

K -Medoids for K -Means Seeding

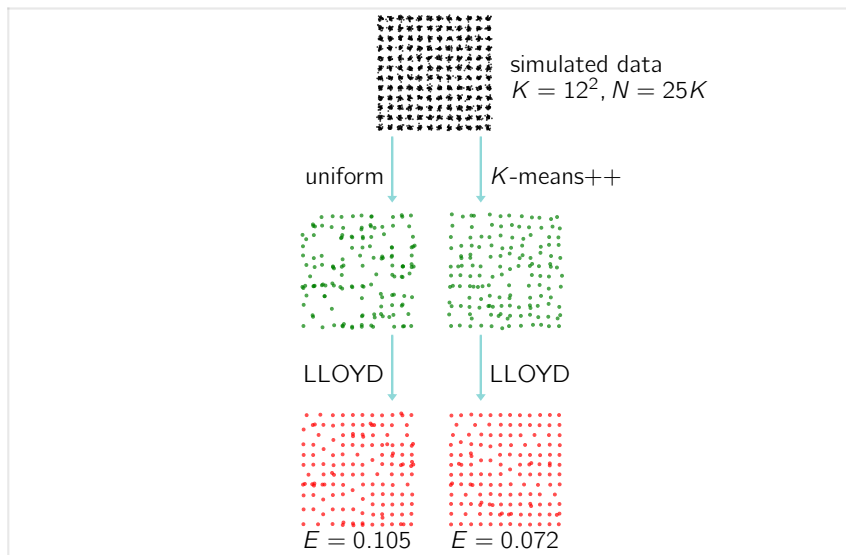
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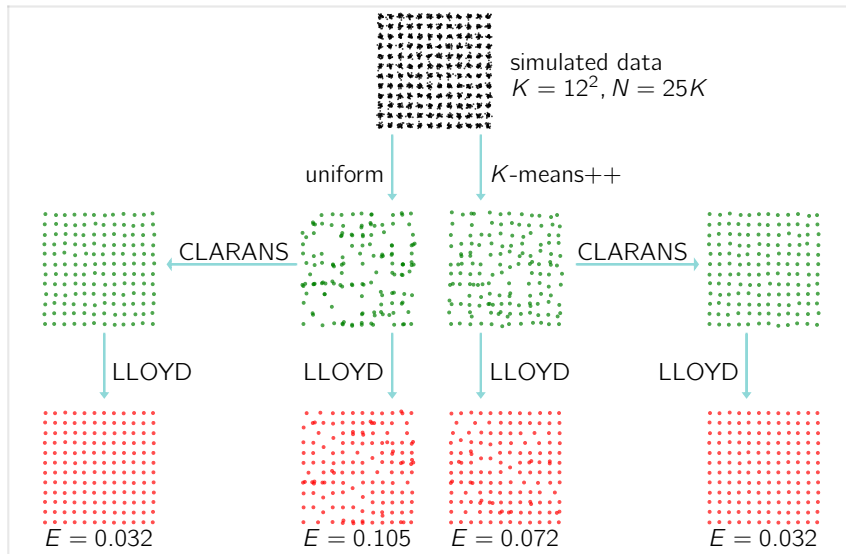
December 5th, 2017

The standard K -means pipeline

First: Seeding. Second: Lloyd's (a.k.a. K -means) algorithm.



The standard K -means pipeline (+CLARANS)



CLARANS of Ng and Han (1994)

- 1: **while** not converged **do**
- 2: randomly choose 1 center and 1 non-center
- 3: **if** swapping them decreases E **then**
- 4: implement the swap
- 5: **end if**
- 6: **end while**

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Avoids local minima of LLOYD by,

- long-range swaps
- updating centers and samples *simultaneously*.

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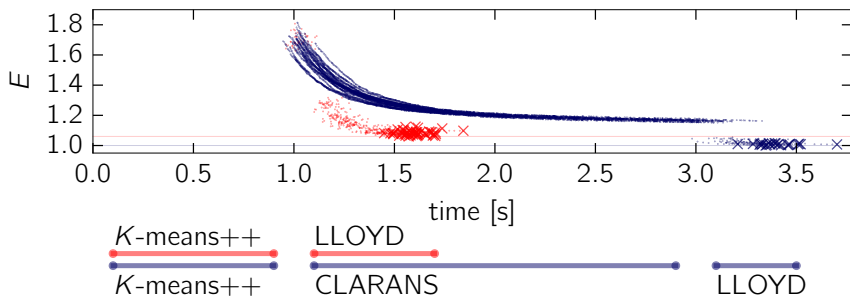
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We present algorithmic improvements, where

- computing new E is $O(N/K)$
- implementing swap is $O(N)$.

Results

- RNA dataset, $d = 8$, $N = 16 \times 10^4$, $K = 400$
- 50 runs without CLARANS (red), 24 runs with (blue).



- On 16 datasets, geometric mean improvement is 3%.

CLARANS with Levenshtein metric for sequence data, $l_0, l_1, \dots, l_\infty$ for sparse/dense vectors, many others, on github.



