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Distributed k-Means

Implementation and performance analysis of distributed K-Means clustering algorithms

F. Bezzi, W. Conte, E. D'Amore, G. Gasparotto

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k-Means Clustering Objective

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k-**Means problem** $\rightarrow$ find set of cluster centers C with $|C| = k$ that minimizes the **clustering cost** $\phi_X(C)$:

$$\min_C \sum_{x \in \mathcal{X}} \|f(C, x) - x\|^2,$$

where $f(C, x)$ returns the nearest cluster center in C to point x, using Euclidean distance.

Cost Function and Centroids

Let $\mathcal{X} = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$ be the dataset and $C = \{c_1, \dots, c_k\} \subset \mathbb{R}^d$ the set of centers.

Centroid of a set $Y \subseteq \mathcal{X}$ (subset of the dataset) is given by the mean across all points:

$$\texttt{centroid}(Y) = \frac{1}{|Y|} \sum_{y \in Y} y$$

Cost of Y w.r.t. C:

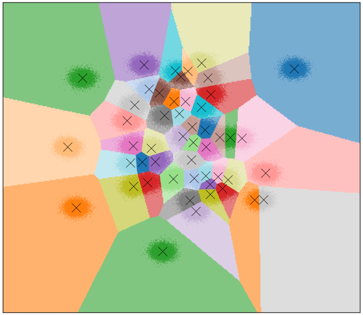
$$\phi_Y(C) = \sum_{y \in Y} \min_{c \in C} \|y - c\|^2$$

Lloyd's Iteration

Simplicity: start with a set of *randomly* chosen *initial centers*, repeatedly assign input points to nearest center, *recompute centers*.

Local search: Lloyd's iteration continues until convergence (early stopping).

Initialization: final solution is *locally optimal*. Better initialization algorithms get closer to *global optimum*.



Voronoi diagram of 2D-Gaussian Mixture synthetic dataset ($n = 10{,}000$ entries, $K = 50$ cluster centers, and variance $R = 100$). Labeling done using `KMeans` from `sklearn`.

k-Means++ Initialization

Algorithm: k-Means++ (k) Initialization

```
1. $C \leftarrow$ sample one point uniformly at random from $\mathcal{X}$
2. while $|C| < k$:
3.     Sample $x \in \mathcal{X}$ with probability $\frac{d^2(x,C)}{\phi_{\mathcal{X}}(C)}$
4.     $C \leftarrow C \cup \{x\}$
```

Algorithm is *sequential*

Computationally expensive depending on k: total running time $O(nkd)$.

k-Means$\|$ Initialization

Algorithm: k-Means$\|$ (k, ℓ) Initialization

```
1. $C \leftarrow$ sample one point uniformly at random from $\mathcal{X}$
2. $\psi \leftarrow \phi_{\mathcal{X}}(C)$
3. for $O(\log \psi)$ times:
4.     $C' \leftarrow$ sample $x \in \mathcal{X}$ independently with $p_x = \frac{\ell \cdot d^2(x, C)}{\phi_{\mathcal{X}}(C)}$
5.     $C \leftarrow C \cup C'$
6. For $x \in C$: assign weight $w_x$ as number of points in $\mathcal{X}$ closest to $x$
7. Recluster the weighted points in $C$ into $k$ clusters
```

Expected number of points in C is $\ell \log \psi$, typically more than k.

Mini-Batch k-Means Algorithm

Inputs: k, batch size b, iterations T, dataset $\mathcal{X}$
Steps:

```
1. Initialize $C$ (with $k$ random points from $\mathcal{X}$ or other init. algo.)
2. $\mathbf{v} \leftarrow \mathbf{0}$ (counts for updates)
3. for $t = 1$ to $T$:
    • Sample mini-batch $M \subset \mathcal{X}$ of size $b$
    • for $x \in M$:
        • Find closest center $c \in C$ and cache it
        • Update counts: $\mathbf{v}[c] \leftarrow \mathbf{v}[c] + 1$
    • for $c \in C$:
        • Learning rate: $\eta = \frac{1}{\mathbf{v}[c]}$
        • Update center: $c \leftarrow (1 - \eta)c + \eta x$
```

Avoids high *computational cost of full batch k-means* on large datasets.

Spark Overview

Spark Application:

- consists of a Driver program → runs user's main and executes parallel operations on a cluster.

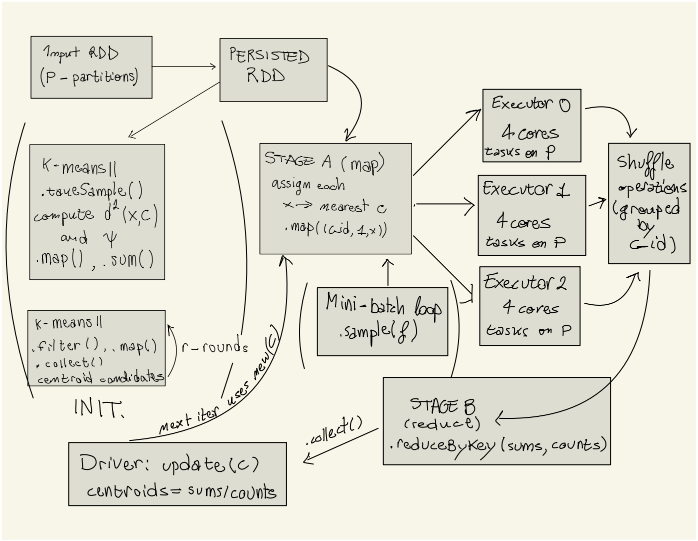
Cluster:

- 1 master, 3 workers, 4 CPU cores and 6.8 GiB RAM per worker.
- Driver runs in the notebook process and orchestrates jobs.

Resilient Distributed Dataset (RDD):

- Slice dataset in `P` partitions to be distributed across the cluster.
- Operate on by:
  transformations → create a new dataset.
  actions → return a value to the driver program after running a computation on the dataset.

Spark Overview



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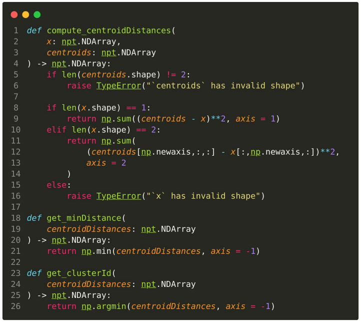
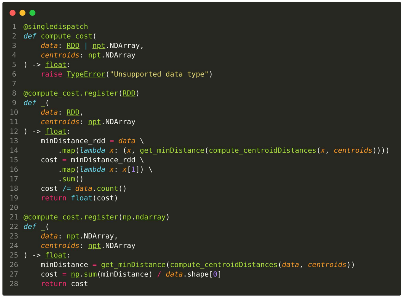
Basic functions



```python
def compute_centroidDistances(
    x: npt.NDArray,
    centroids: npt.NDArray
) -> npt.NDArray:
    if len(centroids.shape) != 2:
        raise TypeError("`centroids` has invalid shape")

    if len(x.shape) == 1:
        return np.sum((centroids - x)**2, axis = 1)
    elif len(x.shape) == 2:
        return np.sum(
            (centroids[np.newaxis,:,:] - x[:,np.newaxis,:])**2,
            axis = 2
        )
    else:
        raise TypeError("`x` has invalid shape")

def get_minDistance(
    centroidDistances: npt.NDArray
) -> npt.NDArray:
    return np.min(centroidDistances, axis = -1)

def get_clusterId(
    centroidDistances: npt.NDArray
) -> npt.NDArray:
    return np.argmin(centroidDistances, axis = -1)
```

- `compute_centroidDistances`: given data and centroids, for each point in data returns the distance to every centroid
- `get_minDistance`: given the distances to every centroid, returns the smallest one
- `get_clusterId`: given the distances to every centroid, returns the index of the smallest one, which is the corresponding `clusterId`

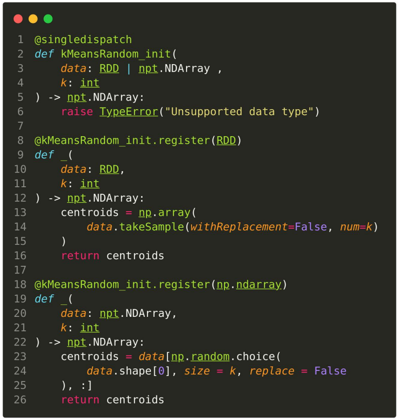
Basic functions



```python
@singledispatch
def compute_cost(
    data: RDD | npt.NDArray,
    centroids: npt.NDArray
) -> float:
    raise TypeError("Unsupported data type")

@compute_cost.register(RDD)
def _(
    data: RDD,
    centroids: npt.NDArray
) -> float:
    minDistance_rdd = data \
        .map(lambda x: (x, get_minDistance(compute_centroidDistances(x, centroids))))
    cost = minDistance_rdd \
        .map(lambda x: x[1]) \
        .sum()
    cost /= data.count()
    return float(cost)

@compute_cost.register(np.ndarray)
def _(
    data: npt.NDArray,
    centroids: npt.NDArray
) -> float:
    minDistance = get_minDistance(compute_centroidDistances(data, centroids))
    cost = np.sum(minDistance) / data.shape[0]
    return cost
```

- `cost` is computed as the sum of all the `minDistances`, normalized by the number of points

kMeansRandom



```python
@singledispatch
def kMeansRandom_init(
    data: RDD | npt.NDArray ,
    k: int
) -> npt.NDArray:
    raise TypeError("Unsupported data type")

@kMeansRandom_init.register(RDD)
def _(
    data: RDD,
    k: int
) -> npt.NDArray:
    centroids = np.array(
        data.takeSample(withReplacement=False, num=k)
    )
    return centroids

@kMeansRandom_init.register(np.ndarray)
def _(
    data: npt.NDArray,
    k: int
) -> npt.NDArray:
    centroids = data[np.random.choice(
        data.shape[0], size = k, replace = False
    ), :]
    return centroids
```

- simplest initialization algorithm: `centroids` are drawn uniformly at random from `data`
- parallel implementation: `takeSample` without replacement

kMeans++

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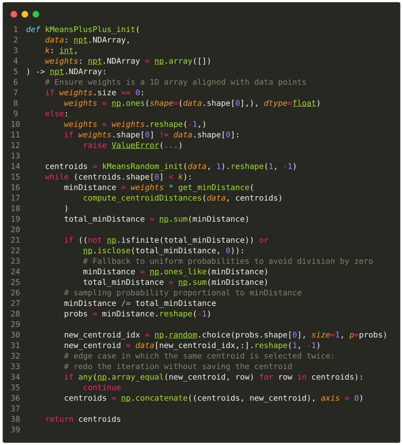
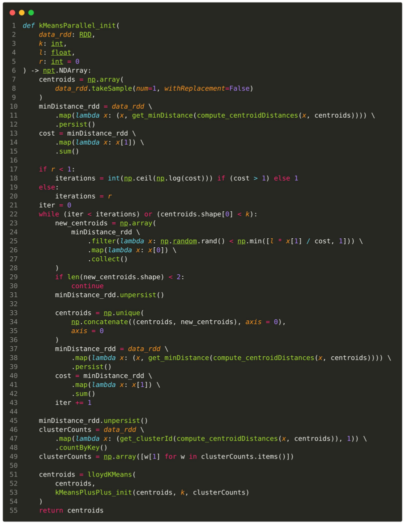


```python
def kMeansPlusPlus_init(
    data: npt.NDArray,
    k: int,
    weights: npt.NDArray = np.array([])
) -> npt.NDArray:
    # Ensure weights is a 1D array aligned with data points
    if weights.size == 0:
        weights = np.ones(shape=(data.shape[0],), dtype=float)
    else:
        weights = weights.reshape(-1,)
        if weights.shape[0] != data.shape[0]:
            raise ValueError(...)

    centroids = kMeansRandom_init(data, 1).reshape(1, -1)
    while (centroids.shape[0] < k):
        minDistance = weights * get_minDistance(
            compute_centroidDistances(data, centroids)
        )
        total_minDistance = np.sum(minDistance)

        if ((not np.isfinite(total_minDistance)) or
            np.isclose(total_minDistance, 0)):
            # Fallback to uniform probabilities to avoid division by zero
            minDistance = np.ones_like(minDistance)
            total_minDistance = np.sum(minDistance)
        # sampling probability proportional to minDistance
        minDistance /= total_minDistance
        probs = minDistance.reshape(-1)

        new_centroid_idx = np.random.choice(probs.shape[0], size=1, p=probs)
        new_centroid = data[new_centroid_idx,:].reshape(1, -1)
        # edge case in which the same centroid is selected twice:
        # redo the iteration without saving the centroid
        if any(np.array_equal(new_centroid, row) for row in centroids):
            continue
        centroids = np.concatenate((centroids, new_centroid), axis = 0)

    return centroids
```

- the sequential nature of the algorithm doesn't allow for a convenient parallel implementation
- variation with `weights`: each data point probability of being sampled is multiplied by its weight $\rightarrow$ used in `kMeans||`

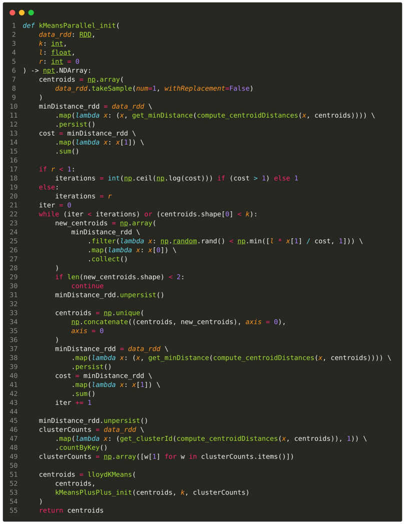
kMeans||



```python
def kMeansParallel_init(
    data_rdd: RDD,
    k: int,
    l: float,
    r: int = 0
) -> npt.NDArray:
    centroids = np.array(
        data_rdd.takeSample(num=1, withReplacement=False)
    )
    minDistance_rdd = data_rdd \
        .map(lambda x: (x, get_minDistance(compute_centroidDistances(x, centroids)))) \
        .persist()
    cost = minDistance_rdd \
        .map(lambda x: x[1]) \
        .sum()

    if r < 1:
        iterations = int(np.ceil(np.log(cost))) if (cost > 1) else 1
    else:
        iterations = r
    iter = 0
    while (iter < iterations) or (centroids.shape[0] < k):
        new_centroids = np.array(
            minDistance_rdd \
                .filter(lambda x: np.random.rand() < np.min([l * x[1] / cost, 1])) \
                .map(lambda x: x[0]) \
                .collect()
        )
        if len(new_centroids.shape) < 2:
            continue
        minDistance_rdd.unpersist()

        centroids = np.unique(
            np.concatenate((centroids, new_centroids), axis = 0),
            axis = 0
        )
        minDistance_rdd = data_rdd \
            .map(lambda x: (x, get_minDistance(compute_centroidDistances(x, centroids)))) \
            .persist()
        cost = minDistance_rdd \
            .map(lambda x: x[1]) \
            .sum()
        iter += 1

    minDistance_rdd.unpersist()
    clusterCounts = data_rdd \
        .map(lambda x: (get_clusterId(compute_centroidDistances(x, centroids)), 1)) \
        .countByKey()
    clusterCounts = np.array([w[1] for w in clusterCounts.items()])

    centroids = lloydKMeans(
        centroids,
        kMeansPlusPlus_init(centroids, k, clusterCounts)
    )
    return centroids
```

- designed with the MapReduce framework in mind: on each iteration multiple centroids are drawn independently
- `data_rdd` is an RDD where each row has a single element: a `np.ndarray`
    - benefits: more general approach to storage
    - downsides: executors require the `numpy` module to execute operations $\rightarrow$ compress and send virtual environment to executors

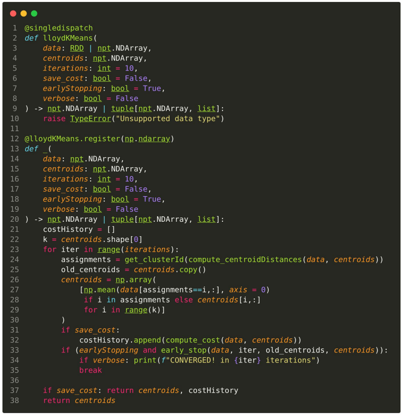
kMeans||



```python
def kMeansParallel_init(
    data_rdd: RDD,
    k: int,
    l: float,
    r: int = 0
) -> npt.NDArray:
    centroids = np.array(
        data_rdd.takeSample(num=1, withReplacement=False)
    )
    minDistance_rdd = data_rdd \
        .map(lambda x: (x, get_minDistance(compute_centroidDistances(x, centroids)))) \
        .persist()
    cost = minDistance_rdd \
        .map(lambda x: x[1]) \
        .sum()

    if r < 1:
        iterations = int(np.ceil(np.log(cost))) if (cost > 1) else 1
    else:
        iterations = r
    iter = 0
    while (iter < iterations) or (centroids.shape[0] < k):
        new_centroids = np.array(
            minDistance_rdd \
                .filter(lambda x: np.random.rand() < np.min([l * x[1] / cost, 1])) \
                .map(lambda x: x[0]) \
                .collect()
        )
        if len(new_centroids.shape) < 2:
            continue
        minDistance_rdd.unpersist()

        centroids = np.unique(
            np.concatenate((centroids, new_centroids), axis = 0),
            axis = 0
        )
        minDistance_rdd = data_rdd \
            .map(lambda x: (x, get_minDistance(compute_centroidDistances(x, centroids)))) \
            .persist()
        cost = minDistance_rdd \
            .map(lambda x: x[1]) \
            .sum()
        iter += 1

    minDistance_rdd.unpersist()
    clusterCounts = data_rdd \
        .map(lambda x: (get_clusterId(compute_centroidDistances(x, centroids)), 1)) \
        .countByKey()
    clusterCounts = np.array([w[1] for w in clusterCounts.items()])

    centroids = lloydKMeans(
        centroids,
        kMeansPlusPlus_init(centroids, k, clusterCounts)
    )
    return centroids
```

- `minDistance_rdd` gets cached as it is used for computing two different quantities during each iteration: `cost` and `new_centroids`
- `clusterCounts` represents the weight of each `centroid` (i.e. how many data points contains its cluster)

lloydKMeans



```python
@singledispatch
def lloydKMeans(
    data: RDD | npt.NDArray,
    centroids: npt.NDArray,
    iterations: int = 10,
    save_cost: bool = False,
    earlyStopping: bool = True,
    verbose: bool = False
) -> npt.NDArray | tuple[npt.NDArray, list]:
    raise TypeError("Unsupported data type")

@lloydKMeans.register(np.ndarray)
def _(
    data: npt.NDArray,
    centroids: npt.NDArray,
    iterations: int = 10,
    save_cost: bool = False,
    earlyStopping: bool = True,
    verbose: bool = False
) -> npt.NDArray | tuple[npt.NDArray, list]:
    costHistory = []
    k = centroids.shape[0]
    for iter in range(iterations):
        assignments = get_clusterId(compute_centroidDistances(data, centroids))
        old_centroids = centroids.copy()
        centroids = np.array(
            [np.mean(data[assignments==i,:], axis = 0)
             if i in assignments else centroids[i,:]
             for i in range(k)]
        )
        if save_cost:
            costHistory.append(compute_cost(data, centroids))
        if (earlyStopping and early_stop(data, iter, old_centroids, centroids)):
            if verbose: print(f"CONVERGED! in {iter} iterations")
            break

    if save_cost: return centroids, costHistory
    return centroids
```

- on each iteration all `data` points are considered in the update of the `centroids`
- `cost` monotonically decreases as iterations pass

lloydKMeans - Parallel implementation

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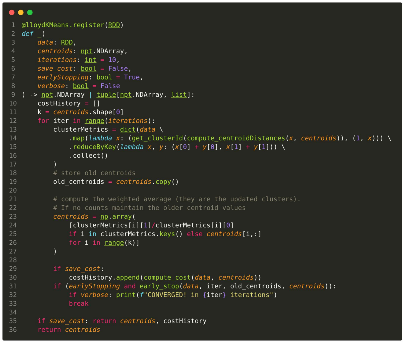
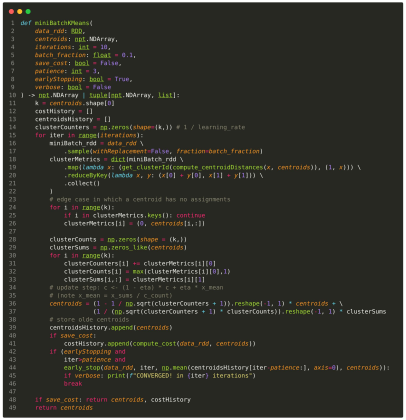


```python
@lloydKMeans.register(RDD)
def _(
    data: RDD,
    centroids: npt.NDArray,
    iterations: int = 10,
    save_cost: bool = False,
    earlyStopping: bool = True,
    verbose: bool = False
) -> npt.NDArray | tuple[npt.NDArray, list]:
    costHistory = []
    k = centroids.shape[0]
    for iter in range(iterations):
        clusterMetrics = dict(data \
            .map(lambda x: (get_clusterId(compute_centroidDistances(x, centroids)), (1, x))) \
            .reduceByKey(lambda x, y: (x[0] + y[0], x[1] + y[1])) \
            .collect()
        )
        # store old centroids
        old_centroids = centroids.copy()

        # compute the weighted average (they are the updated clusters).
        # If no counts maintain the older centroid values
        centroids = np.array(
            [clusterMetrics[i][1]/clusterMetrics[i][0]
            if i in clusterMetrics.keys() else centroids[i,:]
            for i in range(k)]
        )

        if save_cost:
            costHistory.append(compute_cost(data, centroids))
        if (earlyStopping and early_stop(data, iter, old_centroids, centroids)):
            if verbose: print(f"CONVERGED! in {iter} iterations")
            break

    if save_cost: return centroids, costHistory
    return centroids
```

- natural porting of the classic Lloyd's algorithm to the parallel framework
- `reduceByKey` allows the parallel computation of the new centroid

miniBatchKMeans



```python
def miniBatchKMeans(
    data_rdd: RDD,
    centroids: npt.NDArray,
    iterations: int = 10,
    batch_fraction: float = 0.1,
    save_cost: bool = False,
    patience: int = 3,
    earlyStopping: bool = True,
    verbose: bool = False
) -> npt.NDArray | tuple[npt.NDArray, list]:
    k = centroids.shape[0]
    costHistory = []
    centroidsHistory = []
    clusterCounters = np.zeros(shape=(k,)) # 1 / learning_rate
    for iter in range(iterations):
        miniBatch_rdd = data_rdd \
            .sample(withReplacement=False, fraction=batch_fraction)
        clusterMetrics = dict(miniBatch_rdd \
            .map(lambda x: (get_clusterId(compute_centroidDistances(x, centroids)), (1, x))) \
            .reduceByKey(lambda x, y: (x[0] + y[0], x[1] + y[1])) \
            .collect()
        )
        # edge case in which a centroid has no assignments
        for i in range(k):
            if i in clusterMetrics.keys(): continue
            clusterMetrics[i] = (0, centroids[i,:])

        clusterCounts = np.zeros(shape = (k,))
        clusterSums = np.zeros_like(centroids)
        for i in range(k):
            clusterCounters[i] += clusterMetrics[i][0]
            clusterCounts[i] = max(clusterMetrics[i][0],1)
            clusterSums[i,:] = clusterMetrics[i][1]
        # update step: c <- (1 - eta) * c + eta * x_mean
        # (note x_mean = x_sums / c_count)
        centroids = (1 - 1 / np.sqrt(clusterCounters + 1)).reshape(-1, 1) * centroids + \
                    (1 / (np.sqrt(clusterCounters + 1) * clusterCounts)).reshape(-1, 1) * clusterSums
        # store olde centroids
        centroidsHistory.append(centroids)
        if save_cost:
            costHistory.append(compute_cost(data_rdd, centroids))
        if (earlyStopping and
            iter>patience and
            early_stop(data_rdd, iter, np.mean(centroidsHistory[iter-patience:], axis=0), centroids)):
            if verbose: print(f"CONVERGED! in {iter} iterations")
            break

    if save_cost: return centroids, costHistory
    return centroids
```

- a fraction of the dataset is considered on each iteration
- learning rate shrinks as iterations pass
- our modification: $\eta \sim v^{-1/2}$ instead of $\eta \sim v^{-1}$. This leads to slower shrinking and, generally, improved learning (i.e. lower cost)

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Introduction to the initialization analysis

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The goal is to evaluate the performance of different initialization strategies in terms of **initialization time** and **clustering cost**:

- **Random**
- **k-Means++**
- **k-Means**$\|$ with $\ell \cdot k = 0.5$
- **k-Means**$\|$ with $\ell \cdot k = 2$

Each initialization is followed by Lloyd's iterations.

This setup evaluates whether the **parallelization** of **k-Means**$||$ improves clustering, using **Random** and **k-Means++** as baselines. We compare two metrics:

- **Execution time**: Initialization + Lloyd updates
- **Final cost**: $C = \frac{1}{|Y|} \sum_{y \in Y} \min_{i=1,\dots,k} \|y - c_i\|^2$

GaussianMixture dataset

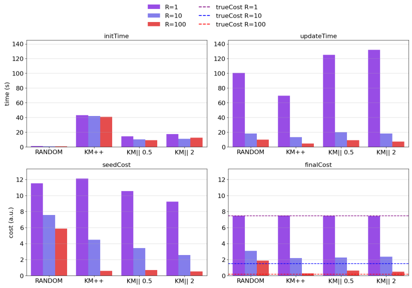
- Synthetic dataset
- k centers sampled from a 15-dimensional spherical Gaussian:

$$\mathcal{N}(0, R), \quad R \in \{1, 10, 100\}.$$

- Around each center, points are Normally distributed
- Result: a mixture of k spherical Gaussians with equal weights

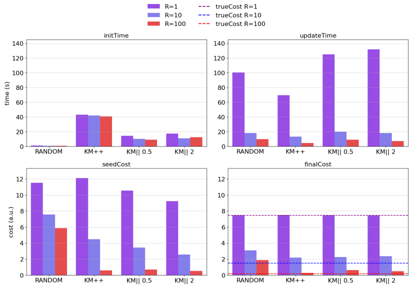
$\Longrightarrow$ Regular dataset with well separated clusters boundaries

Cost and Time analysis



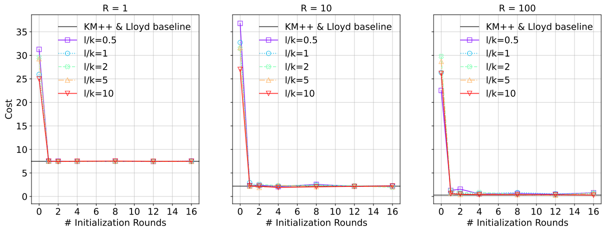
- **Random:** fastest initialization but with an high cost due to stochastic centroid selection
- **k-Means++:** achieves lower cost, but initialization is slower because of its sequential nature
- **k-Means**||: parallelization provides fast initialization and comparable or better cost

Cost and Time analysis: effect of R



- Higher R means that centers are farther apart and clusters are better separated $\Rightarrow$ clustering becomes easier: **lower seed and final costs** as R increases

Cost vs Rounds (GaussianMixture)



- Cost decreases rapidly within the first rounds ⇒ few iterations are sufficient to approach the baseline of k-Means++
- Larger oversampling ratio (ℓ/k) slightly improves centroid coverage

$\Longrightarrow$ **Parallelization is effective:** low and fast initialization cost, scalable for large datasets

KDDcup 1999 dataset (10%)

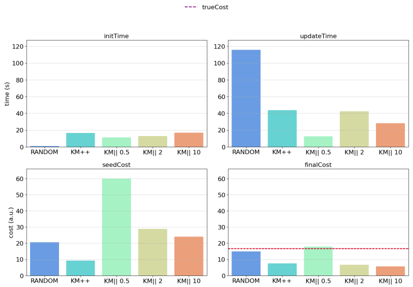
Now our goal is to demonstrate whether these improvements still hold on massive, real-world datasets.

KDDcup99:

- Real-world dataset for anomaly detection in network traffic
- Contains 5M records
- Each record: 41 features
- Clusters are not well-separated as before

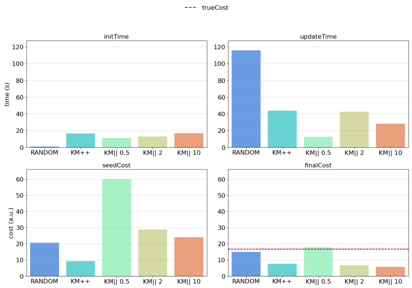
$\Longrightarrow$ Clustering is harder: noisy, heterogeneous, overlapping data

Seed and Final cost



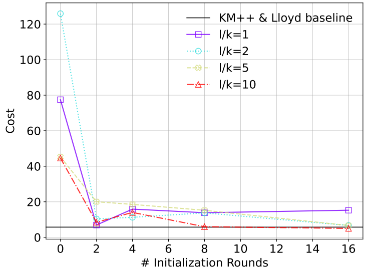
- **k-Means**$\|$: higher seed cost than **k-Means++**, but improves as ℓ/k increases (since we are sampling more points for each centroid k)
- Data heterogeneity makes it harder for parallel sampling to consistently capture the best centers
- All methods converge to similar final costs after Lloyd iterations

Initialization and update time



- **Init Time**:
  - **Random**: almost zero.
  - **k-Means++**: slowest
  - **k-Means||**: more time to sample as ℓ/k increases but better cost
- Lloyd iterations dominate the cost, so gains from faster initialization are less visible overall
- **k-Means||** offers a good balance between time and cost, scaling better than k-Means++

Cost vs Rounds



- The cost decreases sharply in the first rounds and quickly approaches the baseline
- Increasing ℓ/k improves stability but does not change the overall trend

Introduction to the update analysis

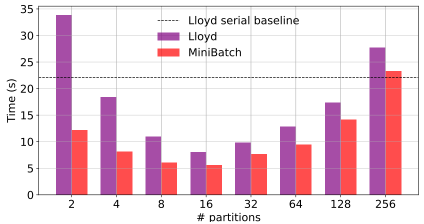
In the **“update”** analysis, we focus on two properties to evaluate algorithms:

- Execution time
- Iterations required to reach convergence

Why?

$\rightarrow$ **Time scaling with the number of partitions**
$\rightarrow$ **Convergence differences/similarities for each algorithm**

time vs $N_{partitions}$

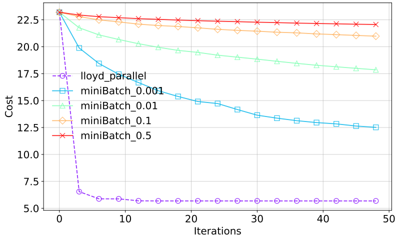


- Minibatch K-Means is **more efficient** than Lloyd-parallel.
- $N_{partitions} = 16$: $\rightarrow$ more than a $2\times$ speedup compared to Lloyd-serial.
- Choosing too many or too few $N_{partitions}$ $\rightarrow$ worse performance than Lloyd-serial.

Why this pattern?

- **Too few partitions:**
  - Large tasks, poor load balancing
  - Limited parallelism, resources underutilized
- **Too many partitions:**
  - Smaller tasks $\rightarrow$ proportionally higher **overhead**
  - Overhead sources: scheduling, communication, coordination
  - Overhead dominates computation

Cost vs iterations



- Lloyd-parallel converges “faster” in terms of iterations.
- Minibatch K-Means is slower and appears to approach different (and worse) “steady states”.
- For Minibatch K-Means, convergence improves when using smaller batch fractions.

$\rightarrow$ **Minibatch K-Means is more time efficient, but requires more iterations w.r.t. Lloyd-parallel**

Remark on Minibatch update

Looking at the centroids update formula for the Minibatch K-Means:

$$c_j^{(t+1)} = (1 - \eta_t)\, c_j^{(t)} + \eta_t\, \bar{x}_j^{(t)}$$

Where:

- η_t is the learning rate used for the update of centroid j at iteration t.
- η_t is proportional to $\left(N_j^{\text{samples}}\right)^{-\frac{1}{2}}$

Larger batch fractions $\rightarrow$ $\boldsymbol{\eta_t}$ drops close to zero more quickly.

$$\downarrow$$

Smaller centroid updates over time $\rightarrow$ slower convergence and poorer minimization of the cost function.

Final Remarks and further improvements

- Overall, the distributed versions of the algorithm are more efficient than the serial one when dealing with large datasets.
- There appears to be a tradeoff between time efficiency and cost minimization for both the initialization and update algorithms.
- Regarding initialization, it would be interesting to repeat the analysis with a dataset containing more centroids, in order to observe clearer performance improvements.
- With sufficient computing resources, an analysis on a larger dataset could also be valuable for the update step, where minibatch K-means generally outperformed the parallel version (assuming an appropriate number of partitions).