K-medoids for *K*-means seeding

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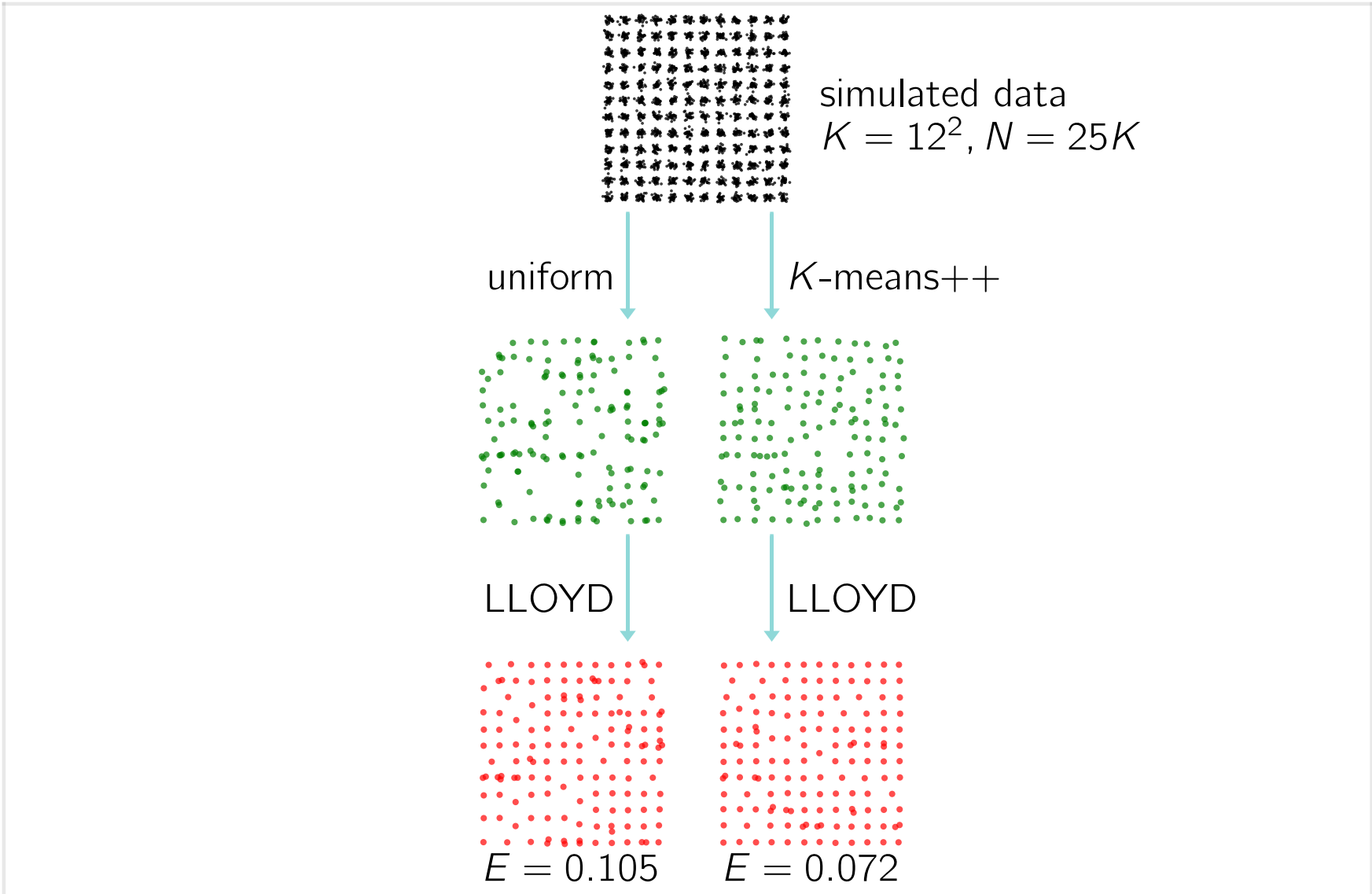
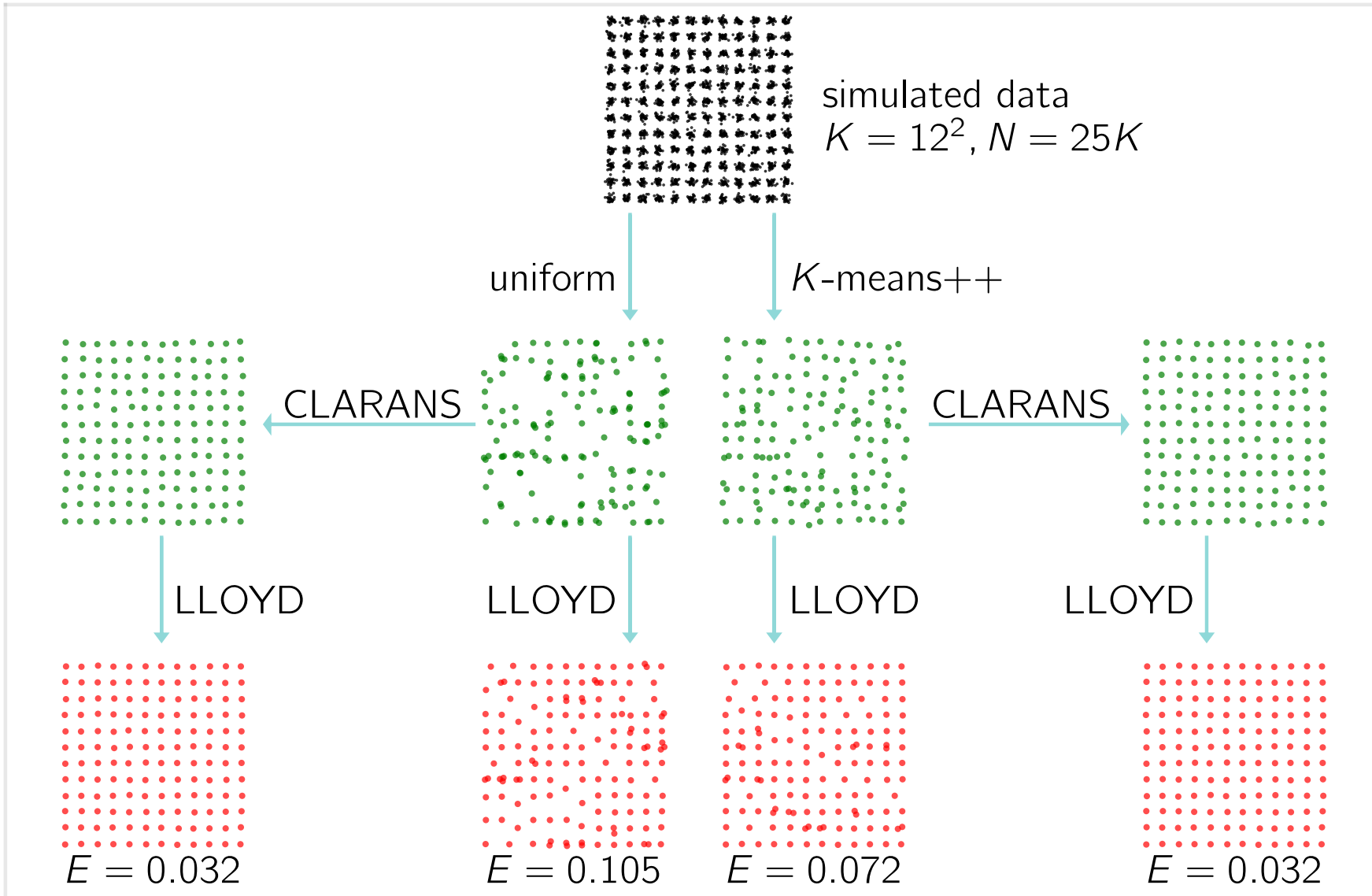
The standard K-means pipeline

First step: Seeding. Second step: Lloyd's algorithm



The standard K-means pipeline (+CLARANS)



Talk Outline

1) K-medoids, K-means++ and LLOYD

2) The CLARANS algorithm of Ng and Han (1994), algorithmic complexity and improvements

3) Results

K-medoids problem

Input :

- N samples $\mathcal{X} = \{x(1), \ldots, x(N)\}$
- Dissimilarity function $diss : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$

Task :

- Find K indices $c(1), \ldots, c(K) \in \{1, \ldots, N\}$ to minimize

$$E = \sum_{i=1}^{N} \min_{k=1:K} diss\left(x(i), x(c(k))\right).$$

- NP-hard.

K-means++ seeding

- Arthur and Vassilvitskii (2007)
- A K-medoids algorithm for

$$diss(x(i), x(i')) = \|x(i) - x(i')\|^2.$$

1: select $c(1)$ uniformly from $\{1, \ldots, N\}$
2: **for** $k = 2 : K$ **do**
3: select $c(k) = i$ with prob $\sim \min_{k'<k} diss(x(i), x(c(k')))$
4: **end for**

- Provides $8 \ln K + 2$ approximation bound to optimal K-means solution in expectation

LLOYD for K-means:

1: $C(k) \leftarrow x(c(k))$ for $k \in \{1, \ldots, K\}$
2: **while** not converged **do**
3: for $i = 1 \rightarrow N$ set $a(i) = \text{argmin}_{k=1:K} \|x(i) - C(k)\|$
4: for $k = 1 \rightarrow K$ set $C(k) \leftarrow \frac{\sum_{i:a(i)=k} x(i)}{||i : a(i) = k||}$
5: **end while**

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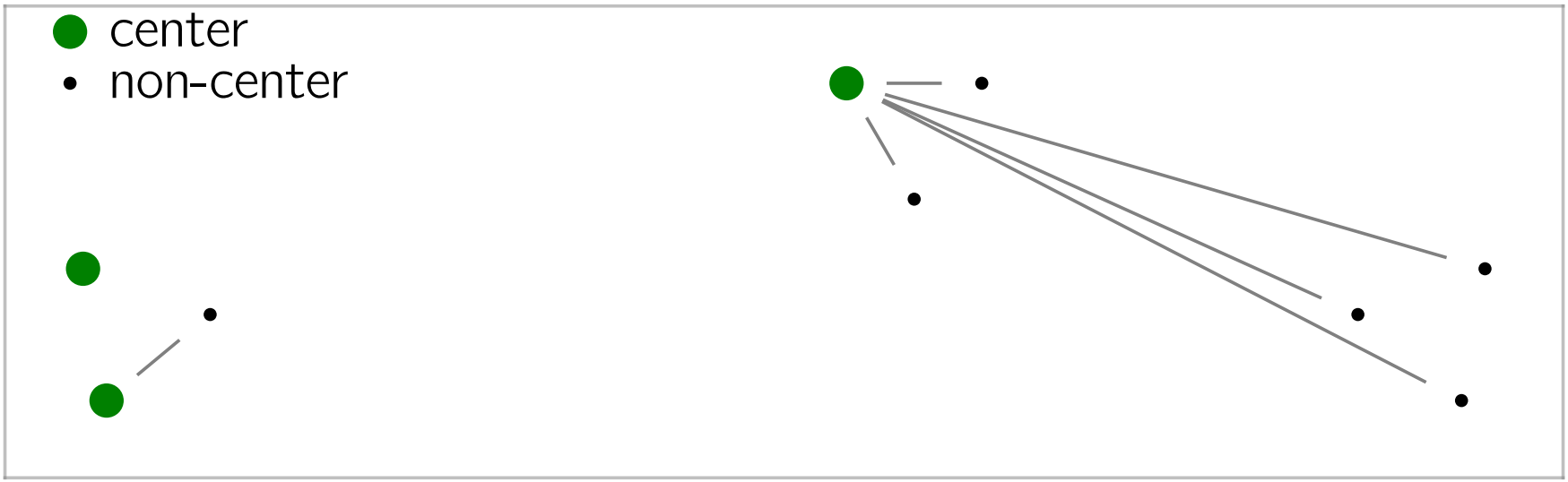
MEDLLOYD for K-medoids similar, with the constraint that centers are always samples,

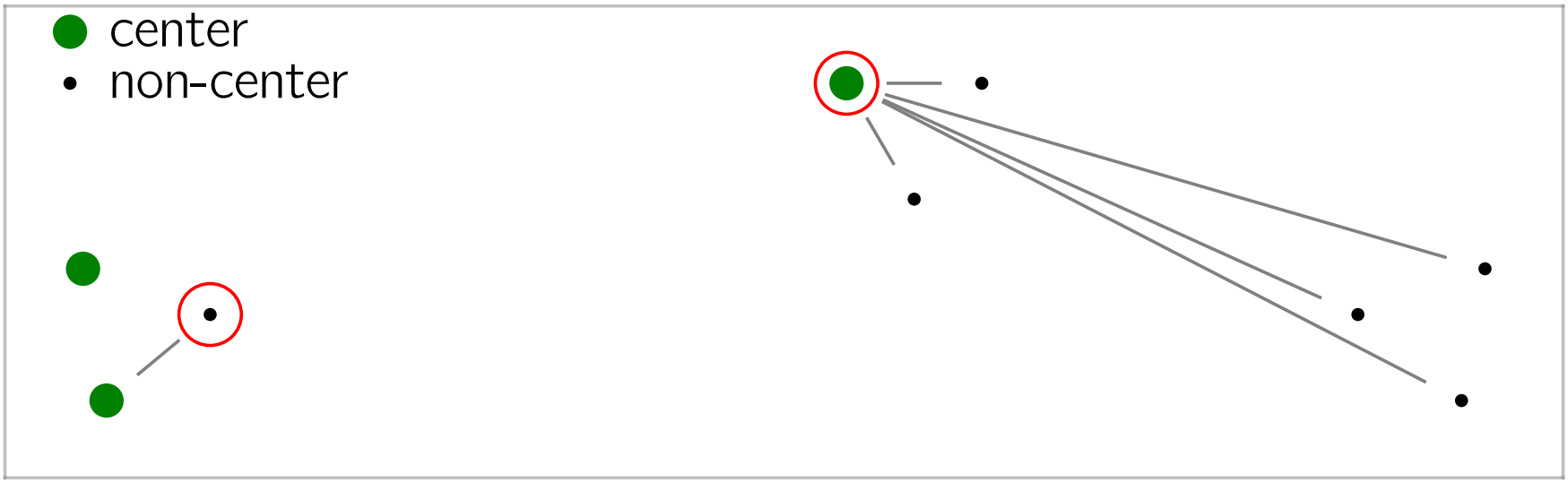
$$C(k) \leftarrow x\left(\underset{i:a(i)=k}{\text{argmin}} \sum_{i':a(i')=k} \|x(i) - x(i')\|^2\right)$$

A very simple K-medoids algorithm:

Randomly propose swaps between 1 center and 1 non-center, accept if E decreases.

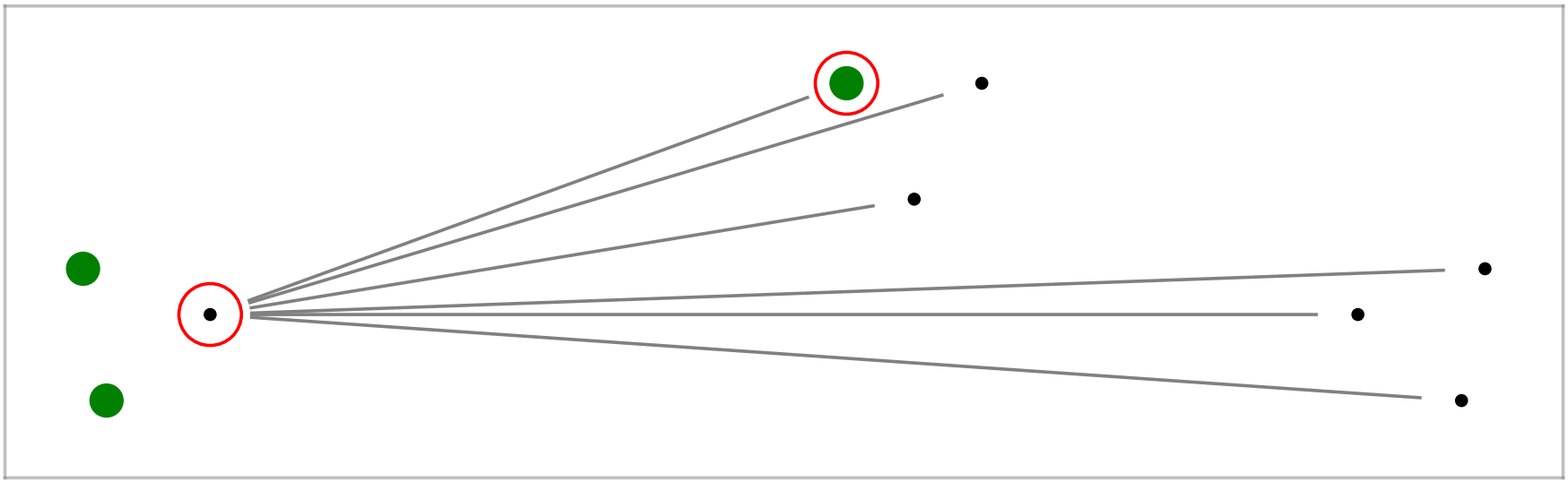
CLARANS
Demonstration



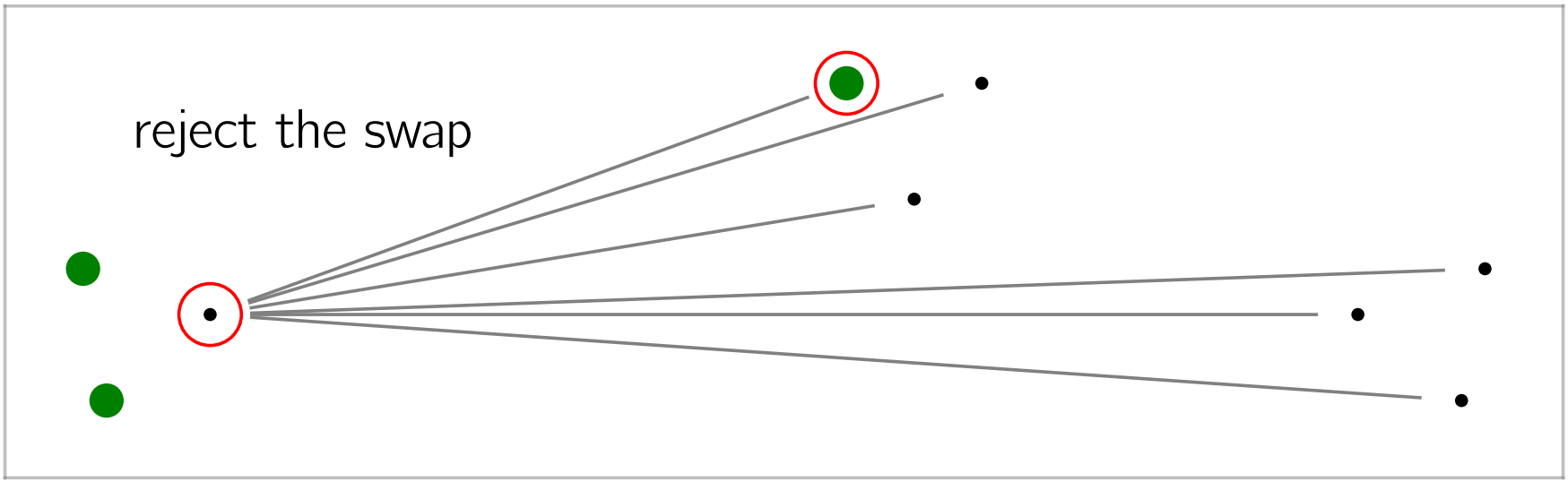


1) propose a swap

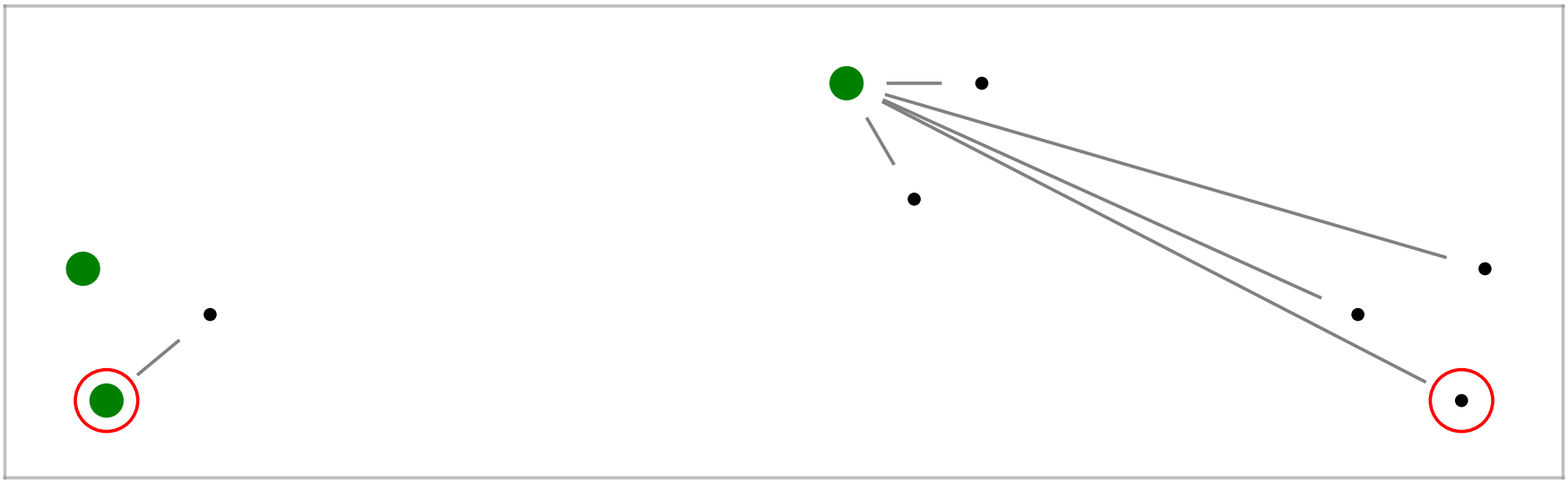
Demonstration



1) propose a swap
2) evaluate energy



1) propose a swap
2) evaluate energy
3) implement or reject



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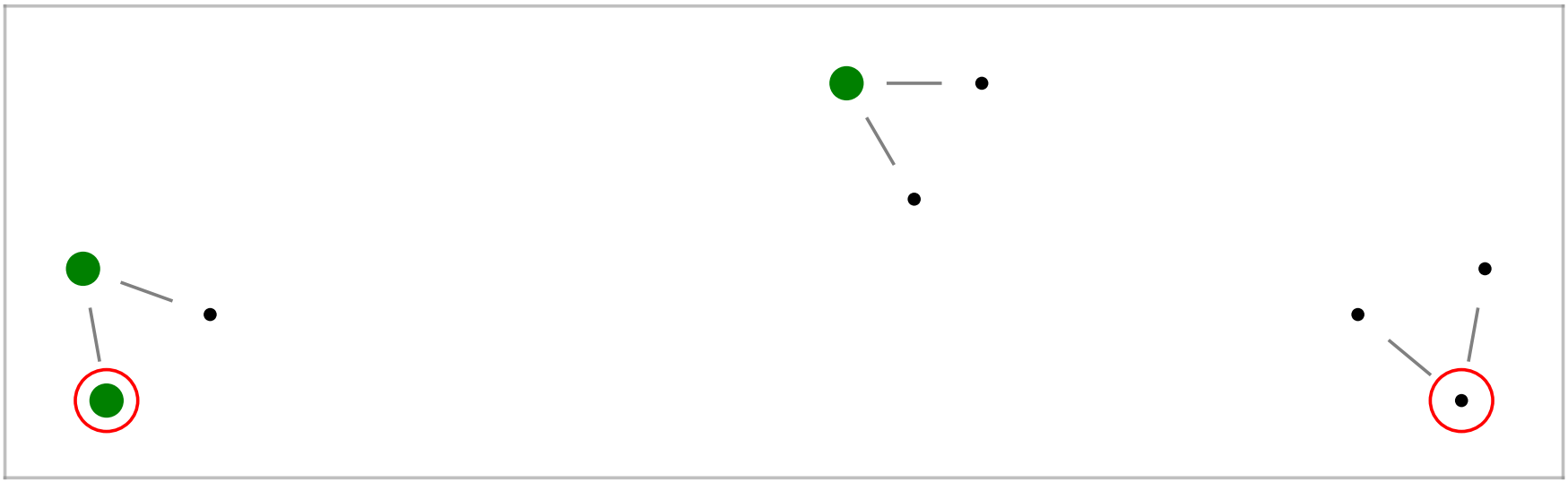

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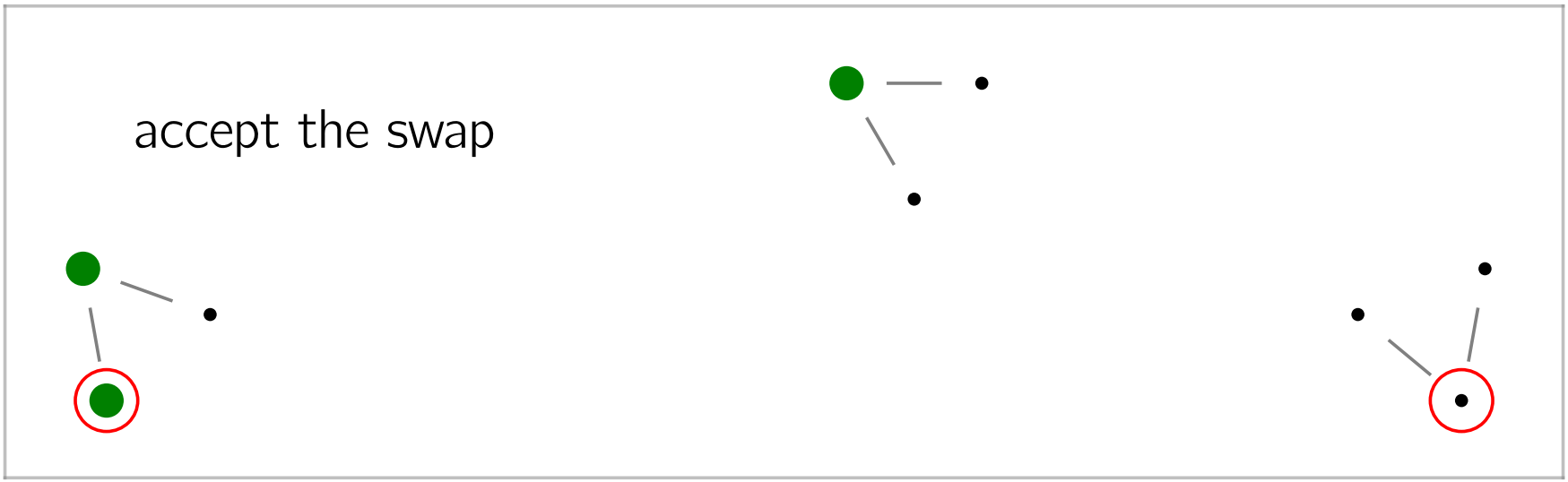

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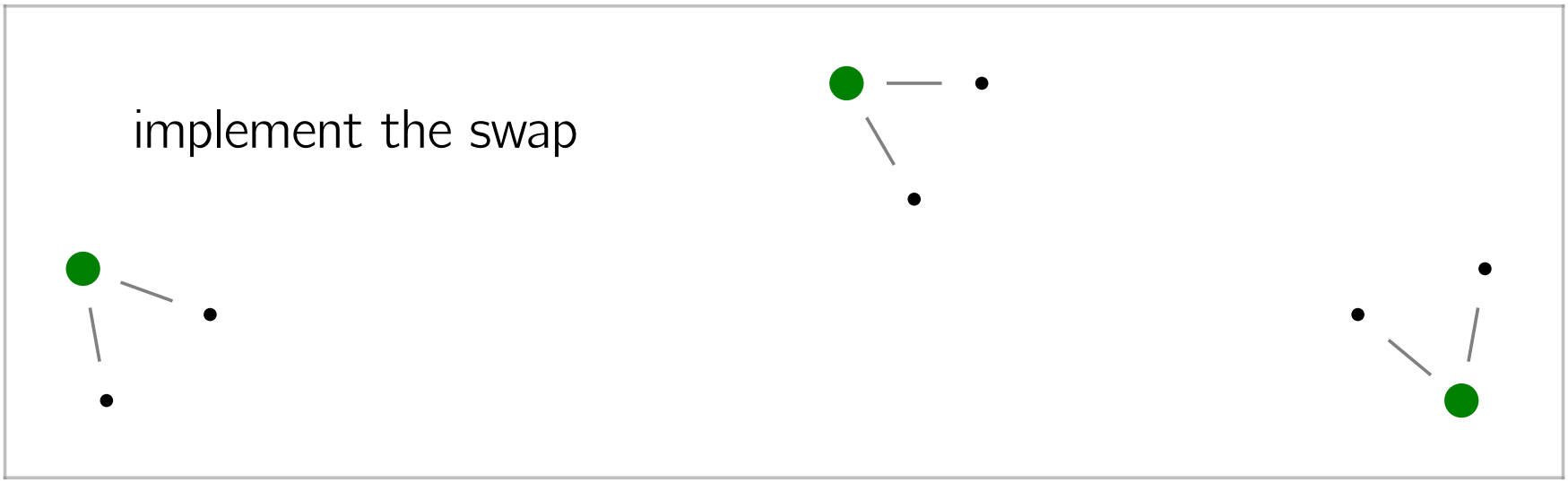

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Advantages of CLARANS over MEDLLOYD (and LLOYD) are,

- updates are *not local*
- assignments and centers change simultaneously

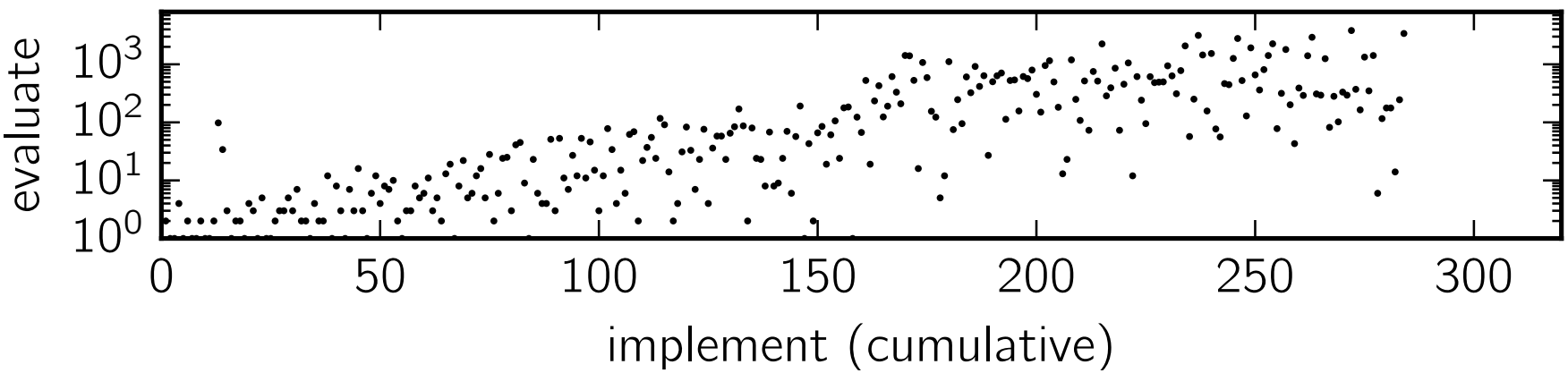
Easy to show that,

- {local minima of CLARANS} $\subseteq$ {local minima of MEDLLOYD}.

Ng and Han use N^2 dissimilarity matrix, infeasible now

Useful to distinguish between evaluate and implement steps:

1: **while** stopping condition is false **do**
2: randomly select center and non-center
3: evaluate proposal energy
4: **if** proposal energy lower **then**
5: implement proposed swap
6: **end if**
7: **end while**



We present different levels of optimization:

1. For all samples, record distances to nearest and second nearest centers (d_1 and d_2 respectively).
2. Also record for all clusters maximum d_1 and d_2, and inter-center distances. $(\triangle)$

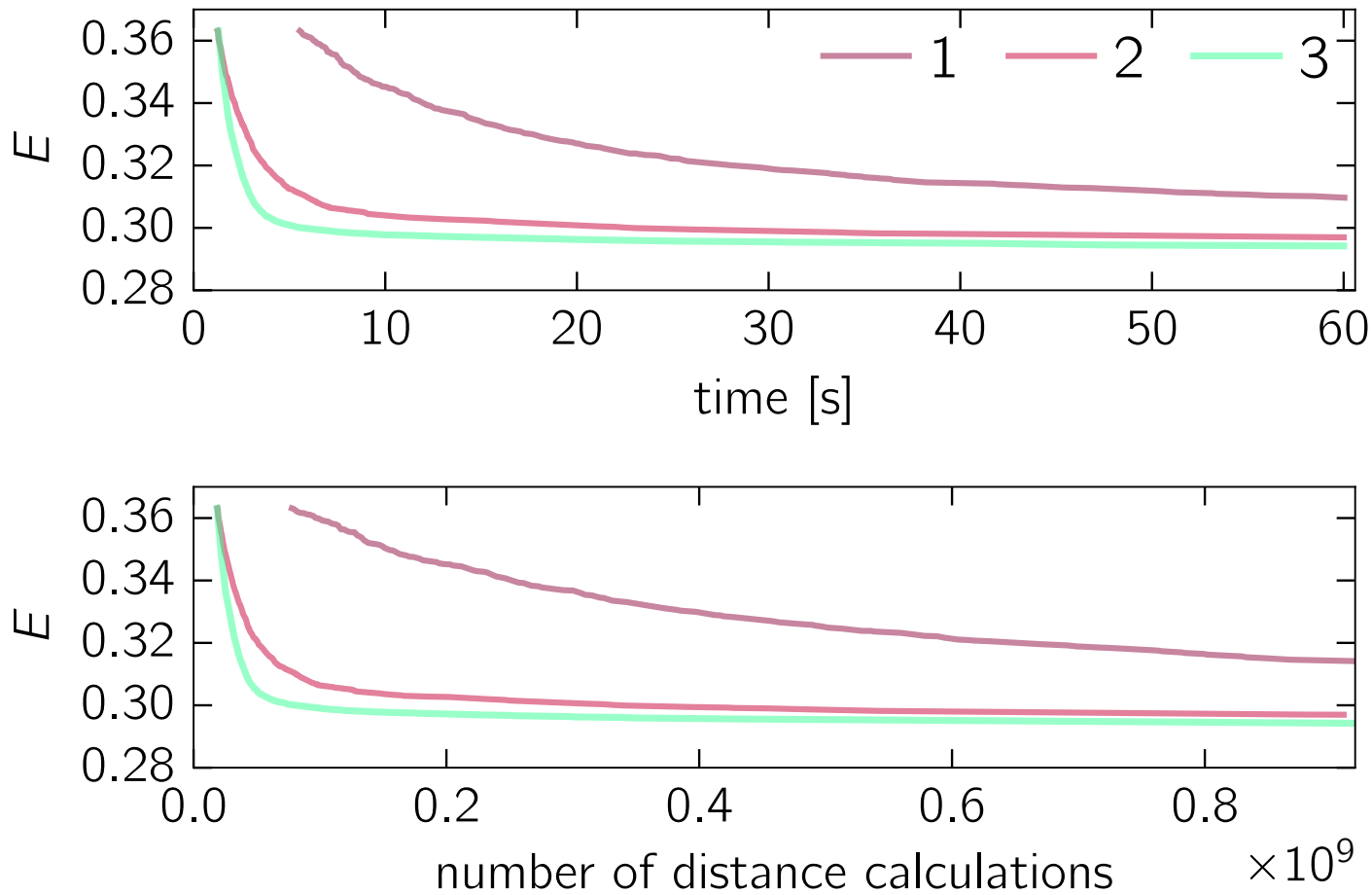
Assuming largest cluster is $O(N/K)$,

	1.	2.
evaluate	$O(N)$	$O(\frac{N}{K})$
implement	$O(N)$	$O(N)$

3. Terminate evaluation early if swap unpromising.

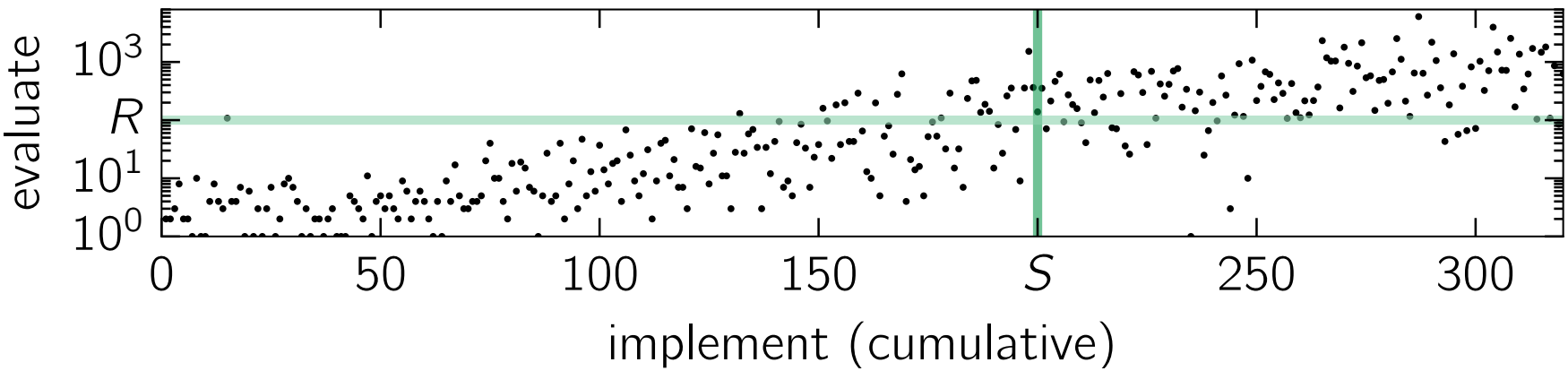
Empirical speed-up

$N = 10^6/2$, $K = 10^3/2$, data from 4-d Gaussian with I covariance .



Two possible stopping criteria

- Ng and Han stop after R consecutive swap rejections
- Can stop after S implementations (swap accepts)

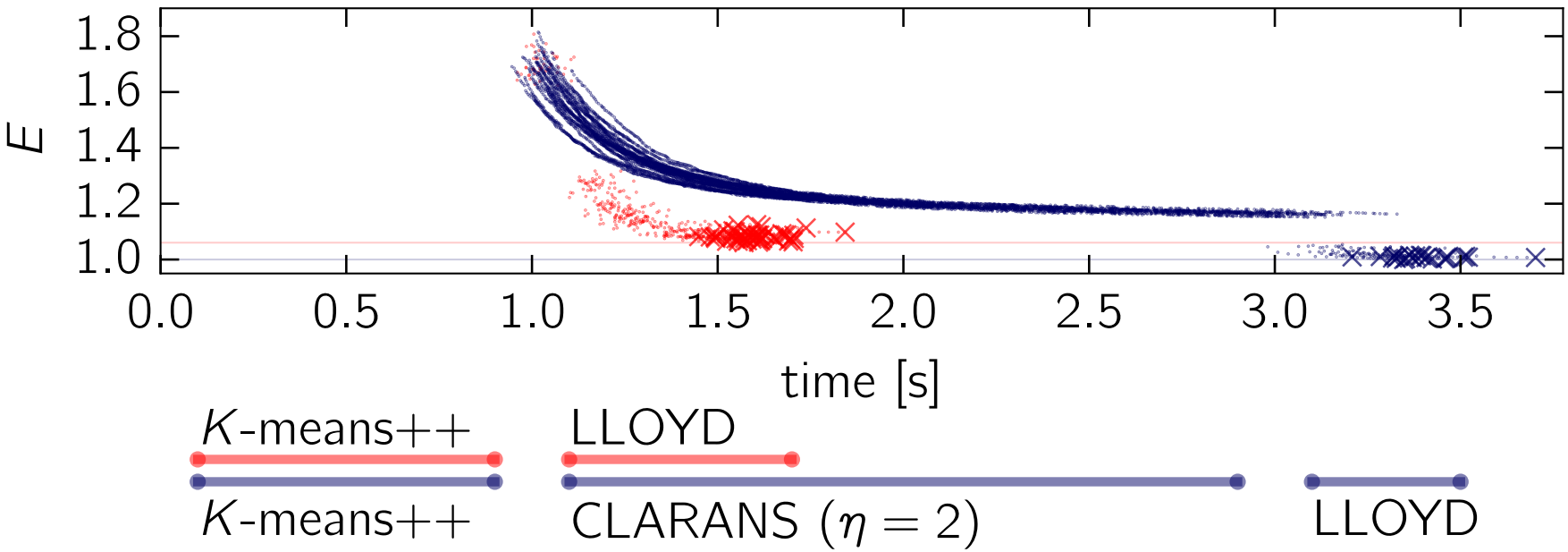


We prefer a time based criterion

- If first seeding (with K-means++) takes T_0, stop afer ηT_0.

Experiment 1

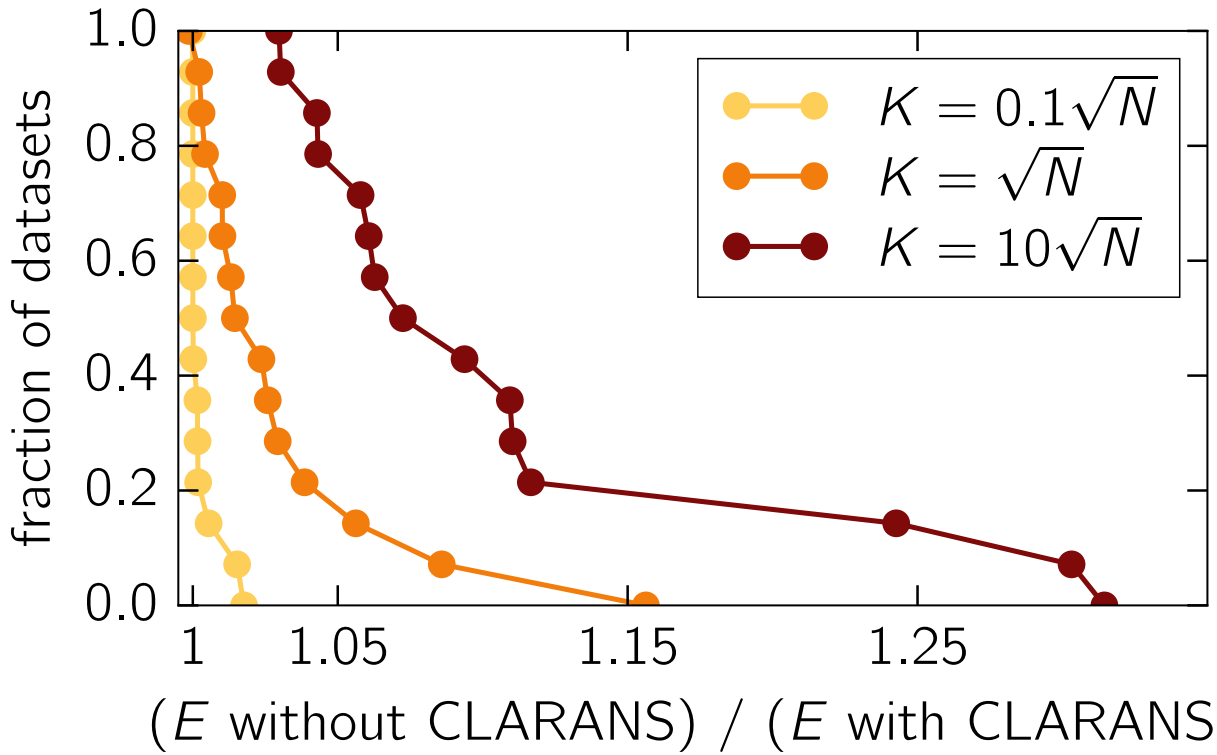
Subset of RNA dataset, $d = 8$, $N = 16 \times 10^4$, $K = 400$.



50 runs of K-means++ $\rightarrow$ LLOYD, and several with CLARANS. Number with CLARANS chosen so total times equal. Comparing best solutions, using CLARANS results in 6% lower E.

Results Summary

Summary of experiments. Each point is an experiment with same setup as previous slide, horizontal position is reduction in E obtained using CLARANS.

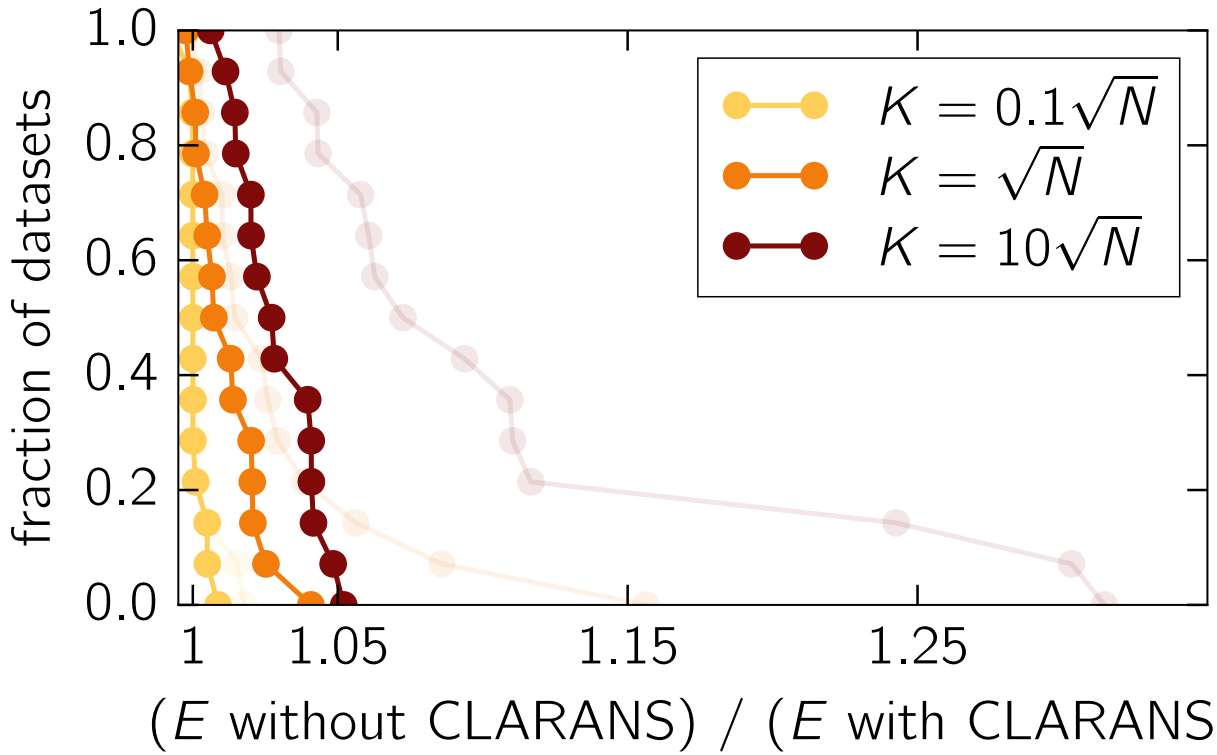


Dataset dimensions range in $d : 2 \to 90$, $N : 1484 \to 488565$.

From conclusion of K-means++ paper of Arthur and Vassilvitskii (2007):

"Also, experiments showed that k-means++ generally performed better if it selected several new centers during each iteration, and then greedily chose the one that decreased E as much as possible. Unfortunately, our proofs do not carry over to this scenario."

K-means++ revisited



Comparison to version of K-means++ referred to in Conclusion of Arthur and Vassilvitskii (2007) (selecting from best of 5 new centers). Using CLARANS still improves results, but by less.

Clustering library: zentas

$(\triangle)$: $diss(x(i), x(i')) = \psi(dist(x(i), x(i')))$, where

- $\psi : \mathbb{R} \to \mathbb{R}$ is non-decreasing
- $dist : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ satisfies the $\triangle$-inequality

Our software `zentas` implements accelerated CLARANS for different metrics. Levenshtein for sequence data, $l_0, l_1, \ldots, l_\infty$ for sparse/dense vectors. Also fast K-means++, LLOYD, many others.

Conclusion

We discussed CLARANS, and how

- to accelerate it
- it improves seeding for K-means
- it is a versatile clustering algorithm in its own right.

The end

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