcal{R}^d)^N$, find centers $(c_k)_{k=1}^K \in (\mathcal{R}^d)^K$ minimising

$$\sum_{i=1}^{N} \min_{k=1:K} \|x_i - c_k\|^2.$$

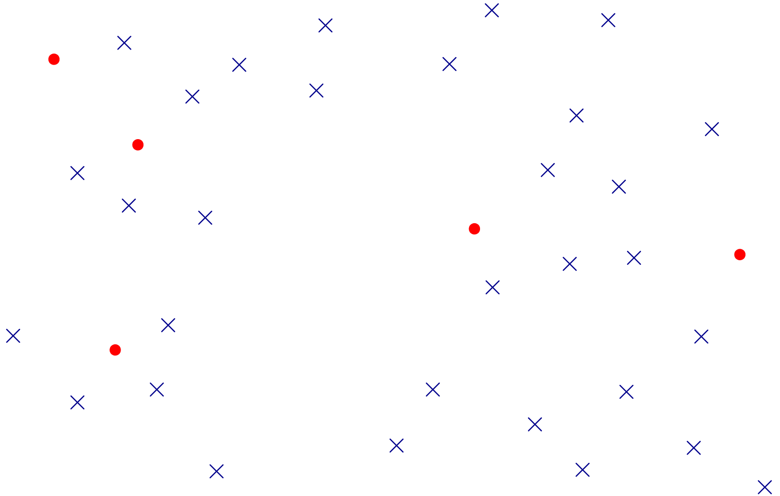
NP-hard, so heuristic algorithms such as Lloyd's are used

Lloyd's algorithm run for T iterations requires $dKNT$ FLOPs

We are interested in making it faster

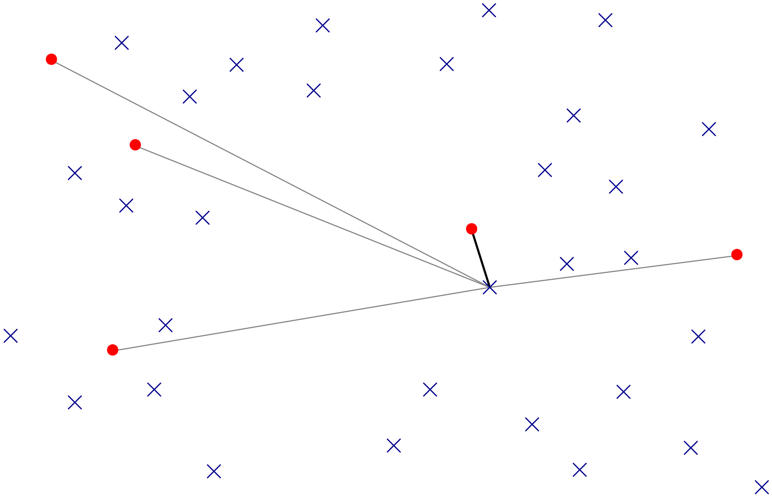
Lloyd's Algorithm

× : data ● : centers

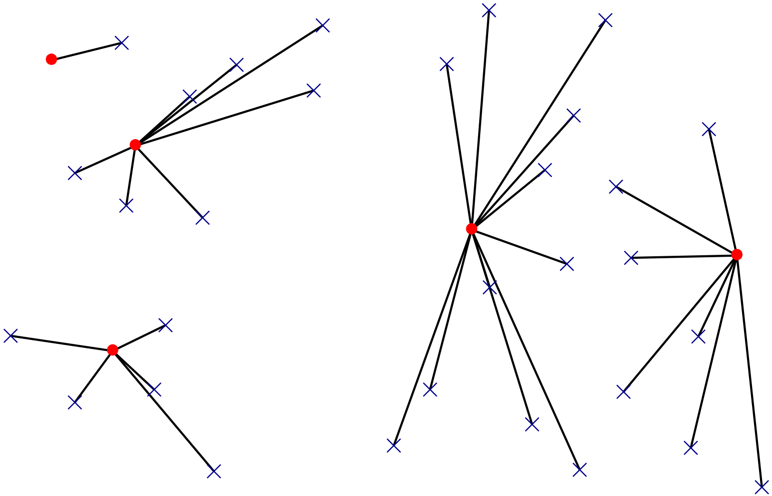


Lloyd's Algorithm

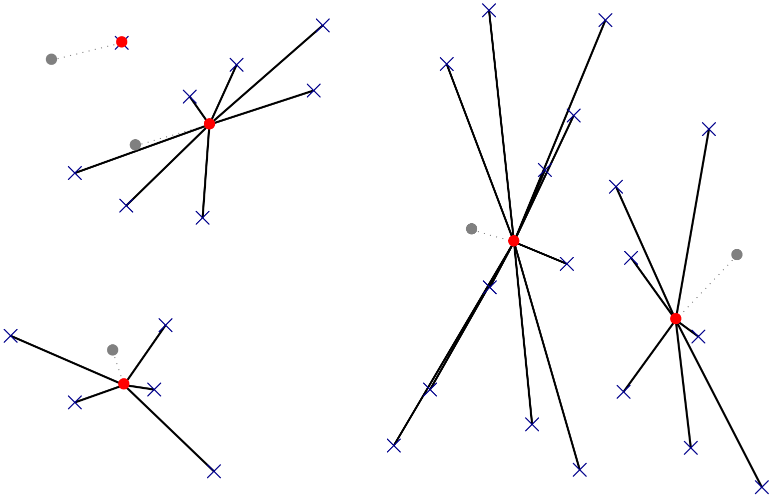
Assignment of datapoint at iteration 1



Lloyd's Algorithm
All assignments at iteration 1

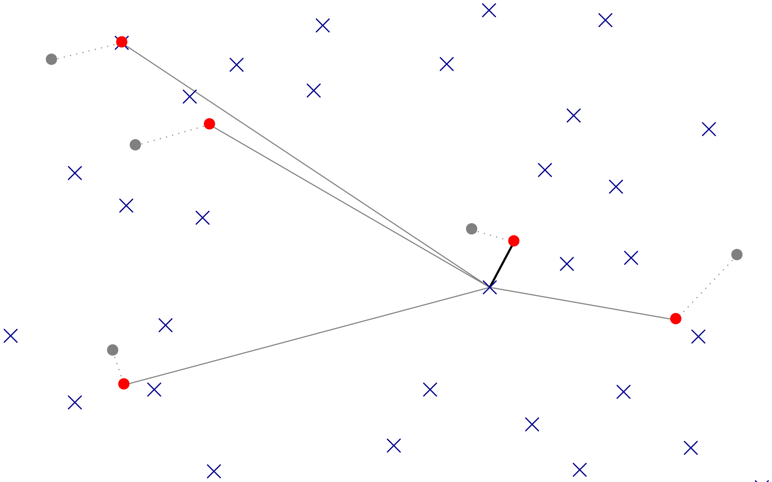


Lloyd's Algorithm
Updates at iteration 1



Lloyd’s Algorithm

Assignment of datapoint at iteration 2



Lloyd's Algorithm
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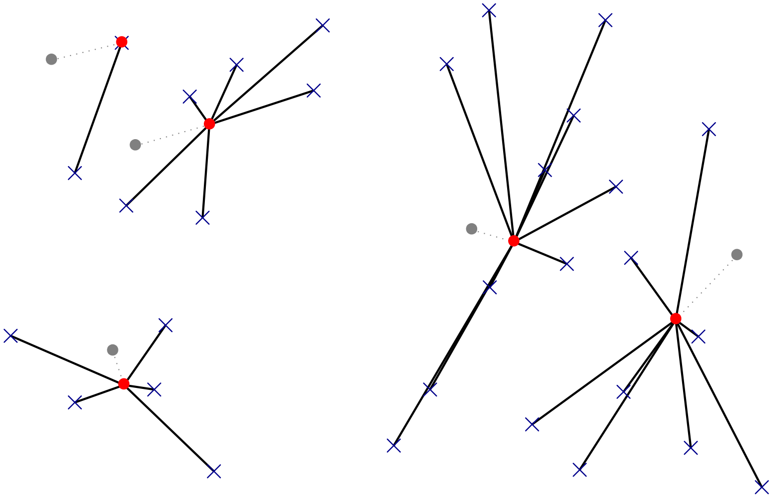

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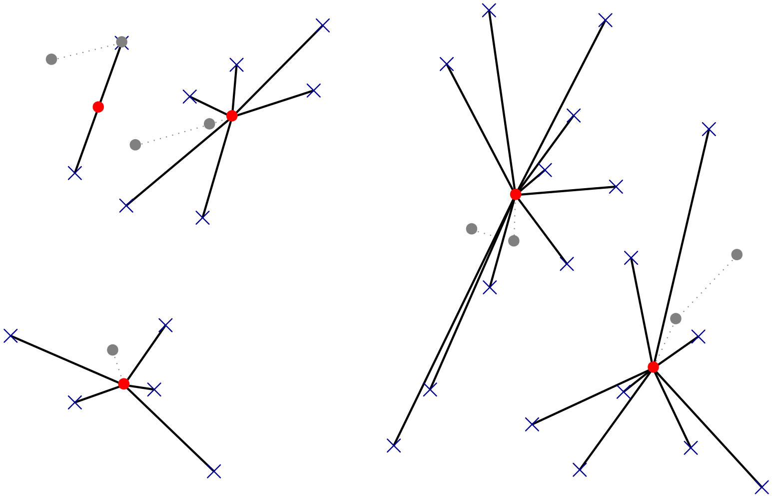
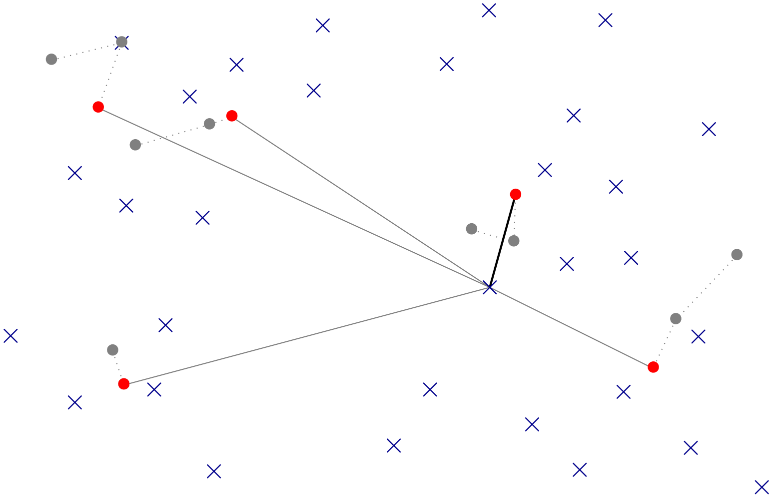
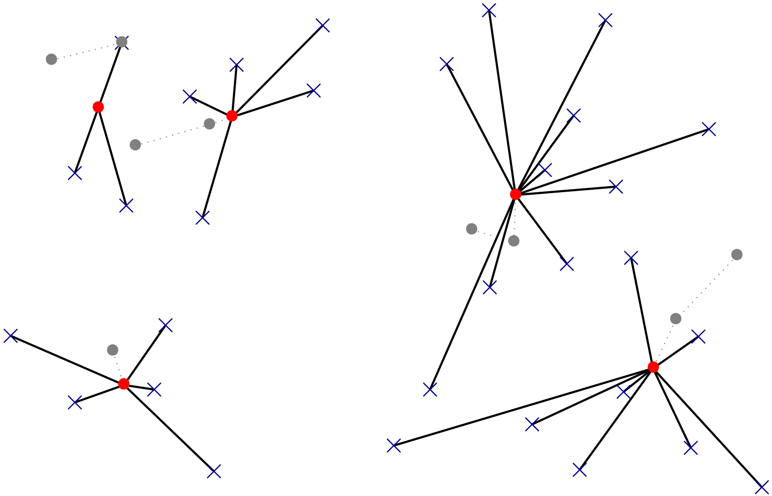


Lloyd's Algorithm
Assignment of datapoint at iteration 3



Lloyd's Algorithm

All assignments at iteration 3



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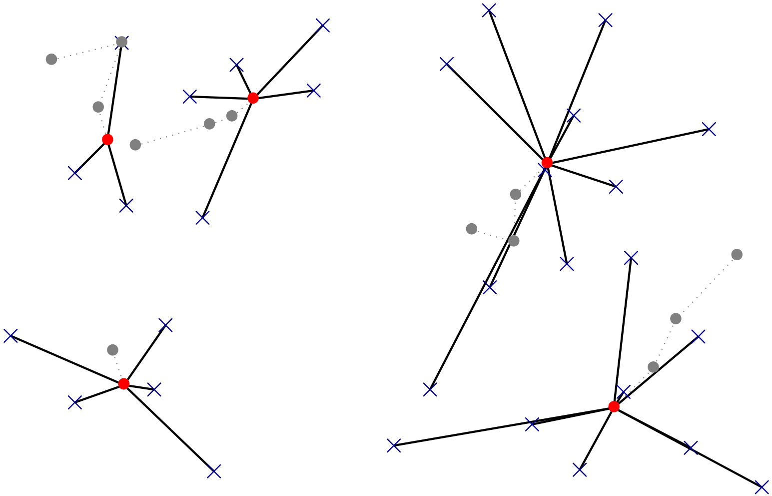
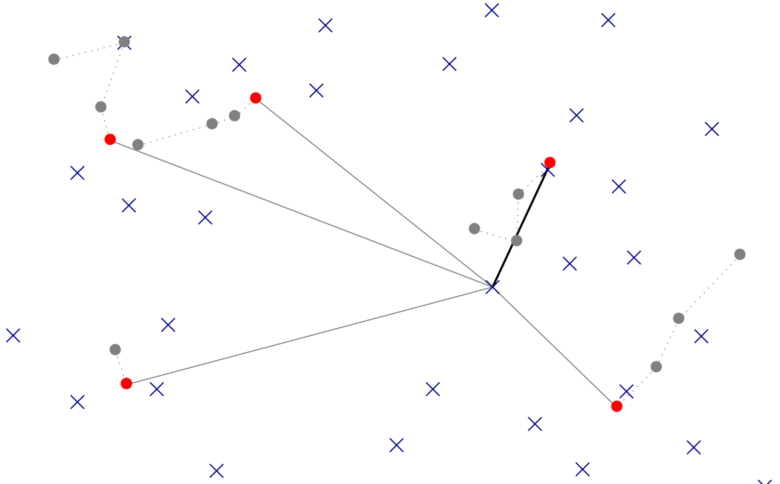


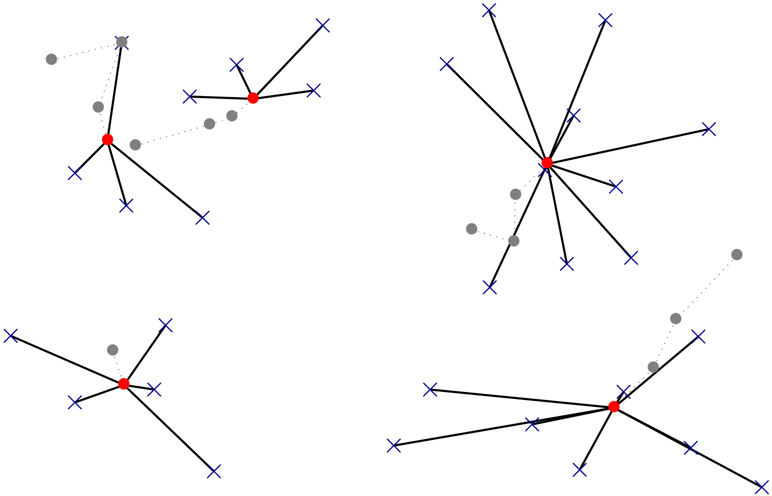
Lloyd's Algorithm

Assignment of datapoint at iteration 4



Lloyd’s Algorithm

All assignments at iteration 4



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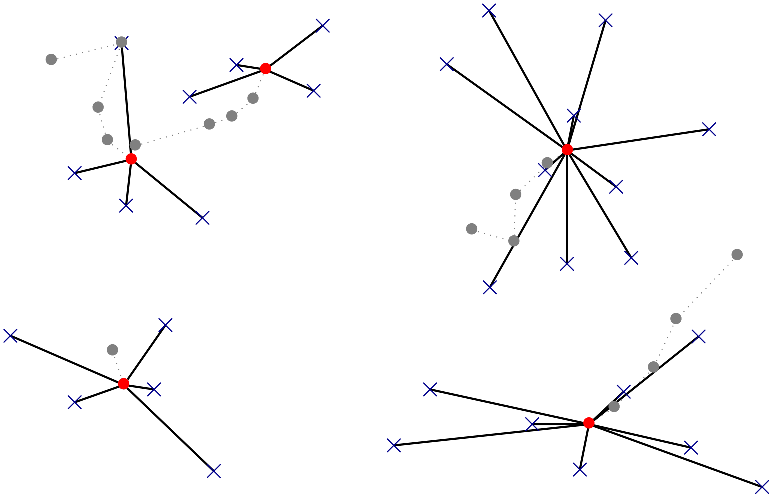

Two approaches :

(1) approximate it

(2) be more efficient – get exactly the same output as Lloyd's algorithm without all data-center distances

- Pelleg et al. (1999)
- Kanungo et al. (2002)
- Δ Hamerly (2010)
- Δ Elkan (2003) best high-*d*
- Δ Yinyang (2015) best mid-*d*
- Δ Annular (2013) best low-*d*

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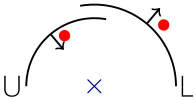
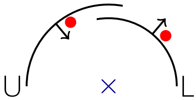
Elkan uses the triangle inequality in two distinct ways

(1) center-center distances to bound data-center distances

(2) directly maintain bounds on data-center distances





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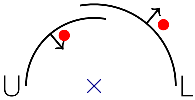
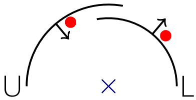
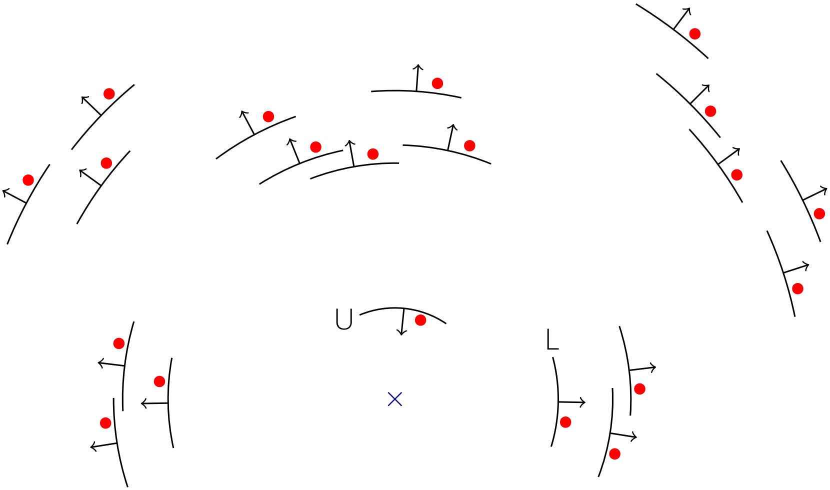




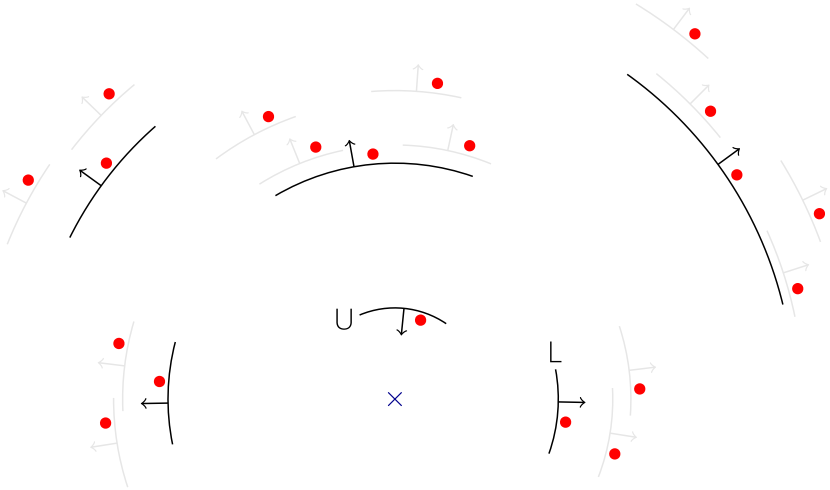
(A) *We show that (1) + (2) is slower than just (2). Simplifying helps!*

Using The Triangle Inequality

Elkan $K - 1$ lower bounds

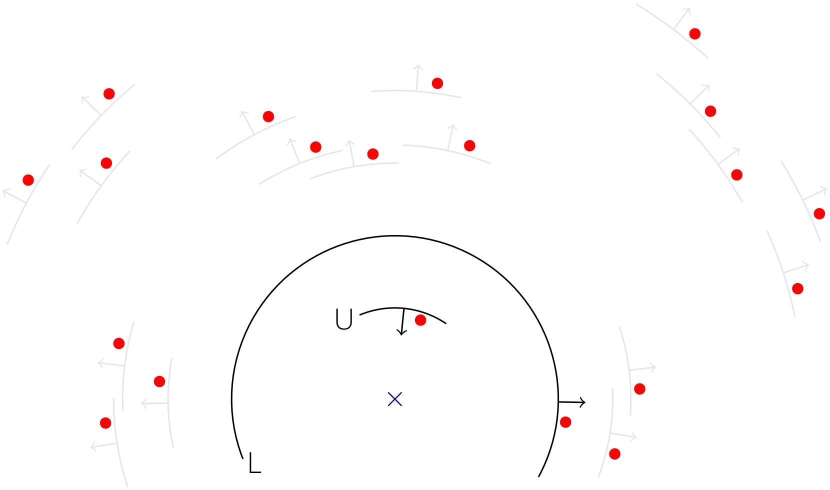


Using The Triangle Inequality
Yinyang group lower bounds

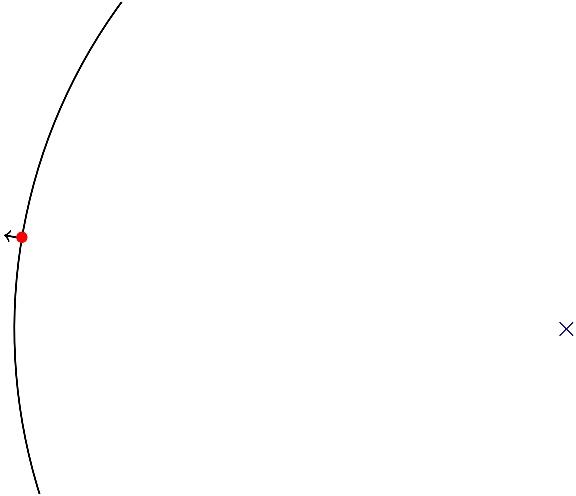


Using The Triangle Inequality

Hamerly 1 lower bound



Lower bound updating



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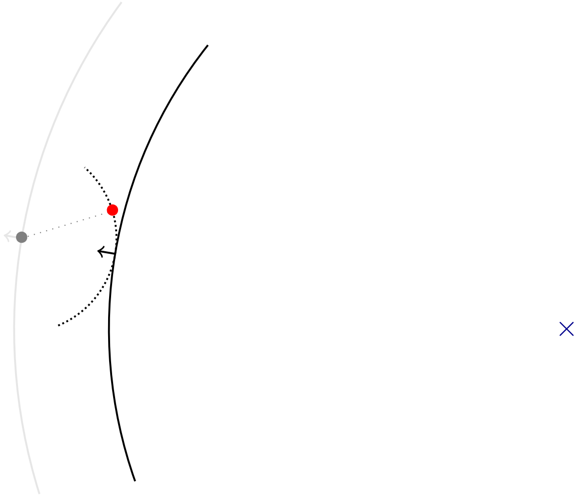

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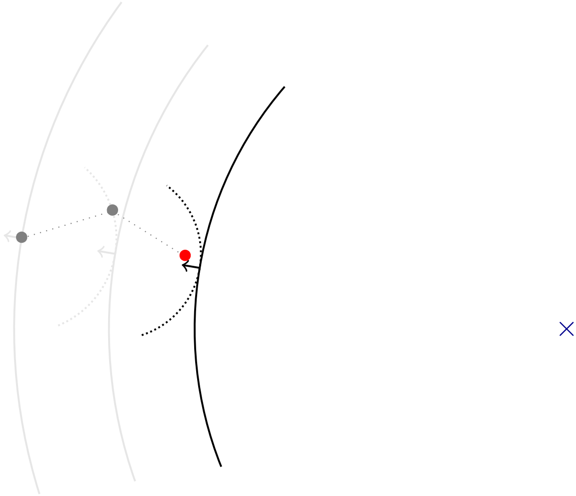

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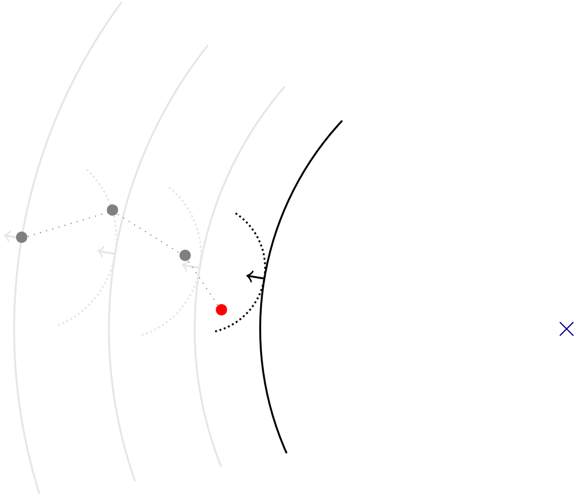

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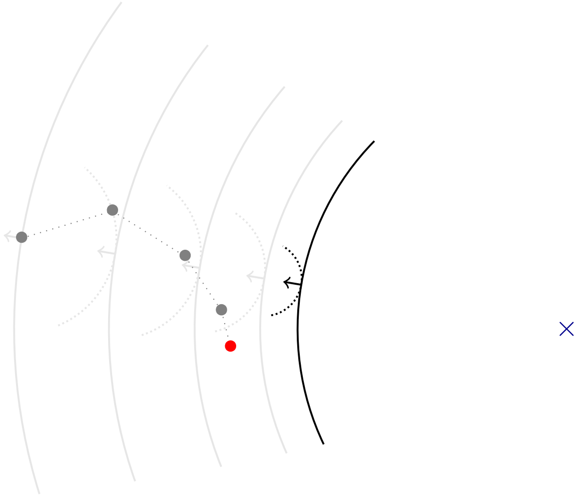

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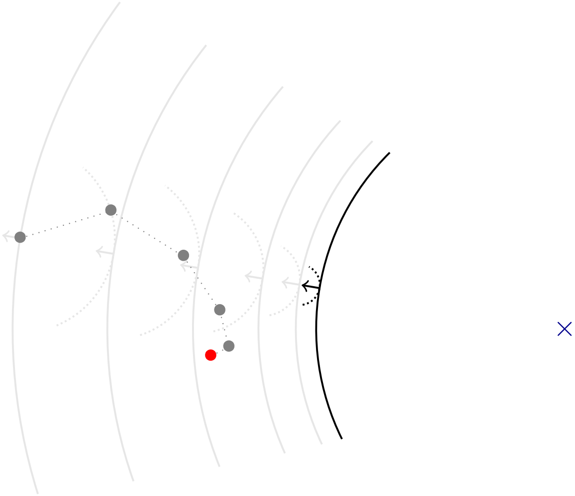

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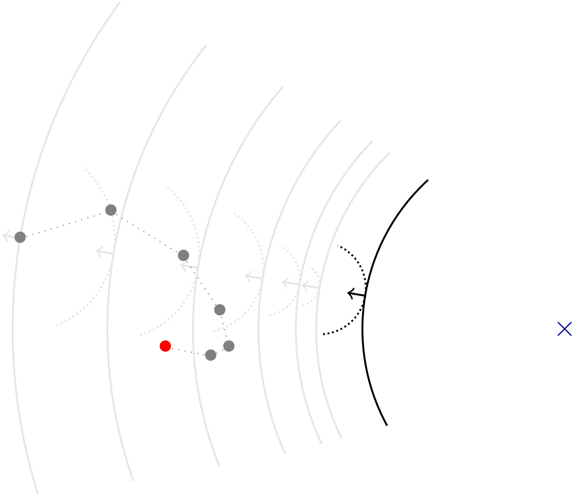

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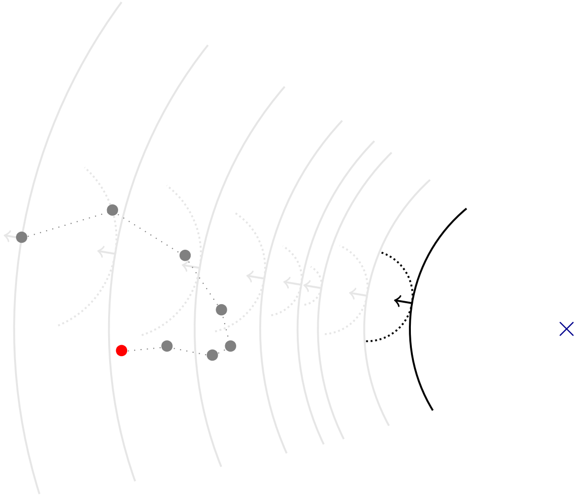

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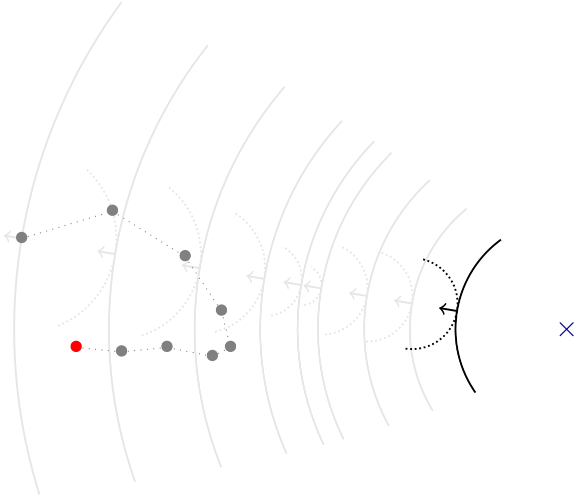

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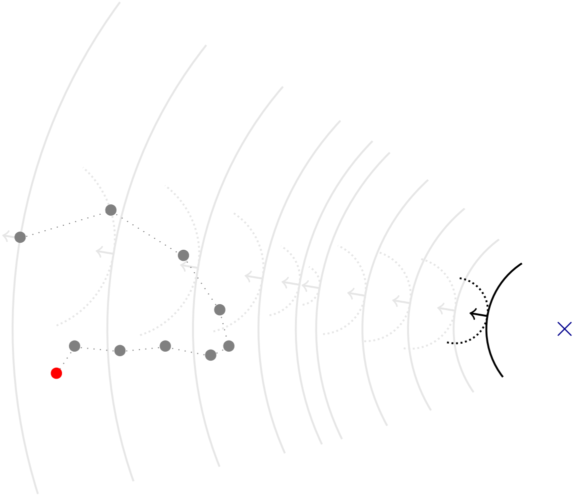

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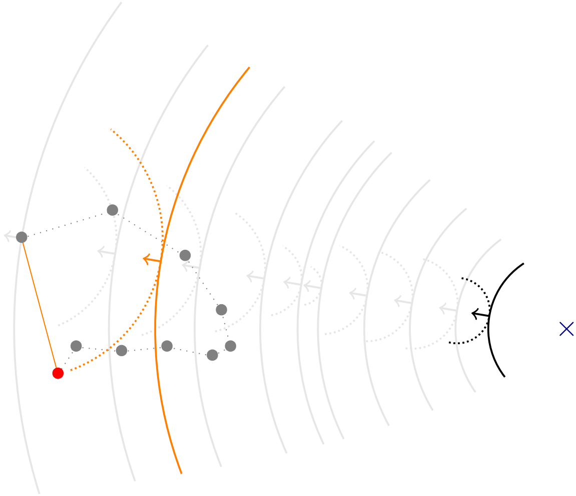

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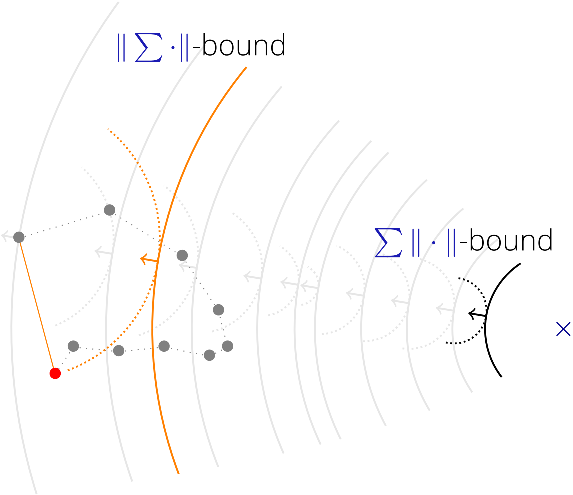

$\| \sum \cdot \|$-bounds

All upper and lower bounds in Elkan, Hamerly, Yinyang, Annular are $\sum \| \cdot \|$-bounds, and can be replaced by tighter $\| \sum \cdot \|$-bounds.

There is a cost to $\| \sum \cdot \|$-bounds, additional memory is required:

- Store historical centers from all rounds
- Store the round in which bounds are made tight

This memory overhead can be controlled by periodically clearing the history, requiring a $\sum \| \cdot \|$-bound update

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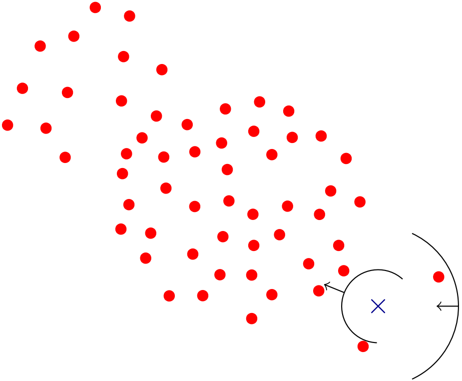
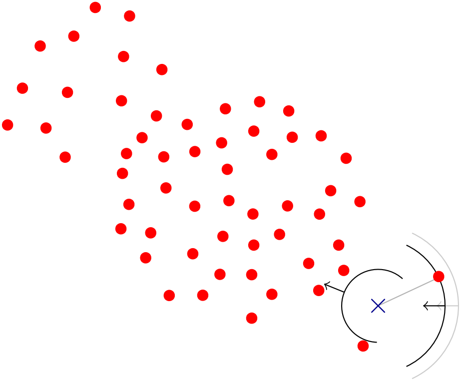
(B) *We show that $\|\sum \cdot\|$-bounding generally improves algorithms.*

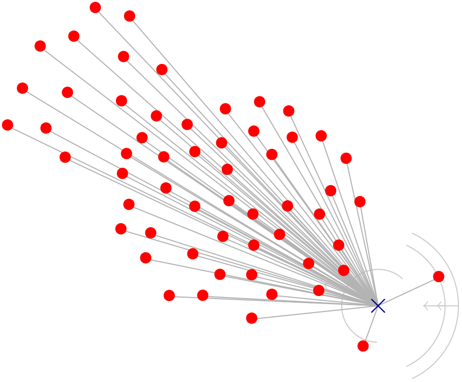
Hamerly (2010) bound test, failure 1



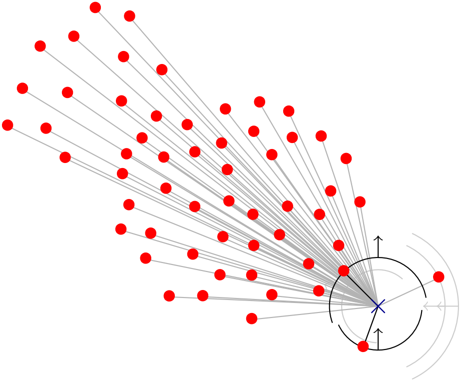
Hamerly (2010) bound test, failure 2



Hamerly (2010) compute all distances

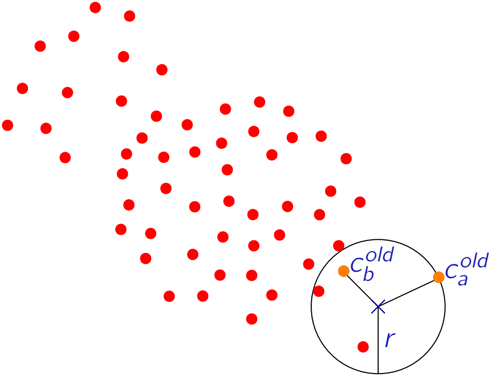


Hamerly (2010) reset bounds



Eliminating distance calculations

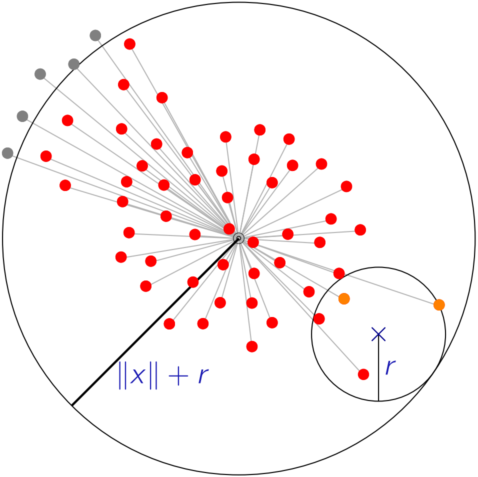
$$c \notin \mathcal{B}(x, r) \Rightarrow c \notin \{c_a^{new}, c_b^{new}\}$$



$$r = \max_{c \in \{c_a^{old}, c_b^{old}\}} \|x - c\|$$

Annular (2013) elimination zone

$\|c\| > \|x\| + r \Rightarrow c \notin \mathcal{B}(x, r)$ (● : centers eliminated)



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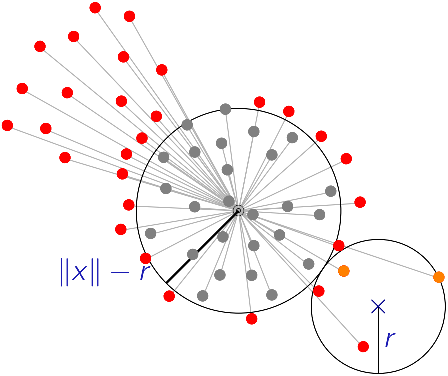

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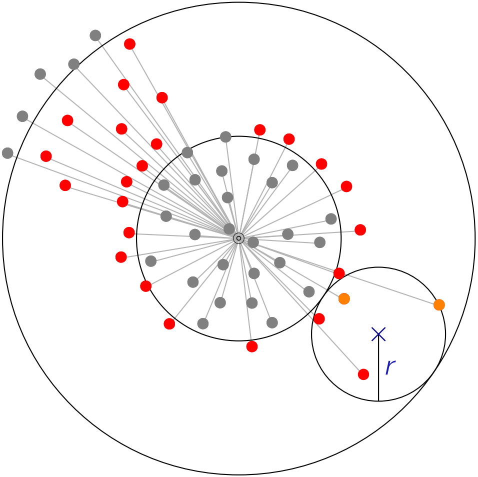

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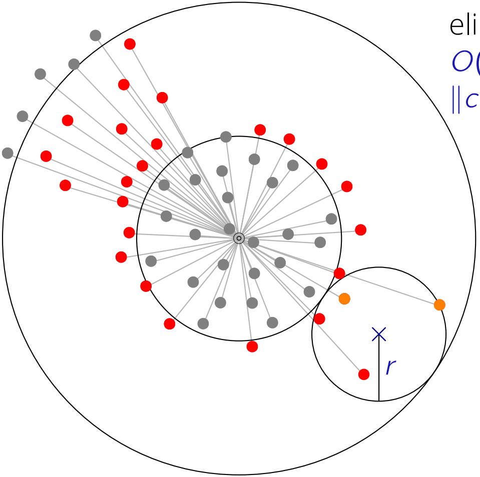

elimination
$O(\log N)$ if
$\|c\|$ sorted

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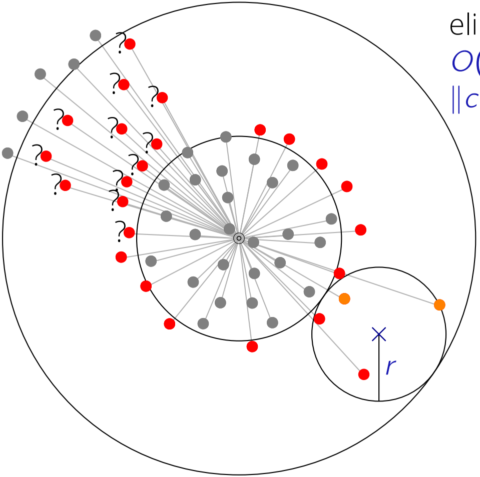

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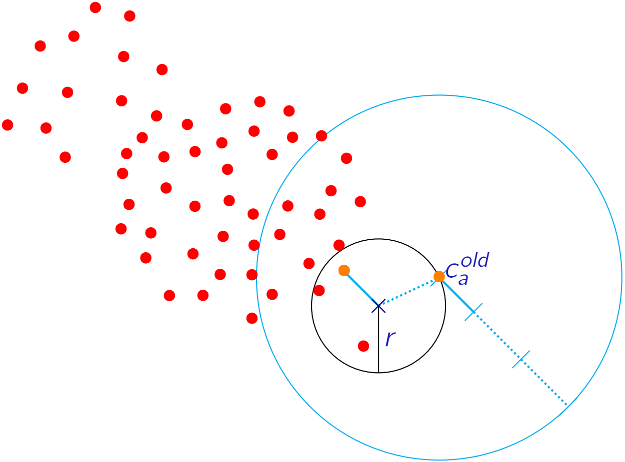
Exponion (ours) elimination zone

$$\|c - c_a^{old}\| > 2\|x - c_a^{old}\| + \|x - c_b^{old}\| \Rightarrow c \notin \mathcal{B}(x, r)$$



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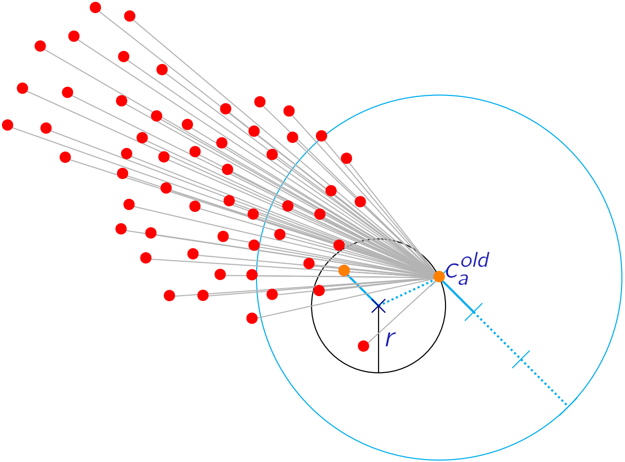

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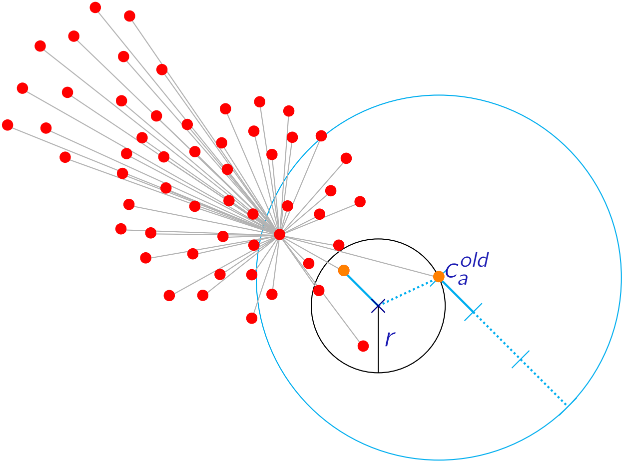

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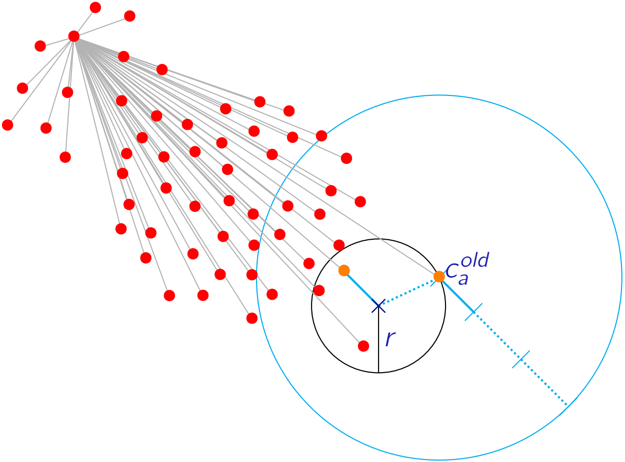

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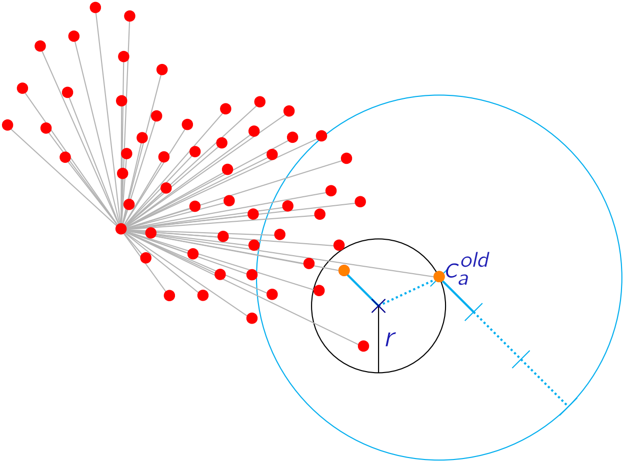

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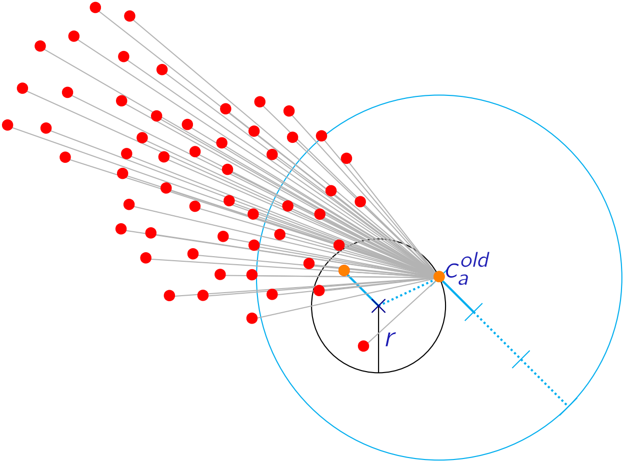

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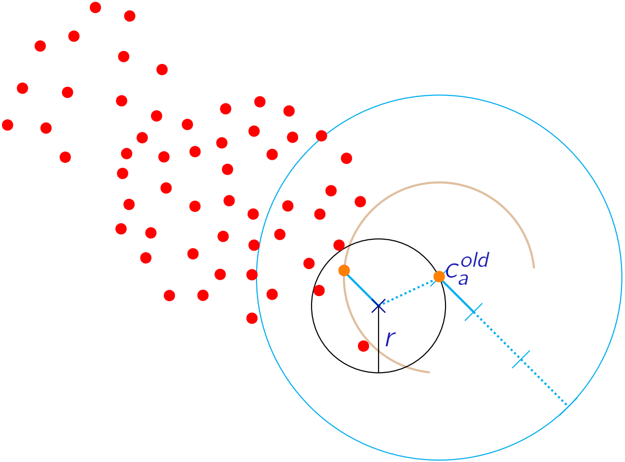

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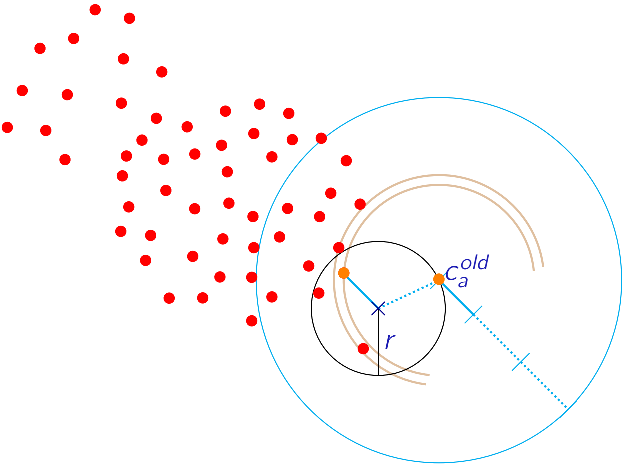

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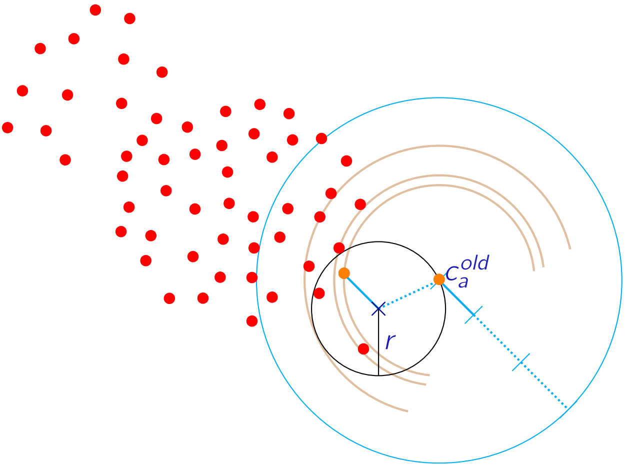

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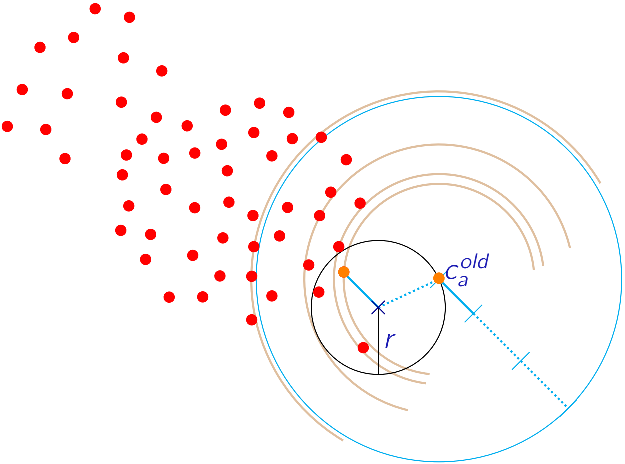

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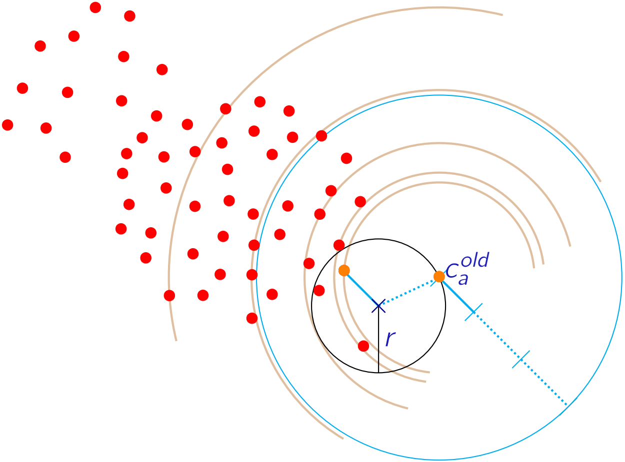

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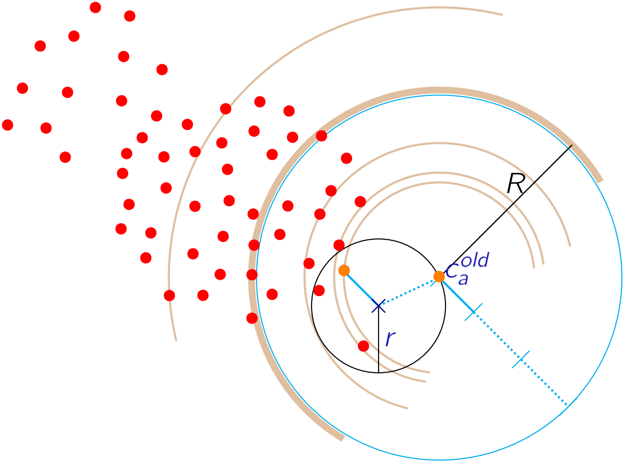
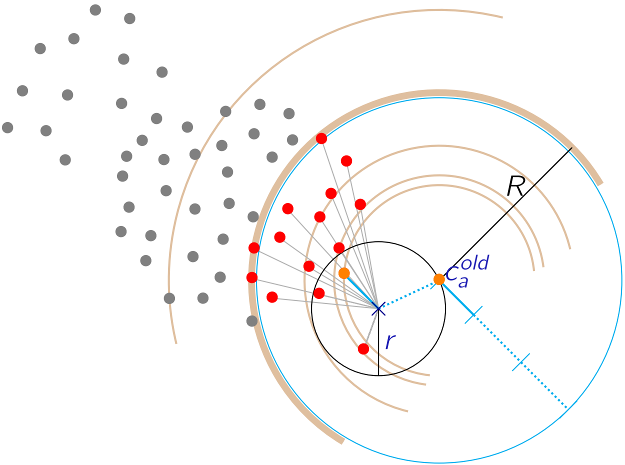


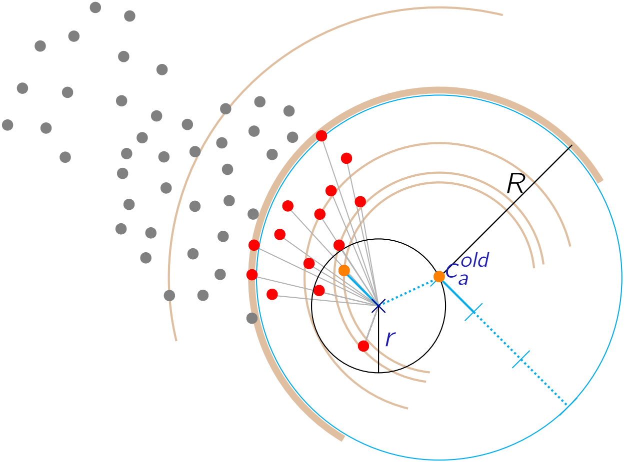
Exponion (ours) elimination zone

$\|c - c_a^{old}\| > R \Rightarrow c \notin \mathcal{B}(x, r)$ (● : centers eliminated)



Exponion (ours) elimination zone

(C) *We find that Exponion is generally faster than Annular*



Experiments and Results

22 datasets ($d : 2 \to 784$, $N : 60k \to 2.6m$) and $K \in \{100, 1000\}$

4 public code bases (mlpack, BaylorML, PowerGraph, VLFeat) +

+ all from scratch

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Experiments and Results

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(C) *Exponion is generally faster than Annular*
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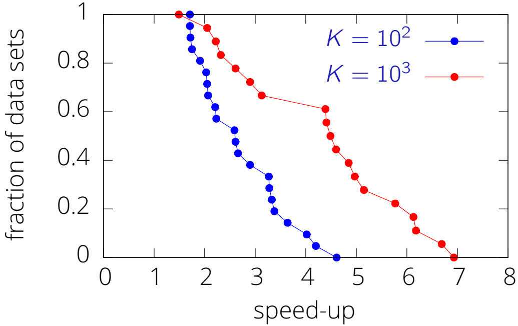
Conclusion

Speed-up: run-times of any of the other 4 implementations of any algorithm relative to our fastest implementations of our algorithms



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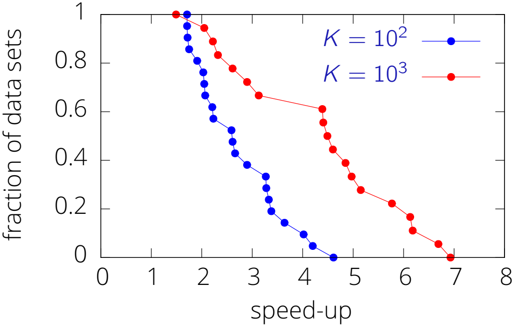

Our multi-threaded & easy-to-use code is available under an open source licence

The end

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