Exponentially consistent K-means clustering algorithm based on Kolmogrov-Smirnov test

Tiexing Wang*, Donald J. Bucci Jr.†, Yingbin Liang⋆, Biao Chen*, Pramod K Varshney*

*Department of EECS, Syracuse University, Syracuse, NY, 13244, USA
†Lockheed Martin - Advanced Technology Labs, Cherry Hill, NJ, 08002, USA
⋆Department of ECE, The Ohio State University, Columbus, OH 43210, USA

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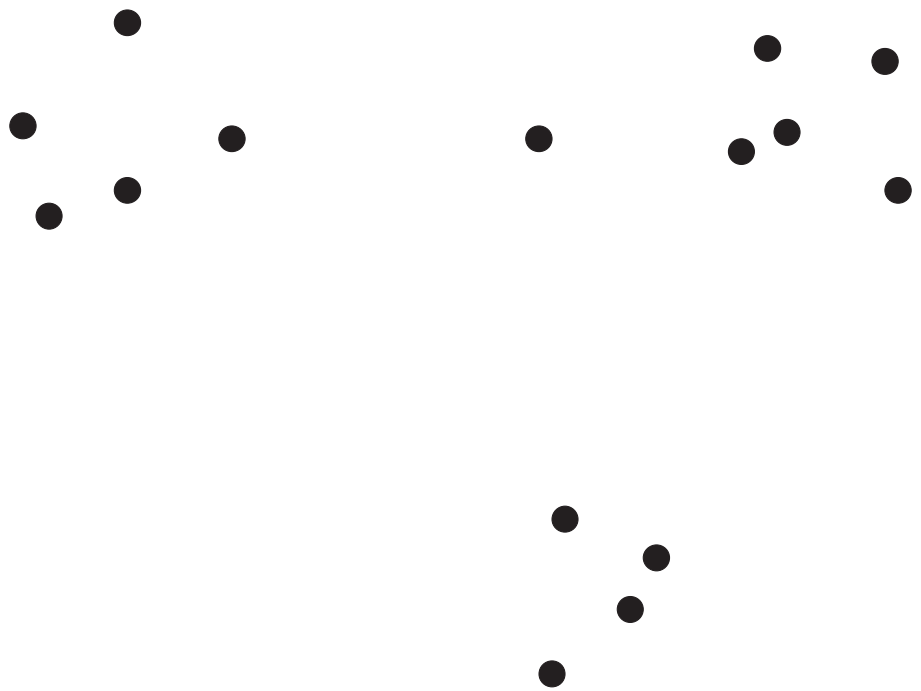
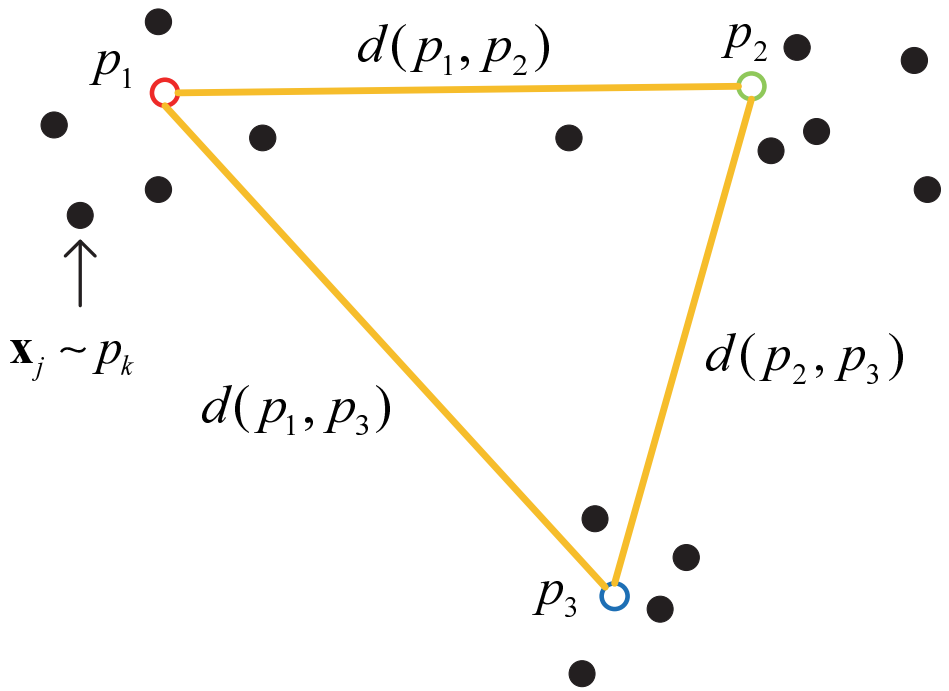
Motivation



- non-parametric
- continuous distribution

Notation



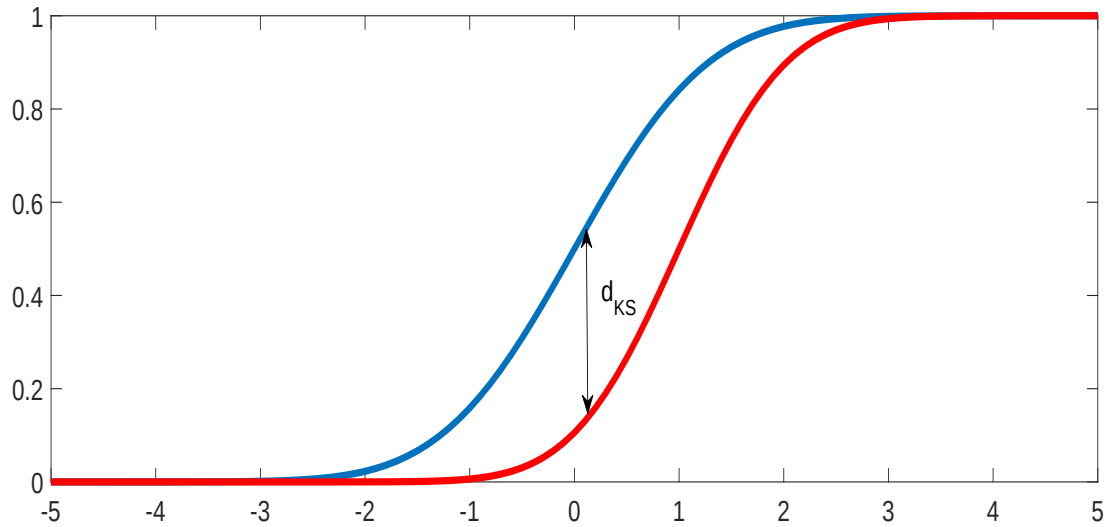
- $K = 3$ - # of distributions
- $M = 15$ - # of sequences

Kolmogrov-Smirnov (KS) distance

- Empirical c.d.f. - $F_{\mathbf{x}}(a) = \frac{1}{n}\sum_{i=1}^{n} 1_{[-\infty,a]} x_i$
  - $\mathbf{x} = \{x_1, \ldots, x_n\}$ - data sequence
  - $1_{[-\infty,x]}$ - indicator function
- KS distance:

$$d_{KS}(\star, *) = \sup_{a \in \mathbb{R}} \left| F_{\star}(a) - F_{*}(a) \right|,$$

  - $\star$, $*$ - sample data or distributions.



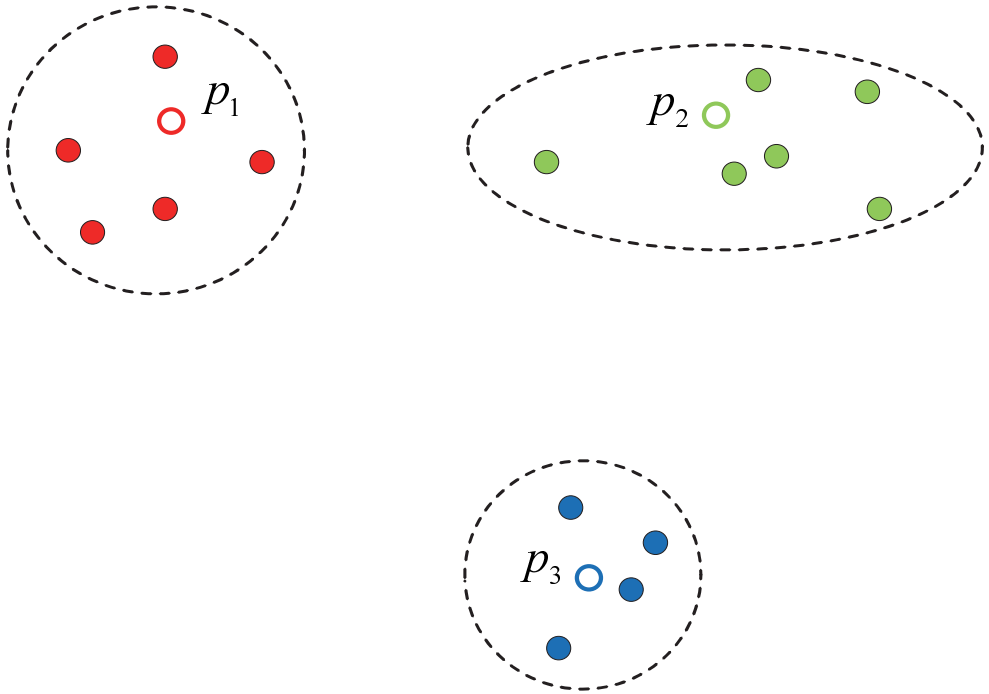
Fundamental lemma

Lemma 1 (Massart1990)

Suppose $\mathbf{x}$ *is generated by* p *and* $F_{\mathbf{x}}(a)$ *is the corresponding empirical c.d.f. Then*

$$P\big(d_{KS}(\mathbf{x}, p) > \epsilon\big) \leq 2\exp\big(-2n\epsilon^2\big).$$

Reasonable clustering result given p_i's



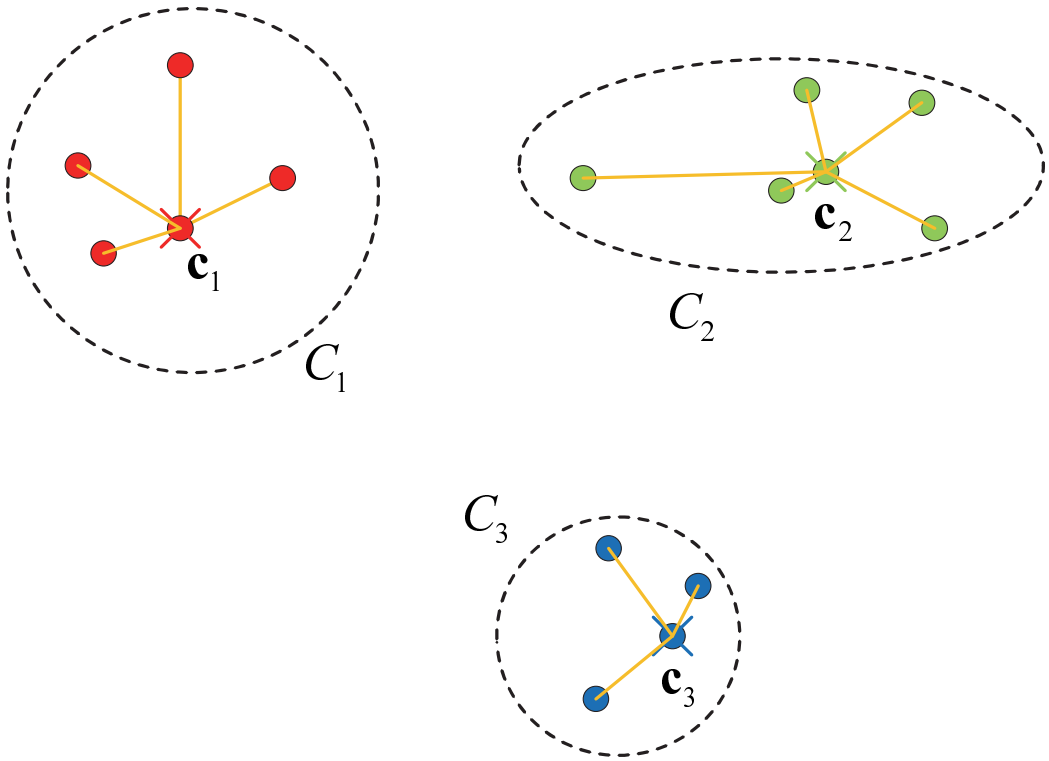
Fundamental lemma cont.

Lemma 2

Suppose $\mathbf{x}$ *and* $\mathbf{z}$ *are generated by* p_1*, and* $\mathbf{y}$ *is generated by* p_2*. Then,*

$$P\left(d_{KS}(\mathbf{x}, \mathbf{z}) > d_{KS}(\mathbf{y}, \mathbf{z}) \right) \leq 6 \exp\left(- \frac{n d_{KS}^2(p_1, p_2)}{8} \right).$$

Reasonable clustering result with unknown p_i's



- Cost function - $J = \sum_{l=1}^{3} \sum_{\mathbf{x}_j \in C_l} d_{KS}(\mathbf{x}_j, \mathbf{c}_l)$

Contributions

- Exponential consistency is established for the proposed algorithm.
  - P_e - the probability of error of a clustering algorithm
  - n - sample size
  - Consistency: $\lim_{n\to\infty} P_e = 0$
  - Exponentially consistency: $\lim_{n\to\infty} -\frac{1}{n} \log P_e > 0$.

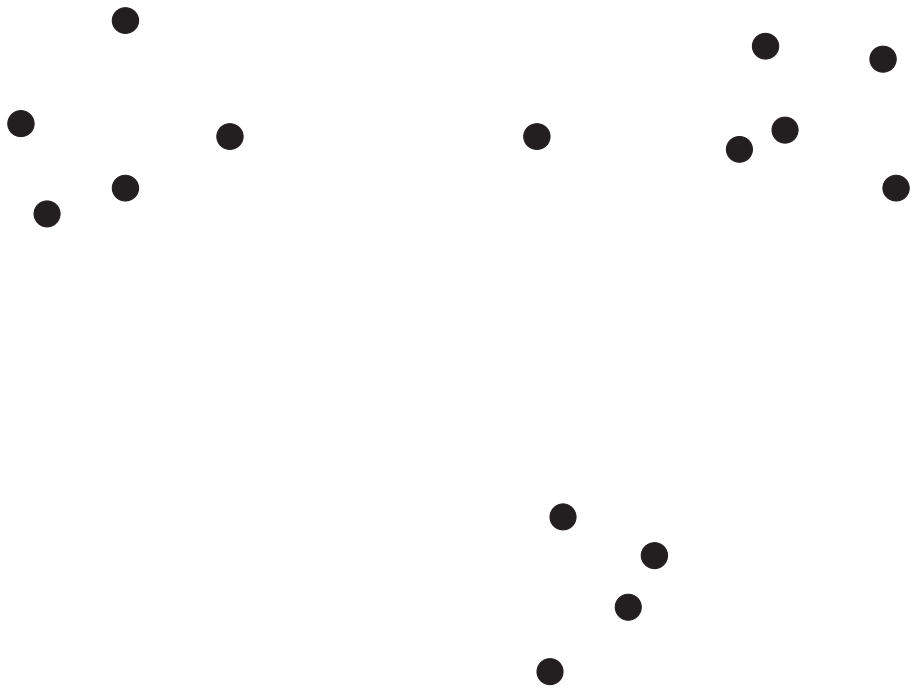
Clustering given K - Initialization

Algorithm 1 KS-based initialization given K for composite distributions

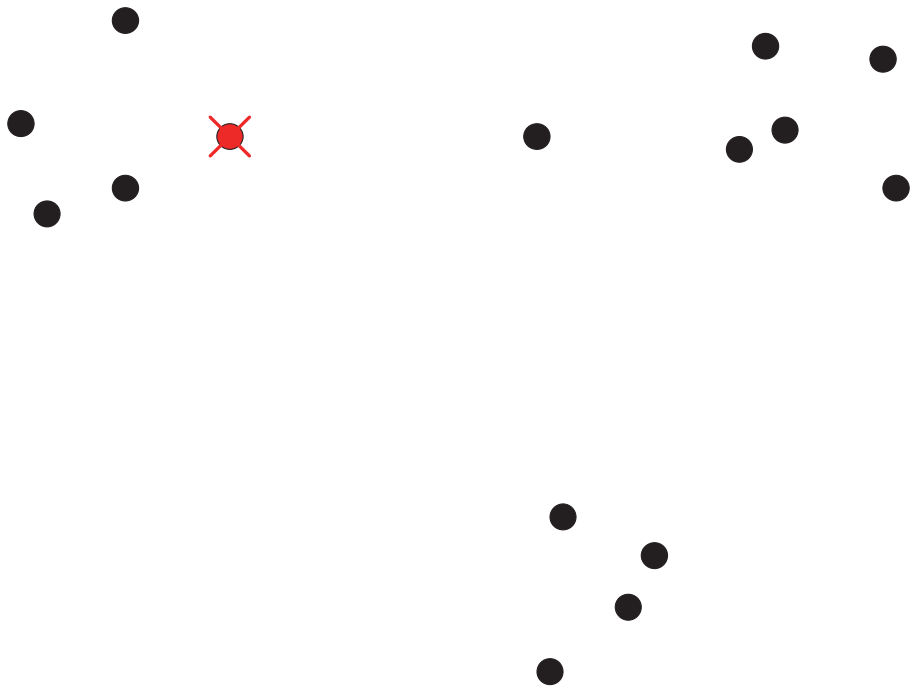
1: **Input**: $\{\mathbf{x}_j\}_{j=1}^{M}$, number of clusters K.
2: {Center initialization}
3: {Cluster initialization}
4: **Output**: $\{\mathcal{C}_k\}_{k=1}^{K}$

- Center initialization
  - Maximize the minimal distance [Katsavounidis-etal 1996]
  - Randomly choose [Moreno-Sáez-etal 2014]

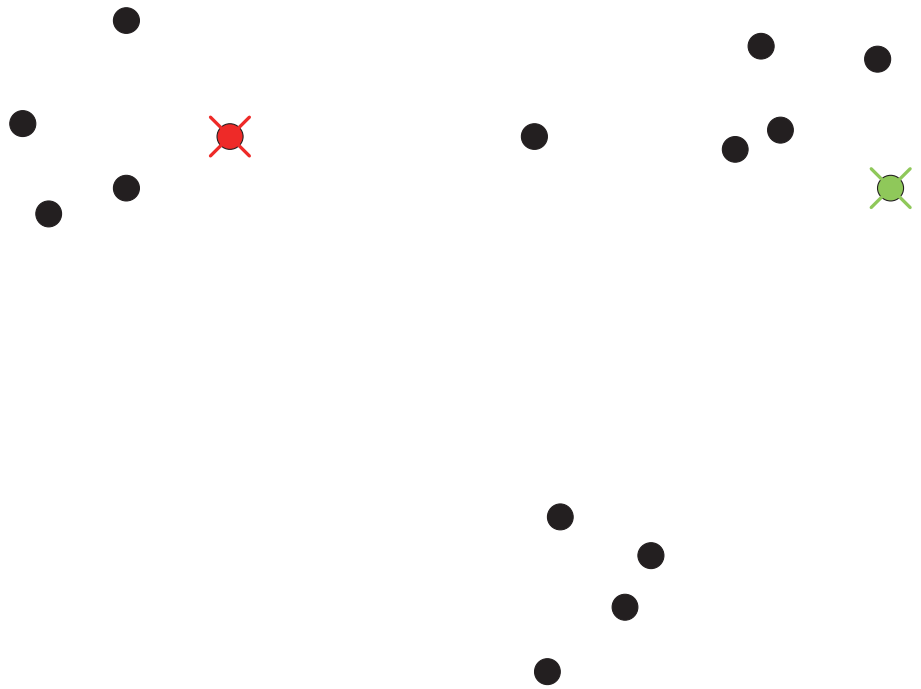
Center initialization illustration



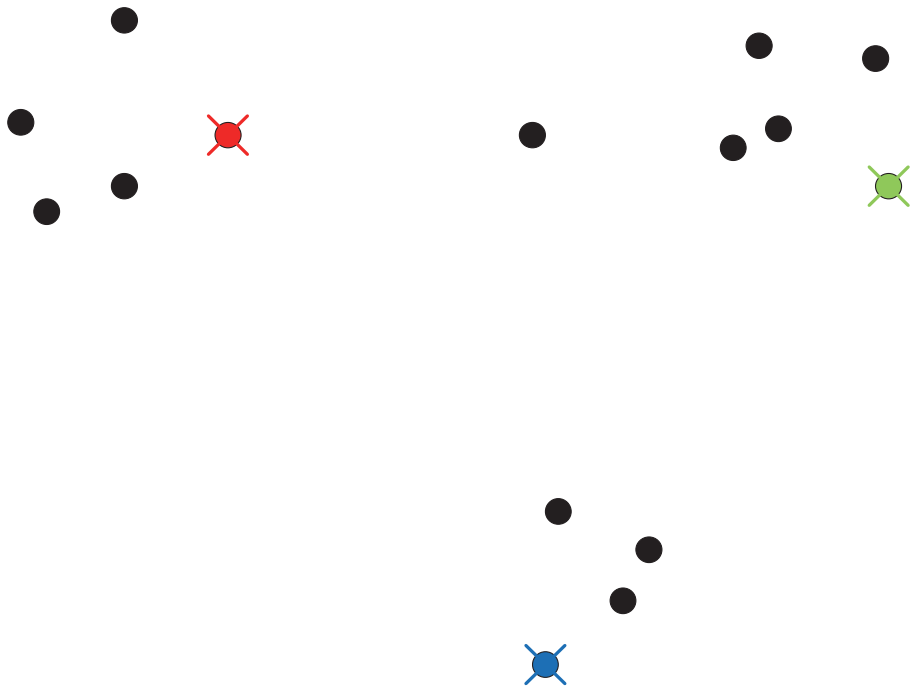
Center initialization illustration cont.



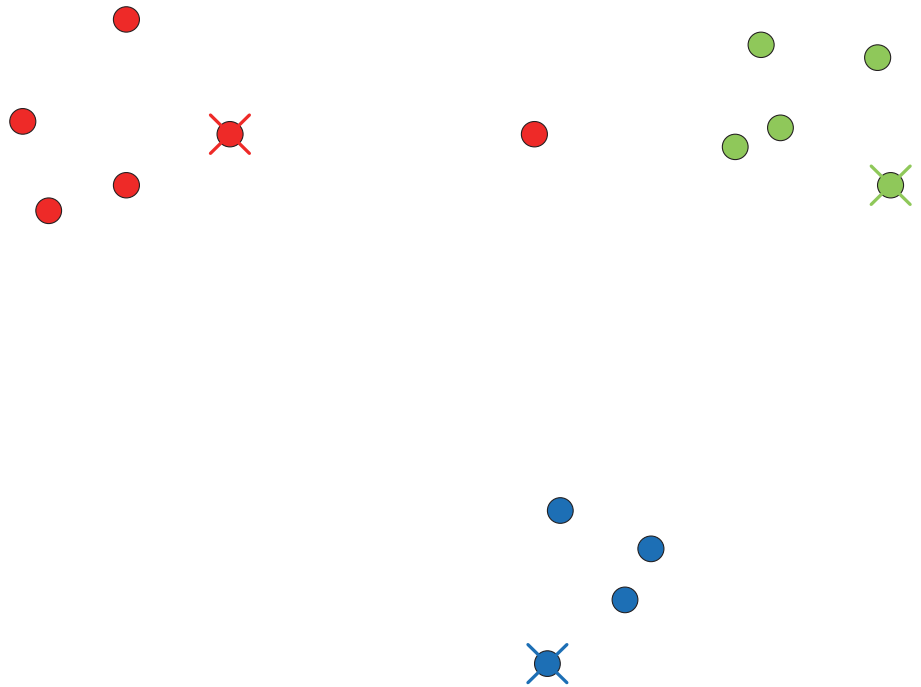
Center initialization illustration cont.



Center initialization illustration cont.



Cluster initialization illustration



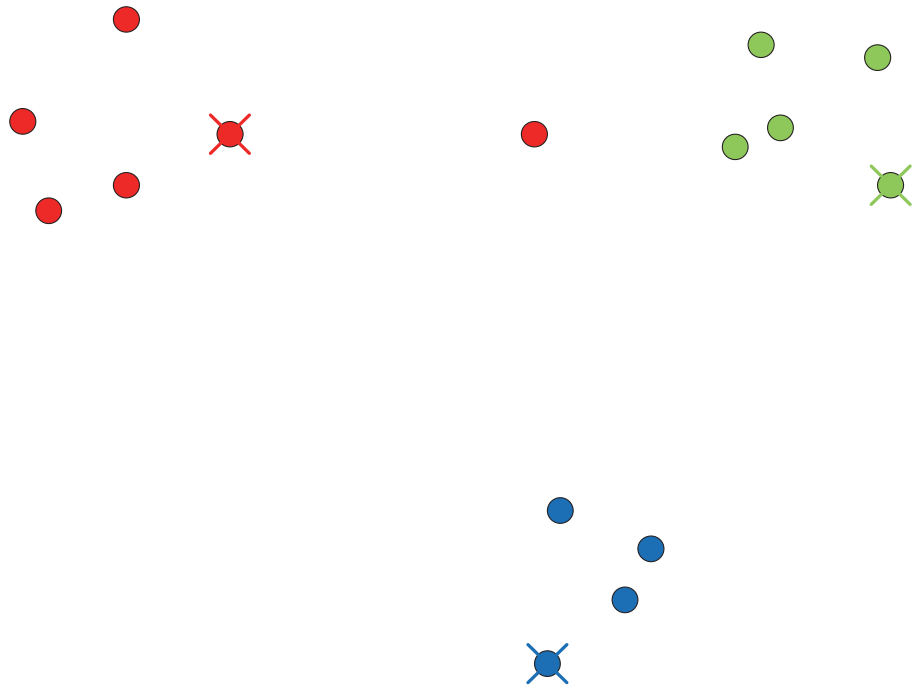
- Cost J_1^0

Clustering given K - Iteration

Algorithm 2 KS based clustering given K for composite distributions

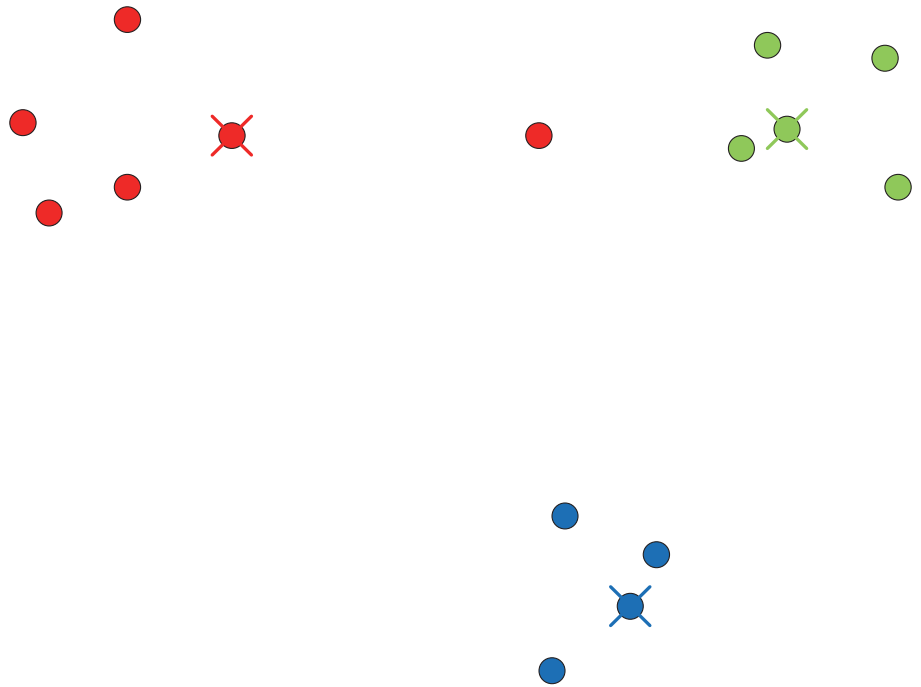
1: **Input**: $\{\mathbf{x}_j\}_{j=1}^{M}$, number of clusters K.
2: **Initialization**: obtain $\{\mathcal{C}_k\}_{k=1}^{K}$ by Algorithm 1.
3: **while** the clustering result does not converge **do**
4: $\quad$ {Center update}
5: $\quad$ {Cluster update}
6: **end while**
7: **Output**: $\{\mathcal{C}_k\}_{k=1}^{K}$.

Iteration one - center update illustration



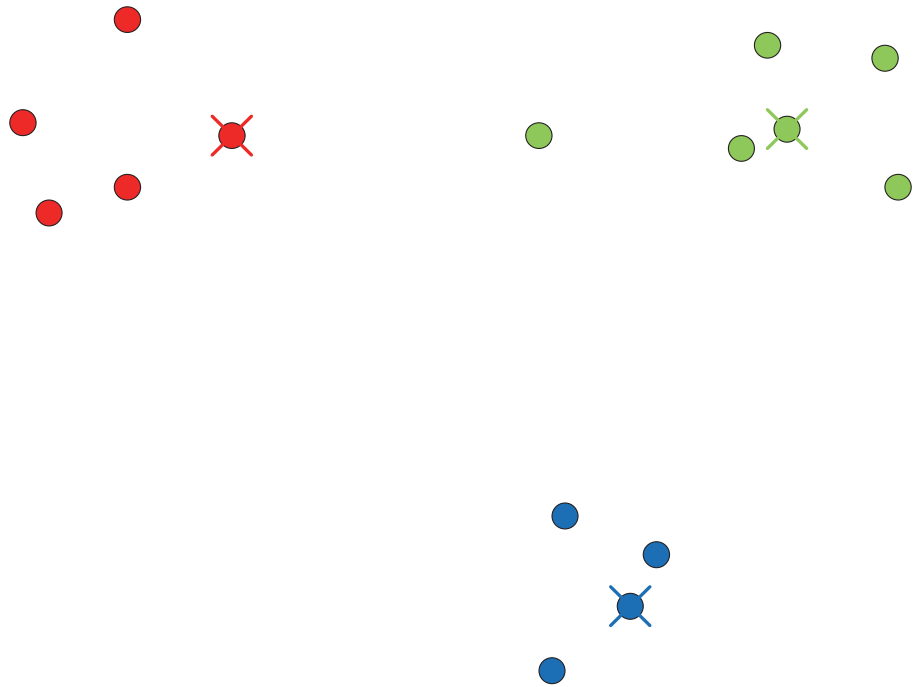
- Cost J_1^0

Iteration one - center update illustration cont.



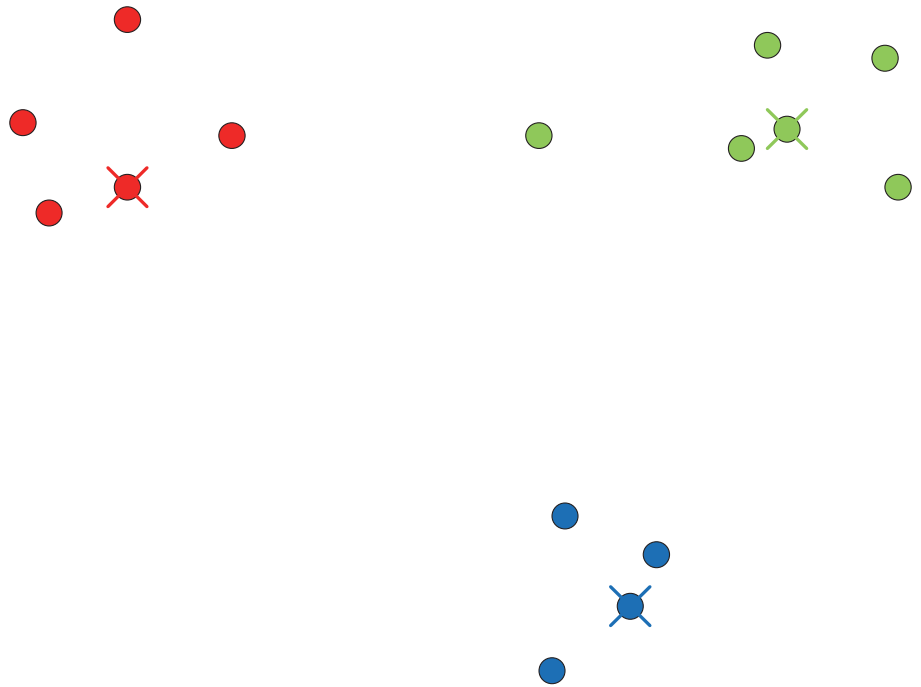
- Cost J_1^1 $(< J_1^0)$

Iteration one - cluster update illustration



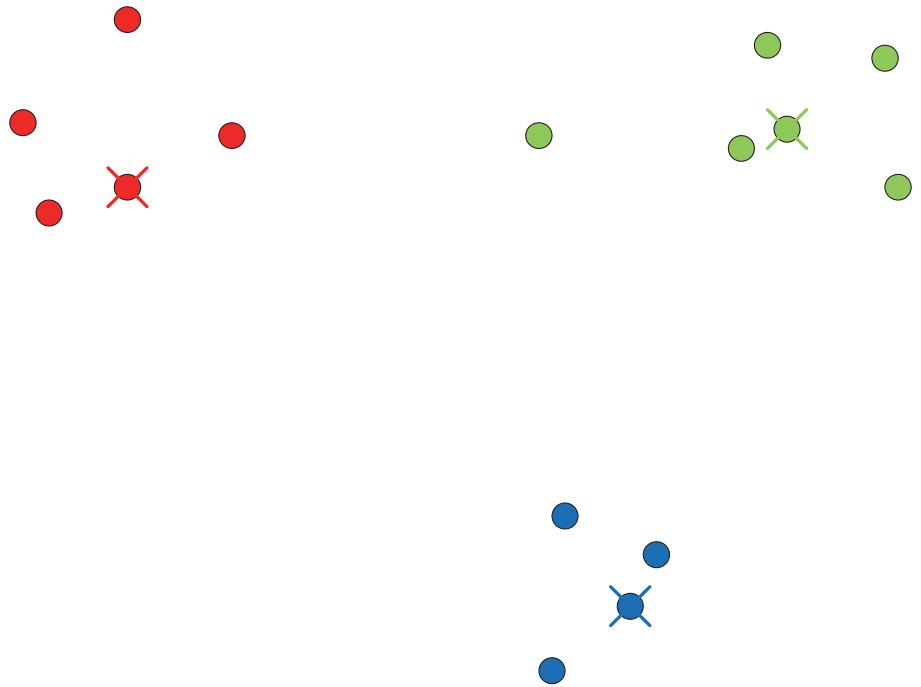
- Cost J_1^2 $(< J_1^1)$

Iteration two - center update illustration



- Cost J_1^3 $(< J_1^2)$

Iteration two - cluster update illustration



- Cost J_1^4 $(= J_1^3)$

Theoretical result - Algorithm 2

Theorem 1

Algorithm 2 converges after finite number of iterations and the error probability after T iterations is upper bounded by

$$P_e \leq 2M(K^2 + 3(T+1)(K-1)) \exp\Big(-\frac{nD_{KS}^2}{8}\Big).$$

Clustering without K

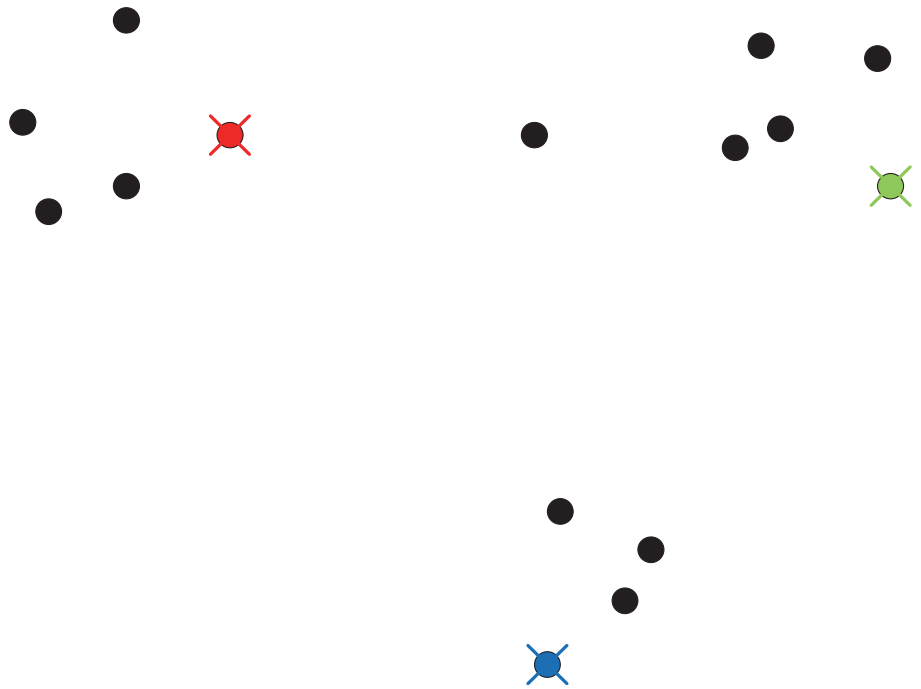
- Question: Is it possible to cluster with unknown K
  - Merge [Wang-etal 2018]
  - Split [Mora-López 2015]

Clustering without K - Merge

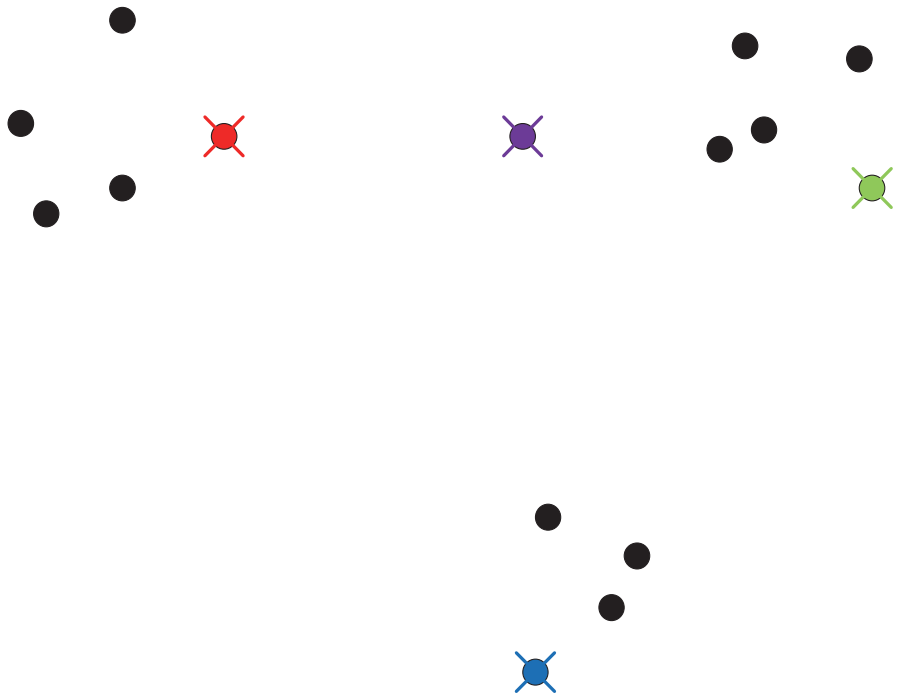
Algorithm 3 KS-based initialization with unknown K for composite distributions - merge

1: **Input**: $\{\mathbf{x}_j\}_{j=1}^{M}$.
2: $\{$Center initialization with threshold $d_{th}\}$
3: Clustering initialization specified in Algorithm 1.
4: **Output**: $\{\mathcal{C}_k\}_{k=1}^{\hat{K}}$.

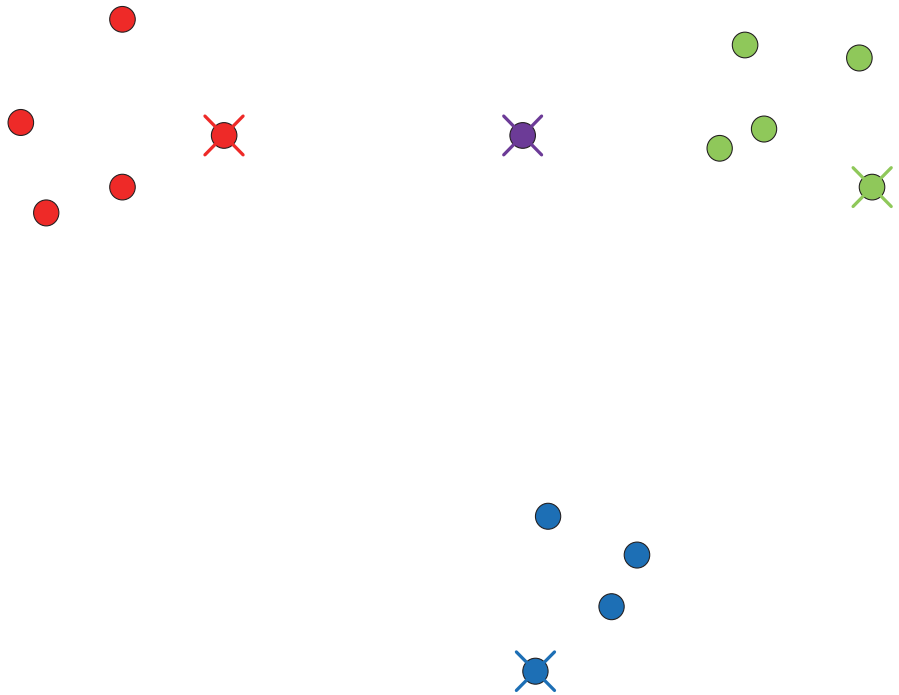
Center initialization illustration



Merge based - center initialization



Merge based - cluster initialization

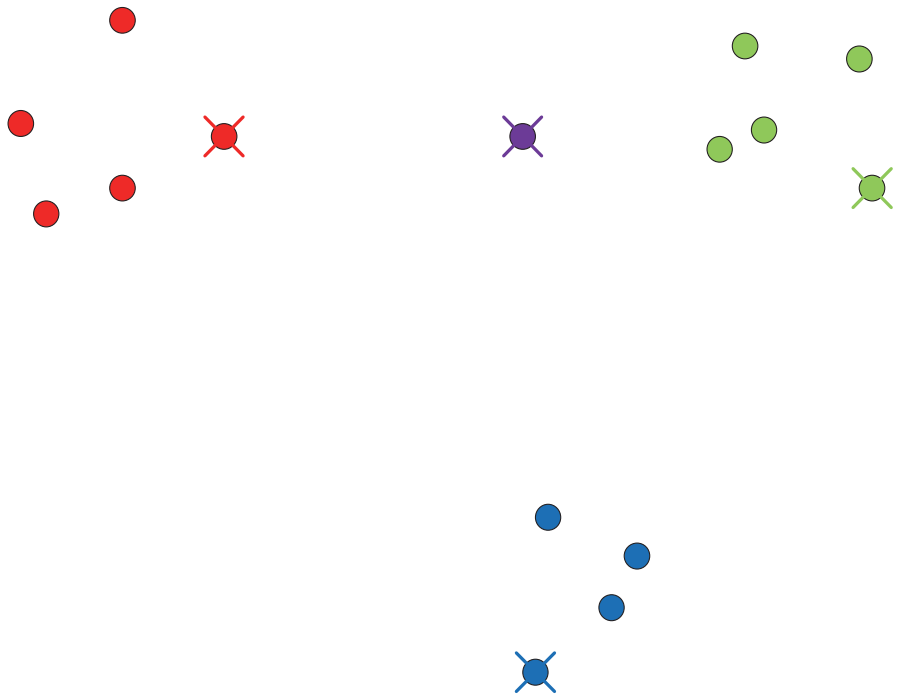


- Cost J_2^0

Algorithm 4 KS based clustering with unknown K for composite distributions - merge

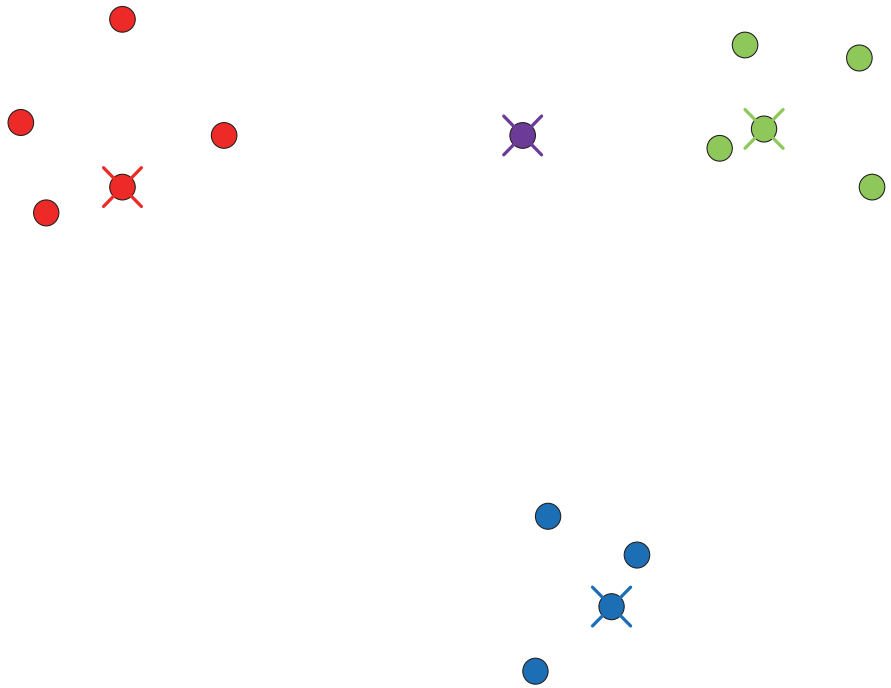
1: **Input**: $\{\mathbf{x}_j\}_{j=1}^{M}$.
2: **Initialization**: $\{\mathcal{C}_k\}_{k=1}^{\hat{K}}$ by Algorithm 3.
3: **while** the clustering result does not converge **do**
4: Center update specified in Algorithm 2.
5: {Merge Step with threshold d_{th}}
6: Cluster update specified in Algorithm 2.
7: **end while**
8: **Output**: Partition set $\{\mathcal{C}_k\}_{k=1}^{\hat{K}}$.

Merge based - center update



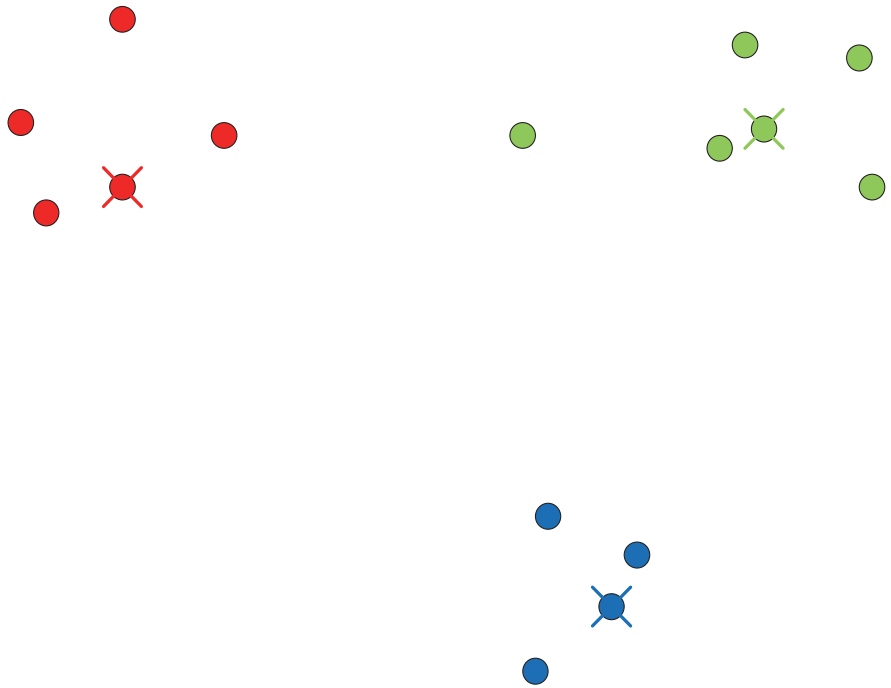
- Cost J_2^0

Merge based - center update cont



- Cost J_2^1 $(< J_2^0)$

Merge based - merge step



- Cost J_2^2

Theoretical result - Algorithm 4

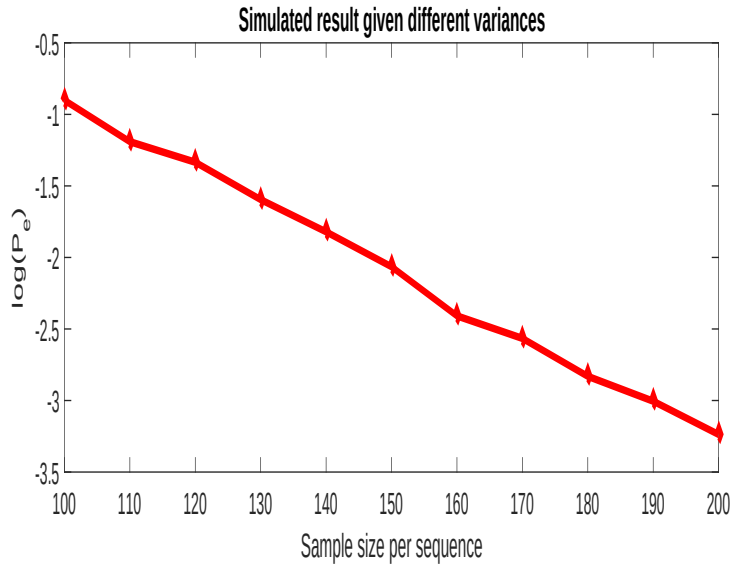
Theorem 2

Given $d_{th} = \frac{D_{KS}}{2}$, *Algorithm 3 and 4 converges after finite number of iterations and the probability of error is upper bounded by*

$$P_e \leq \left(4M^2(K+1) + 6M(K-1)(T+1) + 4TK^2\right) \exp\left(-\frac{nD_{KS}^2}{8}\right).$$

- $0 < D_{KS} \leq \min_{k \neq k'} d_{KS}(p_k, p_{k'})$

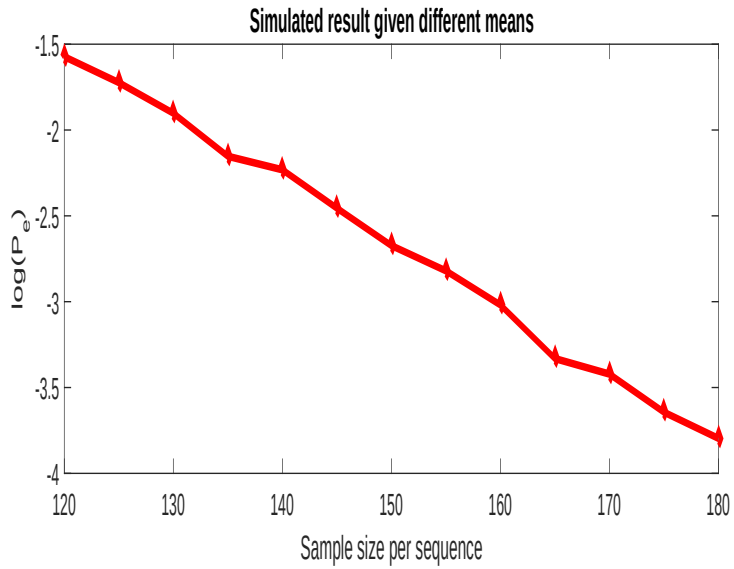
Numerical Result - Given K

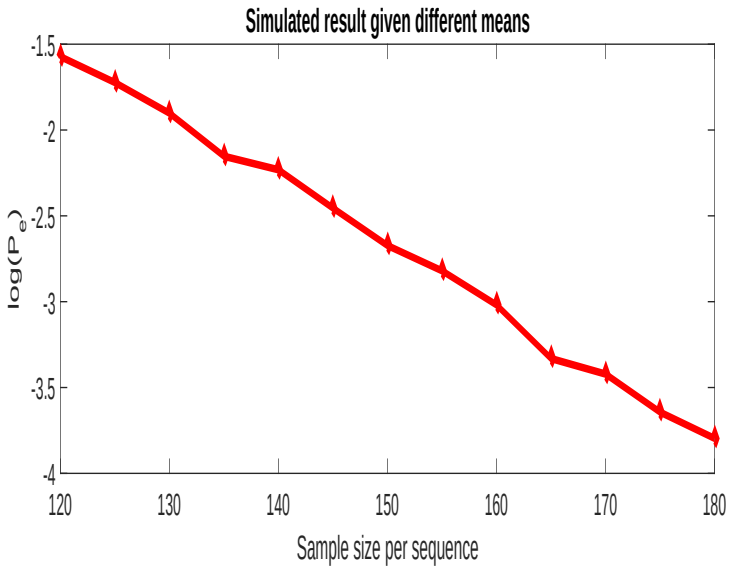


- $\mathbf{x}_j \sim \mathcal{N}(\mu, 1)$
- $\mu \in \{0, 1, 2, 3, 4\}$

- $\mathbf{x}_j \sim \mathcal{N}(0, \sigma^2)$
- $\sigma^2 \in \{1, 2, 4, 8, 16\}$

Numerical Result - Without K





- $\mathbf{x}_j \sim \mathcal{N}(\mu, 1)$
- $\mathbf{x}_j \sim \mathcal{N}(0, \sigma^2)$

Conclusion

- Clustering sequences generated by unknown continuous distributions.
  - Upper bound of P_e
  - Exponential consistency of P_e