Breathing K-Means: Superior K-Means Solutions through Dynamic K-Values

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Abstract

We introduce the breathing k-means algorithm, which on average significantly improves solutions obtained by the widely-known greedy k-means++ algorithm, the default method for k-means clustering in the scikit-learn package. The improvements are achieved through a novel “breathing” technique, that cyclically increases and decreases the number of centroids based on local error and utility measures. We conducted experiments using greedy k-means++ as a baseline, comparing it with breathing k-means and five other k-means algorithms. Among the methods investigated, only breathing k-means and better k-means++ consistently outperformed the baseline, with breathing k-means demonstrating a substantial lead. This superior performance was maintained even when comparing the best result of ten runs for all other algorithms to a single run of breathing k-means, highlighting its effectiveness and speed. Our findings indicate that the breathing k-means algorithm outperforms the other k-means techniques, especially greedy k-means++ with ten repetitions, which it dominates in both solution quality and speed. This positions breathing k-means (with the built-in initialization by a single run of greedy k-means++) as a superior alternative to running greedy k-means++ on its own.

Keywords: k-means, k-means++, generalized Lloyd algorithm, clustering, vector quantization, scikit-learn

1. Introduction

This section defines the k-means problem and describes the classic Generalized Lloyd Algorithm (a.k.a. k-means algorithm), the k-means++ algorithm, and its widely-used variant, greedy k-means++.

1.1 The K-Means Problem

A common task in data analysis or compression is to describe an extensive data set consisting of numeric vectors by a smaller set of representative vectors, often called centroids. This task is known as the k-means problem.

We assume an integer $k$ and a set of $n$ data points $X \subset \mathbb{R}^d$. The k-means problem is to position a set $C = \{c_1, c_2, \ldots, c_k\}$ of $k$ $d$-dimensional centroids such that the error function

$$\phi(C, X) = \sum_{x \in X} \min_{c \in C} ||x - c||^2$$

(1)
is minimized. We will also refer to \( \phi(C, X) \) as Summed Squared Error or shortly SSE. In the context of vector quantization, the centroid set \( C \) is called a codebook, centroids are referred to as codebook vectors, and \( \phi(C, X) \) is denoted as quantization error.

For each centroid \( c_i \), one can determine its so-called Voronoi set, which is the set \( C_i \) of data points for which \( c_i \) is the nearest centroid:

\[
C_i = \{ x \in X | \| x - c_i \| < \| x - c_j \| \forall j \neq i \} \tag{2}
\]

A necessary but not sufficient condition for a solution \( C \) to be optimal is the fulfillment of the centroid condition: Each centroid \( c_i \in C \) must be the mean of its Voronoi set \( C_i \):

\[
c_i = \frac{1}{|C_i|} \sum_{x \in C_i} x \tag{3}
\]

While the term centroid typically refers to the mean of a Voronoi set, we will use it in this article to generally denote a codebook vector, even if is not yet the mean of its Voronoi set. We will also use the term codebook instead of centroid set for brevity.

Finding the optimal solution to the \( k \)-means problem is known to be NP-hard (Aloise et al., 2009). Therefore, approximation algorithms are used to find a solution with an SSE as low as possible.

Please note: In this article, we are not concerned with the general clustering problem or whether solutions to the \( k \)-means problem lead to “good” or even “correct” clusterings. We also do not require the data to fulfill any pre-conditions or criteria beyond the above definition of the \( k \)-means problem. We are exclusively interested in minimizing the SSE as defined in Equation (1) for a given data set \( X \) and a given value of \( k \).

1.2 The Generalized Lloyd Algorithm

The Generalized Lloyd Algorithm, proposed by Linde et al. (1980), is a multidimensional version of a scalar quantization method initially proposed by John Stuart Lloyd in a 1957 technical report and published 25 years later (Lloyd, 1982). It differs from the \( k \)-means algorithm proposed by MacQueen (1967) and described in Section 3.2.1. Despite common misconceptions, the Generalized Lloyd Algorithm is not synonymous with ‘the’ \( k \)-means algorithm, as several \( k \)-means algorithms exist.

Defined in Algorithm 1, the Generalized Lloyd Algorithm starts with the seeding step (the initial codebook choice), followed by repeated Lloyd iterations as long as the SSE decreases. Alternatively, it can stop when the relative SSE improvement falls below a certain threshold.

The algorithm is proven to converge in finite steps (Selim and Ismail, 1984), but solution quality can vary greatly depending on seeding. Hence, it is common to perform multiple runs with different seedings and select the best result (Fränti and Sieranoja, 2019).

1.3 \( K \)-Means++

Arthur and Vassilvitskii (2007) proposed \( k \)-means++, a specific way of seeding the generalized Lloyd algorithm. Centroids are sequentially added by randomly selecting
Algorithm 1: The Generalized Lloyd Algorithm

\[ \mathcal{X} = \{x_1, x_2, \ldots, x_n\}, x_i \in \mathbb{R}^d \] /* data set */

\[ \mathcal{C} = \{c_1, c_2, \ldots, c_k\}, c_i \in \mathbb{R}^d. \] /* seeding */

repeat /* Lloyd Iteration */

• Determine for each centroid \( c_i \) its Voronoi set \( C_i \).
  \[ C_i = \{ x \in \mathcal{X} | \| x - c_i \| < \| x - c_j \| \forall j \neq i \}, \forall i, i \in \{1, \ldots, k\} \]

• Move each centroid \( c_i \) to the center of gravity of its Voronoi set:
  \[ c_i = \frac{1}{|C_i|} \sum_{x \in C_i} x, \forall i \in \{1, \ldots, k\} \]

until \( C \) no longer changes

from the data set. The probability of a data point \( x \) to be selected is proportional to its quadratic distance to the nearest centroid already in the current codebook (see Algorithm 2).

Algorithm 2: \( K \)-means++

\[ \mathcal{X} = \{x_1, x_2, \ldots, x_n\}, x_i \in \mathbb{R}^d \] /* data set */

\[ \mathcal{C} = \{c_1\}, \text{ with } c_1 \text{ chosen at random from } \mathcal{X} \] /* start with one centroid */

repeat

• for each \( x \in \mathcal{X} \) let \( D(x) \) be the distance of \( x \) to the nearest centroid \( c \in \mathcal{C} \)

• Select a new centroid \( q \), choosing \( x \in \mathcal{X} \) with probability \( P(x) = \frac{D(x)^2}{\sum_{x \in \mathcal{X}} D(x)^2} \).

• \( \mathcal{C} = \mathcal{C} \cup \{q\} \) /* add \( q \) to the set of centroids */

until \( |\mathcal{C}| = k \)

\[ \mathcal{C} = \text{GLA}(\mathcal{C}, \mathcal{X}) \] /* apply the generalized Lloyd algorithm */

Arthur and Vassilvitskii (2007) proved the following theorem providing an upper bound for the expected error \( E[\phi] \) of a \( k\)-means++ seeding:

**Theorem.** For any set of data points, \( E[\phi] \leq 8(\log k + 2)\phi_{OPT} \)

Thereby, \( \phi_{OPT} \) is the error of the optimal solution. The theorem provides a significant theoretical improvement over random initialization, which lacks an upper bound for expected error. While seeding is only the algorithm’s initial phase, subsequent Lloyd iterations often lead to substantial error reduction. Yet, there is a lack of theoretical evidence quantifying the expected error reduction during this post-seeding phase.

### 1.4 Greedy \( K \)-Means++

Greedy \( k\)-means++, a variant of \( k\)-means++ introduced by Arthur and Vassilvitskii (2007), draws multiple centroid candidates in each step, choosing the one that maximizes overall error reduction. This reduces the chance of two closely located centroids, which could limit error reduction. Despite reporting improved solution quality, the \( O(\log k) \) approximation no longer holds, as confirmed by Bhattacharya et al. (2020).
The Python library, scikit-learn, uses greedy \textit{k-means++} as its default seeding method, making it the most commonly used seeding approach. It served as our baseline for experimental evaluations. The default number of candidates drawn per step in scikit-learn is \( n_{\text{local trials}} = 2 + \lfloor \log(k) \rfloor \), resulting for example in 4 for \( k = 10 \), 6 for \( k = 100 \), and 8 for \( k = 1000 \).

2. Breathing \( K \)-Means

In this section, we motivate and define the core components of the proposed approach before presenting the complete algorithm.

2.1 Algorithm Outline

The \textit{generalized Lloyd algorithm} is deterministic and only performs local movements of its centroids (by moving them to the center of gravity of their associated data points). This makes this approach very dependent on the initial seeding. To overcome this locality, we added so-called "breathing cycles" consisting of the following steps which are executed after one initial execution of the \textit{generalized Lloyd algorithm}:

1. Insert \( m \) additional centroids ("breathe in").
2. Run the \textit{generalized Lloyd algorithm} on the resulting enlarged codebook of size \( k + m \).
3. Delete \( m \) centroids ("breathe out").
4. Run the \textit{generalized Lloyd algorithm} on the resulting codebook of size \( k \).

The purpose of a breathing cycle is to position the \( m \) additional centroids to minimize the SSE, and subsequently remove \( m \) centroids without significantly increasing the SSE thus leading to an improved solution with \( k \) centroids. Usually, the removed centroids differ from the added ones, effectively leading to non-local movements of the centroids.

Because of the periodic changes in codebook size, we refer to the new algorithm as "\textit{breathing k-means}.” Several questions must be addressed to complete the description of the approach, which are covered in the following sections:

- Where should new centroids be inserted during the “breathe in” step?
- Which centroids should be deleted in the “breathe out” step?
- When should the algorithm terminate?

2.2 Breathe In: Adding Centroids Based on High Error

An established strategy (Fritzke, 1993, 1995) for minimizing error, regardless of the underlying data distribution, involves adding new centroids near those generating significant errors in quantizing their Voronoi sets. Let us denote with \( d(x, \mathcal{C}) \) the \textit{quantization error} made for data point \( x \) using the codebook \( \mathcal{C} \), i.e., the squared distance between \( x \) and the nearest centroid in \( \mathcal{C} \), defined as
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\[ d(x, \mathcal{C}) = \min_{c_i \in \mathcal{C}} \|x - c_i\|^2. \]

Given a codebook \( \mathcal{C} \) and a data set \( \mathcal{X} \), we define for each centroid \( c_i \in \mathcal{C} \) its associated error \( \phi(c_i) \) as

\[ \phi(c_i) = \sum_{x \in C_i} d(x, \mathcal{C}), \quad (4) \]

which is the sum of all \( d(x, \mathcal{C}) \)-values over its Voronoi set \( C_i \) (defined in Equation 2).

We can now define the set of those \( m \) centroids, which will serve as anchors for placing new centroids as

\[ \mathcal{M} = \text{(the } m \text{ centroids with the largest associated error } \phi(c)) \quad (5) \]

One new centroid will be inserted near the position of each centroid in \( \mathcal{M} \), modified by adding a small random offset vector \( v \) to ensure distinct centroid values. To be independent of the scaling of the data, we set the length of these offset vectors proportional to the root-mean-square error \( \text{RMSE}(\mathcal{C}, \mathcal{X}) \), defined as

\[ \text{RMSE}(\mathcal{C}, \mathcal{X}) = \sqrt{\phi(\mathcal{C}, \mathcal{X})/|\mathcal{X}|}. \]

Accordingly, we compute each offset vector \( v \) as

\[ v = \epsilon \text{RMSE}(\mathcal{C}, \mathcal{X}) u \quad (6) \]

with a small constant \( \epsilon \) and a random vector \( u \) drawn uniformly from the \( d \)-dimensional unit hypercube centered at the origin. This leads to the following set \( \mathcal{D}^+ \) of new centroids

\[ \mathcal{D}^+ = \{c + v | c \in \mathcal{M}\} \text{ with each } v \text{ being an offset vector according to (6).} \quad (7) \]

The set \( \mathcal{D}^+ \) is added to the current codebook to finalize the “breathe in” step:

\[ \mathcal{C} \leftarrow \mathcal{C} \cup \mathcal{D}^+ \quad (8) \]

2.3 Breathe Out: Removing Centroids Based on Low Utility

Removing centroids inevitably increases the SSE. To minimize this effect, we select for removal the \( m \) centroids causing the smallest error increase. Fortunately, the subsequent run of the generalized Lloyd algorithm will lower the resulting SSE again to some degree. Following Fritzke (1997), we define the Utility \( U(c_i) \) of a given centroid \( c_i \) as

\[ U(c_i) = \phi(\mathcal{C} \setminus \{c_i\}, \mathcal{X}) - \phi(\mathcal{C}, \mathcal{X}). \quad (9) \]

The utility measures the increase in the overall error caused by removing \( c_i \) from the original codebook \( \mathcal{C} \). If this difference is significant, then \( c_i \) is considered useful.

Using the definition of \( \phi(\mathcal{C}, \mathcal{X}) \) in Eq. (1), the utility of a centroid \( c_i \) can be expressed as
\[
U(c_i) = \sum_{x \in \mathcal{X}} d(x, \mathcal{C} \setminus \{c_i\}) - d(x, \mathcal{C})
\]

\[
= \sum_{x \in C_i} d(x, \mathcal{C} \setminus \{c_i\}) - d(x, \mathcal{C}) + \sum_{x \notin C_i} \underbrace{d(x, \mathcal{C} \setminus \{c_i\}) - d(x, \mathcal{C})}_{0}
\]

\[
= \sum_{x \in C_i} d(x, \mathcal{C} \setminus \{c_i\}) - d(x, \mathcal{C}). 
\] (10)

The second sum in Equation (10) contains only zero summands since for any \(x\) outside the Voronoi region \(C_i\) the following holds (and makes the terms in the second sum to be zero):

\[
\forall_{x \notin C_i} \exists_{j, j \neq i} : x \in C_j \land d(x, \mathcal{C} \setminus \{c_i\}) = \|x - c_j\| = d(x, \mathcal{C}).
\]

Thus, the utility \(U(c_i)\) of a centroid \(c_i\) only depends on the data points in its Voronoi set \(C_i\). Moreover, the utility is always non-negative. This follows from the fact that the expression \(d(x, \mathcal{C} \setminus \{c_i\}) - d(x, \mathcal{C})\) inside the sum in Equation (11) is non-negative since \(d(x, \mathcal{C} \setminus \{c_i\}) \geq d(x, \mathcal{C})\).

This expression inside the sum in Equation (11) can be denoted as the utility \(U_x(c_i)\) of the centroid \(c_i\) for a particular data point \(x \in \mathcal{X}\):

\[
U_x(c_i) = d(x, \mathcal{C} \setminus \{c_i\}) - d(x, \mathcal{C})
\]

The overall utility can now be expressed as the sum of the utilities of the individual data points in the Voronoi region of \(c_i\):

\[
U(c_i) = \sum_{x \in C_i} U_x(c_i)
\]

The utility of a centroid, \(U_x(c_i)\), only becomes zero when another centroid, \(c_j\), is at the same distance from \(x\). This happens when \(x\) lies on the so-called bisecting normal hyperplane of \(c_i\) and \(c_j\), an event with practically zero probability assuming random positions of \(X\) and \(C\). Similarly, the complete utility of a centroid \(c_i\), \(U(c_i)\), becomes zero only when all its associated data points lie on bisecting hyperplanes, another event of virtually zero probability. Figure 1 illustrates the error and utility values for a simple \(k\text{-means}\) problem.

To reduce the codebook back to its original size, one might consider deleting the \(m\) centroids with the lowest utility values. However, there is a fundamental flaw in this approach: If the distance between two centroids, \(c_i\) and \(c_j\), is small, also their utility values \(U(c_i)\) and \(U(c_j)\) are small because they mutually act as the second-nearest centroid for their Voronoi sets (see below). Both seem rather "useless." However, removing both \(c_i\) and \(c_j\) can lead to a colossal error increase, as becomes evident further below.
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Figure 1: Error and utility values are shown for a problem with data from six equal Gaussian kernels and \( k = 6 \), each centroid placed at a cluster center. While error values are similar, the utilities of centroids differ based on the distance between the nearest and second-nearest centroids. The most useful centroid is in cluster A, while the least useful is in cluster D, followed by those in B and C.

Let us first calculate what happens to the utility values of two centroids approaching each other:

\[
\lim_{c_i \to c_j} U(c_i) = \lim_{c_i \to c_j} \sum_{x \in C_i} \frac{d(x, C \setminus \{c_i\}) - d(x, C)}{\|x - c_j\|_2} \|x - c_i\|_2 \\
\leq \lim_{c_i \to c_j} \sum_{x \in C_i} \|x - c_j\|^2 - \|x - c_i\|^2 \\
= 0 \quad \text{for all } c_i, c_j \in C, i \neq j
\]

Since also \( U(c_i) \geq 0 \) holds and because of symmetry reasons, the following is fulfilled:

\[
\lim_{c_i \to c_j} U(c_i) = \lim_{c_j \to c_i} U(c_j) = 0 \quad \text{for all } c_i, c_j \in C, i \neq j
\]

As centroids move closer, their utility values decrease and become zero if they are identical, as they can perfectly substitute for each other in quantizing data points. However, removing such neighboring centroids because of low utility can drastically increase error, especially if the next nearest centroid is far away (see Figure 2). This often occurs in datasets with isolated smaller clusters, where data points from these close centroids are quantized by a distant centroid, leading to substantial error. To counter this, we introduce a "freezing" mechanism to prevent the concurrent removal of neighboring centroids.
2.4 Freezing The Nearest Neighbors

How can we avoid a significant error increase in the “Breathe out” step because of the removal of neighboring centroids? One possible solution would be to remove one centroid at a time, run the generalized Lloyd algorithm, recompute the utility, remove the next centroid, and so on. This strategy avoids large error increases, though it may come at the cost of high computational demands due to the many required runs of the generalized Lloyd algorithm.

To enable the simultaneous removal of multiple centroids, we take the following approach:

1. Initialize empty sets for ”frozen” centroids ($\mathcal{F}$) and centroids to be removed ($\mathcal{D}^-$).
2. Rank the centroids by increasing utility.
3. Scan through the centroids; skip ”frozen” ones. Add the first non-frozen centroid to $\mathcal{D}^-$. 
4. After selecting a centroid for removal, add its nearest neighbor to $\mathcal{F}$ (i.e., ”freeze” it).
5. Repeat steps 3 and 4 until $|\mathcal{D}^-|$ equals $m$.

One can construct cases where the above procedure would deliver less than $m$ centroids to remove since too many have been “frozen.” To prevent this, we perform freezing (step 4) only as long as the following condition holds:

$$|\mathcal{F}| + m < |\mathcal{C}|.$$
Together with this condition, the above strategy effectively prevents the problematic case of concurrently removing two closely neighboring centroids.

2.5 Ensuring Termination

To define a termination criterion, we demand a decrease in error after each “breathe out” step (the error after a “breathe in” step is irrelevant because of the enlarged number of centroids). Moreover, we empirically found that once the error stops sinking for a given value of \( m \), additional breathing steps with reduced \( m \)-values can further lower the error.

The above results in the simple approach to guarantee termination shown in Algorithm 3: For each value of \( m \), breathing cycles are repeated as long as the error \( \phi \) strictly decreases.

\[
\text{Algorithm 3: Ensuring Termination}
\]

\[
m = m_0. \quad /\!* \text{initialize the breathing size} */!
\]

\[
\phi_{\text{best}} = \infty. \quad /\!* \text{initialize the error} */!
\]

\[
tol = (\text{small positive number, e.g., } 0.0001) \quad /\!* \text{tolerance for error decrease} */!
\]

\[
\text{repeat} \quad /\!* \text{breathing cycles} */!
\]

\[
\text{Perform one breathing cycle with the current } m.
\]

\[
\text{Compute current error } \phi.
\]

\[
\text{if } (\phi_{\text{best}} - \phi)/\phi_{\text{best}} > tol \text{ then} \quad /\!* \text{error improved sufficiently?} */!
\]

\[
\phi_{\text{best}} = \phi. \quad /\!* \text{update the best error} */!
\]

\[
\text{else}
\]

\[
m = m - 1. \quad /\!* \text{decrement breathing size} */!
\]

\[
\text{until } m = 0
\]

which each time requires finding a previously unseen solution. Since both \( m_0 \) and the number of partitions of the data into \( k \) Voronoi sets are finite and positive, termination occurs in finitely many steps.

2.6 The Breathing K-Means Algorithm in Pseudo-Code

The complete algorithm in pseudo-code is shown in Figure 4.

3. Related Work

The literature on algorithms for the \( k \)-means problem is vast and can not be fully surveyed here. In the following, we describe two relevant groups of approaches. The first group contains methods for finding a good seeding of the centroids before finally running the generalized Lloyd algorithm. The second group employs the generalized Lloyd algorithm also in intermediate phases or not at all.

3.1 Seeding Methods

Many methods proposed in the literature focus on finding a seeding used as a starting configuration for the generalized Lloyd algorithm. Here several relevant examples are described in the order they were historically developed.
Algorithm 4: The Breathing K-Means Algorithm

\[ X = \{x_1, x_2, \ldots, x_n\}, x_i \in \mathbb{R}^d; \] /* data set */
\[ m = m_0 \text{ (default: 5) } \] /* number of centroids to add and remove */
\[ k = k_0; \] /* the \( k \) in \( k \)-means */
\[ C = \text{result of greedy \( k \)-means++ without repetition} \] /* seeding */
\[ \text{tol} = \text{tol}_0 \text{ (default: 0.0001) } \] /* tolerance to declare convergence */
\[ \phi_{\text{best}} = \phi(C, X) \] /* store best error so far */
\[ C_{\text{best}} = C \] /* store best codebook so far */

repeat /* breathing cycles */
  breathe in
  (Compute error \( \phi(c) \) for each \( c \in C \)) /* see Eq.(4) */
  \( c_1, c_2, \ldots, c_m, \ldots, c_k = \text{partial_sort_by_error}(C, \text{“descending”}, m) \)
  /* first \( m \) centroids sorted */
  \( M = \{c_1, c_2, \ldots, c_m\} \) /* subset of \( m \) largest-error centroids */
  \( D^+ = \{c + v | c \in M\} \) with offset vectors \( v \) according to Eq. (6)
  \( C = C \cup D^+ \) /* insert \( m \) additional centroids ("breathe in") */
  \( C = \text{GLA}(C, X) \) /* run the generalized Lloyd algorithm */
  breathe out
  (Compute utility \( U(c) \) for each \( c \in C \)) /* see Eq.(9) */
  \( c_1, c_2, \ldots, c_{k+m} = \text{sort_by_utility}(C, \text{“ascending”}) \) /* sorted sequence */
  \( D^- = \emptyset \) /* initialize set of to-be-deleted centroids */
  \( F = \emptyset \) /* initialize set of frozen centroids */
  forall \( c \) in \( \{c_1, c_2, \ldots, c_{k+m}\} \) do
    if \( c \notin F \) then /* only remove un-frozen centroids */
      \( D^- = D^- \cup \{c\} \) /* add centroid to to-be-deleted set */
      if \( |F| + m < |C| \) then /* not yet too many centroids frozen */
        \( \hat{c} = \arg \min_{x \in C \setminus \{c\}} ||c - x|| \) /* find nearest neighbor \( \hat{c} \) of \( c \) */
        \( F = F \cup \{\hat{c}\} \) /* freeze nearest neighbor \( \hat{c} \) */
      if \( |D^-| = m \) then /* found \( m \) centroids to delete */
        break
    \( C = C \setminus D^- \) /* delete \( m \) centroids ("breathe out") */
    \( C = \text{GLA}(C, X) \) /* run the generalized Lloyd algorithm */
  possibly reduce “breathing depth”
  if \( (\phi_{\text{best}} - \phi(C, X))/\phi_{\text{best}} > \text{tol} \) then
    \( \phi_{\text{best}} = \phi(C, X) \) /* improvement: update best error */
    \( C_{\text{best}} = C \) /* update best codebook */
  else
    \( m = m - 1 \) /* no improvement: reduce "breathing depth" */
until \( m = 0 \)
return \( C_{\text{best}} \)
3.1.1 FORGY’S METHOD

Forgy (1965) randomly assigns each data point to a cluster and then calculates the centroids as the means of these clusters. Consequently, all centroids are typically very close together near the mean of the whole data set, and one can expect a large number of Lloyd iterations before convergence.

3.1.2 MACQUEEN’S FIRST METHOD

In his first method, MacQueen (1967) proposed using the first \( k \) elements of the data set \( X \) as initial centroids. A drawback of this method is that it may initialize all centroids to similar positions in the case of ordered data.

3.1.3 MACQUEEN’S SECOND METHOD

In his second (and more popular) method, MacQueen (1967) proposed to pick random elements from the data set \( X \). This avoids the possible problem of ordered data which his first method has. A drawback of this method is that it may initialize many centroids to similar positions, e.g., if the data set contains a large high-density cluster of data points and a smaller number of spaced-out data points.

3.1.4 MAXIMIN

In the Maximin method (Gonzalez, 1985), the first centroid \( c_1 \) is chosen arbitrarily. The \( i \)-th \( (i \in 2, 3, ..., k) \) centroid \( c_i \) is chosen to have the largest minimum distance to all previously selected centroids, i.e., \( c_1, c_2, ..., c_{i-1} \). The method can be seen as a deterministic ancestor of \( k\)-means++ (see sections 1.3 and 3.1.6) and avoids positioning centroids close to each other even if the data contains high-density clusters.

3.1.5 METHOD OF BRADLEY AND FAYYAD

Bradley and Fayyad (1998) proposed a method to efficiently produce an initial codebook for large data sets. Initially, \( J \) small random sub-samples \( S_i, i \in \{1, \ldots, J\} \) are drawn from the original data set \( C \), and the generalized Lloyd algorithm is performed on each of the sub-samples \( S_i \). Thereafter, the \( J \) solutions \( M_i, i \in \{1, \ldots, J\} \), are merged to a data set \( M \) of size \( J \times K \) on which the generalized Lloyd algorithm is run \( J \) times with the solutions \( M_i \) from the first step as seedings. From all obtained solutions in the second step, the one with the smallest SSE when encoding \( M \) is chosen.

3.1.6 K-MEANS++

The \( k\)-means++ algorithm (Arthur and Vassilvitskii, 2007) is described in detail in Section 1.3 and can be interpreted as a randomized version of the Maximin method (see Section 3.1.4) since it uses a point’s minimum distance to all previous centroids to set the probability of choosing this point as the next centroid.
3.1.7 Greedy K-Means++

Greedy $k$-means++ (Arthur and Vassilvitskii, 2007) differs from $k$-means++ by drawing several new centroid candidates in each step and selecting the one that maximally reduces the overall error (see Section 1.4). Greedy $k$-means++ is the default $k$-means method for the scikit-learn package (Pedregosa et al., 2011).

3.1.8 Better K-Means++

The “better” $k$-means++ variant (Lattanzi and Sohler, 2019) extends the $k$-means++ initialization by continuing to select centroid candidates beyond $k$ and possibly replacing existing centroids if there is an improvement (see Algorithm 5).

**Algorithm 5: Better K-Means++**

\[
\mathcal{X} = \{x_1, x_2, \ldots, x_n\}, x_i \in \mathbb{R}^d \quad /\!*\text{data set}*/\!
\]

Initialize codebook with $k$-means++: \( C = \{x_1, \ldots, x_k\}, x_i \in \mathcal{X} \)

repeat \( Z \) times
  - Select a new centroid candidate \( q \), choosing \( x \in \mathcal{X} \) with probability 
    \[
p(x) = \frac{D(x)^2}{\sum_{x \in \mathcal{X}} D(x)^2}\] 
    whereby \( D(x) \) denotes the distance from a data point \( x \) to the nearest centroid in \( C \). 
    \( D(x) = \min_{c \in C} \|x - c\| \)
  - Compute the minimal error \( \phi_{\text{min}} \) resulting from replacing one of the centroids in \( C \) with \( q \): 
    \[
    \phi_{\text{min}} = \min_{i \in \{1, \ldots, k\}} \phi(C \setminus \{c_i\} \cup \{q\})
    \]
  - if \( \phi_{\text{min}} < \phi(C, \mathcal{X}) \) then
    - Perform the replacement resulting in the minimal error \( \phi_{\text{min}} \)

return \( C_{\text{best}} \)

Lattanzi and Sohler (2019) proved the following theorem guaranteeing that with a sufficiently large computational budget (parameter \( Z \)), the expected cost of the solution produced by better $k$-means++ will be close to the optimal cost (within a constant factor).

**Theorem 1** Let \( P \subseteq \mathbb{R}^d \) be a set of points and \( C \) be the output of Algorithm 1 with \( Z \geq 100000k \log \log k \) then we have \( E[\text{cost}(P, C)] \in O(\text{cost}(P, C^*)) \), where \( C^* \) is the set of optimum centers. The algorithm’s running time is \( O(dnk^2 \log \log k) \).

3.2 Integrated Methods

The approaches described here have in common that they cannot be described as seeding methods for the generalized Lloyd algorithm. Rather, they perform various operations on the codebook (e.g., splitting, merging, adding, removing, or replacing centroids), and most of them alternate this with Lloyd iterations.

3.2.1 MacQueen’s K-Means

MacQueen (1967) proposed an algorithm he called $k$-means (thereby coining the term $k$-means) described as follows (excerpt from the article):

Informally, the $k$-means procedure consists of simply starting with \( k \) groups, each consisting of a single random point, and then adding each new point to the
group whose mean the new point is nearest. After a point is added to a group, the mean of that group is adjusted to take the new point into account. Thus at each stage, the $k$ means are, in fact, the means of the groups they represent (hence the term $k$-means).

This highly efficient algorithm recalculates the mean (centroid) by shifting towards the new point by $\frac{1}{n}$ of total distance upon adding the n-th point to a group. While the means situate at the gravity center of all nearest points when added, a full data sweep does not always ensure the centroid condition, implying each mean is not necessarily at the gravity center of its Voronoi set. As the centroid condition is key for optimality, additional Lloyd iterations often enhance MacQueen's $k$-means solutions, even if only towards a local optimum.

3.2.2 THE HARTIGAN-WONG ALGORITHM

The Hartigan-Wong Algorithm (Hartigan and Wong, 1979) skips Lloyd iterations. It starts by randomly choosing $k$ centroids, forming initial clusters using MacQueen's Second Method (Section 3.1.3). It then reassigns a random data point $x$ from its cluster $S$ to another cluster $T$ if it reduces the sum of intra-cluster variances of $S$ and $T$, choosing $T$ to maximize variance reduction. Termination occurs when no reassignment reduces overall variance (Algorithm 6).

Hartigan and Wong’s implementation introduces a Quick Transfer phase, where $T$ is the centroid second-nearest to $x$, reducing computation. This phase iterates until no improvement occurs. The Optimal Transfer phase, involving a complete search among all clusters (Algorithm 6), alternates with the Quick Transfer phase. Termination occurs when the Optimal Transfer phase finds no improvement.

This algorithm is the default $k$-means algorithm in the stats package of R (R Core Team, 2019). While Telgarsky and Vattani (2010) reported improvements over "online" $k$-means, we generally found better results with vanilla $k$-means++ and greedy $k$-means++ than Hartigan-Wong (see Table A.6).

3.2.3 LBG WITH BINARY SPLITTING

When the generalized Lloyd algorithm (a.k.a. LBG) was proposed by Linde et al. (1980), the authors also discussed a method to produce a series of increasingly large codebooks. In particular, given a codebook consisting of $m$ centroids, one can produce a codebook consisting of twice as many centroids by “splitting” each centroid, adding small offsets to enforce distinct values, and applying the generalized Lloyd algorithm to the resulting enlarged codebook. If one starts with a codebook of size one and performs $p$ splitting steps, the resulting codebook has the size $k = 2^p$. In each splitting step, all existing centroids are split. Thus, this method does not consider which centroids are most suited for splitting to reduce the overall error. This can limit the quality of the results compared to approaches splitting based on error reduction.

3.2.4 LBG-U

Fritzke (1997) proposed the LBG-U algorithm to improve the generalized Lloyd algorithm by non-local movements of centroids. Central to this approach is the concept of
Algorithm 6: Hartigan and Wong

\[ \mathcal{X} = \{x_1, x_2, \ldots, x_n\}, x_i \in \mathbb{R}^d \] /* data set */

Select \( k \) centroids \( c_1, c_2, \ldots, c_k \) randomly from \( \mathcal{X} \).

Form \( k \) clusters \( C_1, C_2, \ldots, C_k \) by assigning each \( x \in \mathcal{X} \) to its nearest centroid.

Recompute centroids \( c_1, c_2, \ldots, c_k \) as means of their associated clusters.

repeat

Select a data point \( x \in \mathcal{X} \).

Let \( S \in \{C_1, C_2, \ldots, C_k\}, T \neq S \) do

Compute the error improvement \( \Phi(x; S; T) \) of re-assigning \( x \) from \( S \) to \( T \)

taking into account the resulting centroid updates of \( S \) and \( T \).

\[ \Phi(x; S; T) = \frac{|S|}{|S|-1} \|\mu(S) - x\|^2 - \frac{|T|}{|T|+1} \|\mu(T) - x\|^2 \]

if \( \exists T \in \{C_1, C_2, \ldots, C_k\}, T \neq S \) \& \( \Phi(x; S; T) > 0 \) then

Re-assign \( x \) to cluster \( T \) with \( T = \arg \max_T \Phi(x; S; T) \).

until no error improvement for a complete sweep through all data points \( x \in \mathcal{X} \)

Utility (thus the “U” in the name) initially defined in that work and also used for breathing \( k\)-means (see Equation 9). The core mechanism of LBG-U is to repeatedly move the least useful centroid to the centroid with maximum error and perform the generalized Lloyd algorithm after each such move. LBG-U delivered better solutions than the generalized Lloyd algorithm (\( k\)-means++ was not yet invented) at the price of additional compute time. Lacking the idea of nearest neighbor freezing introduced in the current article, LBG-U could only insert and delete one centroid at a time which led to larger computational effort and smaller improvements than breathing \( k\)-means.

3.2.5 Splitting

This algorithm (Fränti et al., 1997) starts with a codebook of size one and iteratively enlarges the codebook by a splitting procedure until it reaches size \( k \). Different approaches for selecting the cluster to be split (largest variance, largest width, largest skewness) and for technically performing the splitting (fixed offset vector, random choice of new centroids, mutually furthest data points, local PCA) are discussed. Also the question of how to refine the partition of the data set and the centroids after the splitting is addressed.

3.2.6 Tabu Search

Fränti et al. (1998) proposed an algorithm adapted from a previous clustering method by Al-Sultan (1995). Tabu search generates new solution candidates through random operations, allowing for potentially worse solutions and possible cyclic behavior. To prevent non-termination, the algorithm employs a tabu list—a record of previously visited solutions that helps avoid considering them multiple times. For larger data sets, the exact recurrence of \( k\)-means solutions is rare. To exclude similar solutions as well, the authors propose checking candidates for a minimum distance from all tabu list elements using a suitable distance measure. Two methods for the randomized generation of new solutions are con-
sidered: (1) randomly assigning a fraction of the data set to different (but nearby) clusters and (2) adding noise to existing cluster centers.

3.2.7 Iterative Splitting and Merging

Kaukoranta et al. (1998) describe an iterative splitting and merging algorithm for vector quantization codebook generation. Repeatedly the following steps are performed: (1) a cluster is selected which is split. (2) Two clusters are selected which are merged. (3) Some Lloyd iterations are performed to refine the codebook. For (1) a local optimization strategy is applied where each cluster is tentatively split, and the one decreasing the distortion most is chosen. For (2) the pairwise nearest neighbor (PNN) approach as described by Equitz (1989) is employed. This approach determines the neighboring pair of clusters, \( m_c \) and \( C_k \), which least increases the overall error when merged. For (3) the authors suggest performing a fixed small number (e.g., 2) of Lloyd iterations.

This approach is somewhat similar to breathing k-means with breathing depth \( m = 1 \). Breathing k-means, however, avoids the effort to split each cluster by splitting only the cluster with the largest quantization error. Moreover, breathing k-means avoids the computation of many possible merges by always deleting the centroid with the smallest utility.

3.2.8 Bisecting K-Means

The bisecting k-means (Steinbach et al., 2000) has large similarities to the splitting method proposed by Fränti et al. (1997). It starts with one single cluster and iteratively “bisects” (i.e., “splits”) one of the present clusters into two by performing k-means with \( k = 2 \) on the selected cluster. This bisection step is repeated several times (say \( m \) times) with different random initializations before choosing the bisection with the lowest error. This is iterated until a predefined number of clusters is reached or the overall error falls below a threshold. Optionally, the generalized Lloyd algorithm can be applied to the resulting codebook after each bisecting step. If this optimization is not done, the algorithm produces a hierarchical clustering (obtained by considering all intermediate codebooks). To select the cluster to be split, Steinbach et al. (2000) propose to use either the size of the cluster or the SSE of the cluster as a criterion. In the latter case, there is a similarity to the error-based insertion proposed by Fritzke (1993, 1994).

3.2.9 Genetic Algorithm with Deterministic Cross-Over

Genetic algorithms typically make use of a condensed “genetic” representation of the candidate solutions. They do attempt to simulate natural evolution by employing concepts such as selection (survival of the fittest), cross-over (recombination of several different genetic representations), and mutation (random modifications of genetic representations). Here we consider the genetic algorithm described by Fränti (2000), which is specifically adapted to the problem of vector quantization.

The top-level algorithm is shown in Algorithm 7 and does not show any problem-specific properties apart from the use of the generalized Lloyd algorithm for fine-tuning. The problem-specific properties proposed by Fränti (2000) are the representation of a solution and the cross-over operation. Each solution is represented as a pair \((C, P)\) where \( C \) is a codebook, and \( P \) is a corresponding partition of the data set. Maintaining both types of
Algorithm 7: Genetic Algorithm

Generate S initial solutions.;
Sort the solutions by error.;
repeat T times /* T = number of generations */
  repeat S times /* S = number of individuals per generation */
    Select two solutions for cross-over.;
    Generate a new solution by crossing the selected solutions.;
    Optionally mutate the new solution.;
    Fine-tune the new solution by generalized Lloyd algorithm.;
  Sort the solutions by error.;
  Store the best solution.;
return best solution

Information makes it possible to perform the cross-over operation of two solutions \((C^1, P^1)\) and \((C^2, P^2)\) in a very effective and efficient way:

- A new codebook \(C^{\text{new}}\) is created as the union of \(C^1\) and \(C^2\):
  \[ C^{\text{new}} = C^1 \cup C^2. \]
- The partitions \(P^1\) and \(P^2\) are combined to form a new partition \(P^{\text{new}}\) by mapping each data point to its cluster from \(P^1\) or \(P^2\), depending on which corresponding centroid is closer.
- \(C^{\text{new}}\) is updated to contain the centroids of the clusters in \(P^{\text{new}}\).
- Empty clusters are removed from \(P^{\text{new}}\).
- The number of clusters in \(P^{\text{new}}\) is reduced to the desired number \(k\) of clusters by using the pairwise-nearest-neighbor (PNN) approach on \((C^{\text{new}}, P^{\text{new}})\). PNN is performed on the \(2 \times k\) (fewer if empty clusters were removed) centroids instead of the full data set. The partition is updated accordingly by combining merged clusters.

Mutation was considered but not performed in Fränti (2000) because of the concentration on efficiency.

3.2.10 Global K-Means

“Global k-means” (Likas et al., 2003) is a deterministic method that finds an approximate solution for a given k-means problem \((\mathcal{X}, k)\) by starting with the trivial solution for a codebook size of one. This solution is used to find a solution for codebook size two by combining the size-one solution sequentially with each element of the data set \(\mathcal{X}\) and running the generalized Lloyd algorithm starting from there. The best solution found is taken as the solution for size two. This is iterated for all codebook sizes until a solution for codebook size \(k\) is found. The algorithm requires \(k \times n\) runs of the generalized Lloyd algorithm leading to very high computation demand for data sets of non-trivial size.
3.2.11 Iterative Shrinking

Fränti and Virmajoki (2006) describe an iterative shrinking algorithm for vector quantization codebook generation. The method starts by assigning each data vector to its own cluster. This huge codebook is then stepwise reduced by deleting the single centroid leading to the smallest error increase. The major difference between the “shrinking” described in this algorithm and the “merging” described in Kaukoranta et al. (1998) (see section 3.2.7) is the following: During “shrinking,” a centroid $c_i$ is removed, and each associated data point $x \in C_i$ is assigned to the respective nearest other centroid $c \in C \setminus \{c_i\}$, whereas during “merging,” two neighboring clusters, $C_i$ and $C_k$ are combined into a new cluster $C_m$, i.e., all affected data points end up in the same cluster $C_m$ (before any further optimizations, e.g., Lloyd iterations, are done.).

3.2.12 Random Swap Clustering

Random swap clustering (Fränti, 2018) is based on the idea of repeatedly replacing a randomly chosen centroid $c \in C$ with a randomly chosen data vector $x \in X$. This operation, also called “swap,” is followed by a small number of Lloyd iterations. If the resulting error is lower than before the swap, the swap is “accepted,” and the algorithm continues. If the resulting error is higher than before the swap, the algorithm continues from the codebook state before the swap (basically ignoring the swap). The algorithm is shown in Algorithm 8. This number of required Lloyd operations after a swap operation can be reduced by locally repartitioning the data points associated with the deleted centroid and by specifically determining which data points will be assigned to the new centroid. This is merely an efficiency measure and is denoted as optional by Fränti (2018) if two or more Lloyd iterations are performed.

Algorithm 8: Random Swap Clustering

```
X = \{x_1, x_2, \ldots, x_n\}, x_i \in \mathbb{R}^d  \quad /* data set */
C = \{c_1, \ldots, c_k\}  \quad /* random seeding from X */
repeat Z times
    Randomly select a centroid $c, c \in C$.
    Randomly select a data vector $x \in X$.
    $C_{new} = C \cup \{x\} \setminus \{c\}  \quad /* replace c with x */
    Optional: Locally repartition data points.  \quad /* see text */
    Perform a few Lloyd iterations on $C_{new}$.
    if $\phi(C_{new}, X) < \phi(C, X)  \quad /* is the new codebook better? */$
    then
        $C = C_{new}  \quad /* Accept the new codebook. */$
return C
```

3.2.13 Improvement by Multiple Runs

A general method to improve results for any randomized algorithm is selecting the best result from multiple repeated runs (Fränti and Sieranoja, 2019). The improvements obtained
depend on the variance of the results produced by the algorithm at hand. The required amount of computation is proportional to the number of repetitions.

4. Algorithms Selected for Comparison

The following algorithms were selected as contenders for breathing \( k \)-means (a brief reasoning is given for the inclusion of each approach):

**greedy \( k \)-means++**
(see Section 1.4). This method was selected as the baseline algorithm for all other methods since it probably is the most widely-used algorithm for \( k \)-means because of being the default \( k \)-means method in the popular scikit-learn package (Pedregosa et al., 2011). The implementation is the class \texttt{KMeans} of \texttt{scikit-learn}. Sources: \url{https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html}

**vanilla \( k \)-means++**
(see Section 1.3). The original (non-greedy) variant of \( k \)-means++. For this method, an \( O(\log k) \) upper bound was proven. The implementation stems from the \texttt{scikit-learn} package (Pedregosa et al., 2011), in particular from the function \texttt{kmeans++} with default parameters, except for setting \texttt{n_local_trials=1}. Sources: \url{https://scikit-learn.org/stable/modules/generated/sklearn.cluster.kmeans++.html}

**better \( k \)-means++**
(see Section 3.1.8). A modification of \( k \)-means++ that was selected after being independently suggested by two reviewers. The algorithm was implemented by the author in Python since no open-source (or other) implementation could be found. The parameter \( Z \) for the number of additional centroid selections was set to 25, following the experiments described in the original paper of Lattanzi and Sohler (2019).

**Hartigan-Wong**
(see Section 3.2.2). This method was selected since it is the default \( k \)-means algorithm in the \texttt{stats} package of the R programming language (\{R Core Team\} 2019). The approach is special since it does not rely on the Generalized Lloyd Algorithm. Parameter settings: \texttt{iter.max=500, nstart=1, algorithm="Hartigan-Wong"}. Implementation: Fortran code from the \texttt{stats} package of R. Sources: \url{https://cloud.r-project.org}

**genetic algorithm**
(see Section 3.2.9). We included this approach following a reviewer’s suggestion and promising results in a pre-study. The implementation used is part of a C-Package published on github by the authors of the original publication (Fränti, 2000). The default parameters defined by the package were used in the experiments. Sources: \url{https://github.com/uef-machine-learning/CBModules}

**random swap**
(see Section 3.2.12). We included this approach following a reviewer’s suggestion and
promising results in a pre-study. The implementation used is part of a C-Package published on github by the authors of the original publication (Fränti, 2018). The default parameters defined by the package were used in the experiments. Sources: https://github.com/uef-machine-learning/CBModules

5. Empirical Results

We first list the algorithms selected for comparison with breathing k-means. Then, the k-means problems used for the experiments are described. Finally, the empirical results are presented.

5.1 K-Means Problems Investigated

We used four groups of two-dimensional problems (9 problems per group) and one group of high-dimensional problems (15 members) for a total of 51 k-means problems. These groups were selected to showcase the algorithms’ strengths and weaknesses. The problems included varied point densities, reflecting the diversity of real datasets, unlike the mixtures of identically shaped Gaussians found in many textbook examples. Of the 51 problems, 24 are from the literature, and 27 are self-generated. The following subsections describe the problems in detail.

5.1.1 Problems with known optimum

Each problem in this group is constructed with a known optimal solution. The datasets consist of g identical, well-separated macro-blocks, each comprising b adjacent quadratic base blocks of data points, where b can be 1, 3, or 4. The number of centroids k is set to \( k = g \times b \). The optimal solution places one centroid at the center of each base block, as shown in Figure 3 with optimal solutions in red.

The optimality is justified because the macro-blocks are identical and well-separated, ensuring an optimal solution distributes centroids evenly among them. Thus, the overall solution’s optimality equates to that of an individual macro-block.

For b = 1, the optimal solution is the centroid of the single block, thus satisfying the centroid condition. For b = 3 or b = 4, it is assumed that the optimal partial solution involves placing one centroid in each base block’s center. Hence, the optimal solution for the entire problem is to center one centroid in each base block across all macro-blocks.

5.1.2 Literature Problems

The problems in this group are based on data sets from the literature. The k-values were freely chosen, resulting in the problems listed in Table 1 and displayed in Figure 4.

5.1.3 Modified Literature Problems

The problems in this group were generated from the “literature problems” in the previous section as follows.

- Randomly select 200 data points from the literature problem.
Figure 3: Problems with known optimum. The data points are shown in green, and the optimal centroids are in red.
Breathing K-Means

| data set     | origin                        | n   | k  |
|--------------|-------------------------------|-----|----|
| “Aggregation” | Gionis et al. (2007)          | 788 | 200|
| “Compound”   | Zahn (1971)                   | 399 | 50 |
| “D31”        | Veenman et al. (2002)         | 3100| 100|
| “Flame”      | Fu and Medico (2007)          | 240 | 80 |
| “Jain”       | Jain and Law (2005)           | 373 | 30 |
| “R15”        | Veenman et al. (2002)         | 600 | 30 |
| “S2”         | Fränti and Virmajoki (2006)   | 5000| 100|
| “Spiral”     | Chang and Yeung (2008)        | 312 | 80 |
| “Pathbased”  | Chang and Yeung (2008)        | 312 | 80 |

Table 1: Two-dimensional data sets from the literature with chosen k-values. All data sets were obtained from http://cs.joensuu.fi/sipu/datasets/.

Figure 4: K-means problems based on two-dimensional data sets from the literature (see Table 1).
Figure 5: Modified literature problems. The data sets were constructed from the problems shown in Figure 4 by taking a random subset of size 200 and adding a high-density cluster consisting of 4000 data points below the centroid of the subset. The $k$-values remain the same as in Table 1.

- Add a very dense cluster of 4000 data points below the area occupied by the selected 200 data points.

The purpose of this modification is to test the algorithms’ ability to deal with data sets having a large variation in density.
5.1.4 “Evil Spiral” Problems

This group of problems (see Figure 6) was designed to check the effect of letting an increasing fraction of the data originate from high-density clusters. One common part of all data sets consists of 500 data points located in 25 Gaussian clusters of 20 points, each positioned on a spiral. The other part of the data sets consists of one or more high-density Gaussian clusters arranged on a second spiral intertwined with the first one. The number of high-density clusters, each consisting of 500 data points, varies from one to 25 in steps of three. The value of $k$ is always set to 100.
5.1.5 High-Dimensional Problems

The problems in this group are based on three data sets (see Figure 7) used in the original paper on *k*-means++ (Arthur and Vassilvitskii, 2007) where the *k*-values were chosen from \( k \in \{10, 25, 50\} \). We added two larger *k*-values resulting in \( k \in \{10, 25, 50, 100, 200\} \). The data sets are described below.

**Norm25:** This data set consists of \( n = 10000 \) vectors of dimension \( d = 15 \). The original data used by Arthur and Vassilvitskii (2007) is not publicly available anymore, but their paper contains the following description (and also states that the number of data points is 10000):

“The first data set, Norm25, is synthetic. 25 “true” centers were drawn uniformly at random from a 15-dimensional hypercube of side length 500. Then points from Gaussian distributions of variance 1 around each true center were added, resulting in 25 well-separated Gaussians with the true centers providing a close approximation to the optimal clustering.”

Using this information, we generated a new data set, Norm25, with statistical properties similar to those of the original one.

**Cloud:** This data set consists of \( n = 1024 \) vectors of dimension \( d = 10 \). It is the Cloud data set from the UCI Machine Learning Repository (Dua and Graff, 2017) and is available at https://archive.ics.uci.edu/ml/datasets/Cloud. The data was derived from two 512 \times 512-pixel satellite images of clouds (one image in the visible spectrum and one in the infrared spectrum) taken with an AVHRR (Advanced Very High-Resolution Radiometer) sensor. The images were divided into 1024 super-pixels of size 16 \times 16, and from each pair of super-pixels, ten numerical features were extracted to form the final data set.

**Spam:** This data set consists of \( n = 4601 \) vectors of dimension \( d = 58 \). It is the Spam data set from the UCI Machine Learning Repository (Dua and Graff, 2017) and is available at https://archive.ics.uci.edu/ml/datasets/Spambase. According to the data set description, the data was generated from spam and non-spam emails. Most of the features (48 of 58) are word frequencies from different words. Other features measure the occurrence frequencies of certain characters or capital letters.

5.2 Solution Quality

The primary findings on solution quality are summarized below, with detailed results in Appendix A. Table 2 presents the core results, with each row representing a problem group and each column an algorithm. The values denote the mean relative MSE improvement over the baseline greedy *k*-means++ algorithm, marked as 0.0%. Positive values indicate improvements, while negative values denote poorer results.

The following observations can be made regarding solution quality:

- Only breathing *k*-means and better *k*-means++ consistently beat the baseline algorithm for all problem groups. Thereby, the improvements found by breathing *k*-means were much larger than those found by better *k*-means++.
Figure 7: Three high-dimensional data sets which were also used by Arthur and Vassilvitskii (2007). Descriptions are in the text. The \( k \)-values used with each data set were 10, 25, 50, 100, and 200, resulting in 15 different problems. The figures display projections of the high-dimensional data onto two selected axes.

Figure 8: Color mapping used for the “SSE improvements” tables.

- **Random swap** found the best solutions for the “Literature” problems.
- **Vanilla \( k \)-means++** (the original \( k \)-means++ variant with the \( O(\log k) \) upper bound) found significantly worse solutions than the baseline algorithm.
- **Hartigan-Wong** (the default \( k \)-means algorithm in the stats package of the R programming language) always produced the worst results of all methods (far below the baseline algorithm).

In Table 3, the average standard deviation corresponding to Table 2 is shown. A noticeable pattern is that the standard deviations for **breathing \( k \)-means** are tiny, indicating a quite homogeneous quality of the solutions. Overall there seems to exist a negative correlation between SSE improvement and standard deviation: the higher the SSE improvement, the smaller the standard deviation, and vice versa.

5.3 CPU Time Usage

Here we present the primary findings on CPU time usage from our experiments which were performed on a Linux PC (AMD FX™-8300 eight-core Processor, 16GB RAM) running Ubuntu 22.04 LTS. Detailed, problem-specific results are provided in Appendix B. To reduce bias in the experimental results, we selected the most widely used open-source implementation of each algorithm. For **better \( k \)-means++**, no implementation was available, so we implemented it in Python based on scikit-learn with reasonable effort to obtain an efficient implementation. Overall, this approach resulted in three different programming
Table 2: SSE improvements relative to \textit{greedy} \textit{k-means}++. Both \textit{better} \textit{k-means++} and \textit{breathing} \textit{k-means} consistently found improvements for all problem groups. With the exception of the “Literature” problems (where \textit{random swap} performed best), \textit{breathing} \textit{k-means} always found the largest improvements. The values have been colorized according to the mapping shown in Figure 8. The best results in each row are boxed.

| problem group    | greedy km++ | vanilla km++ | better km++ | Hartigan-Wong | genetic algorithm | random swap | breathing k-means |
|------------------|-------------|--------------|-------------|---------------|-------------------|-------------|------------------|
| Known Optimum    | 0.0%        | -15.5%       | 5.2%        | -30.4%        | 9.1%              | 9.6%        | 9.7%             |
| Literature       | 0.0%        | -6.5%        | 1.8%        | -9.2%         | 7.9%              | 9.6%        | 7.5%             |
| Modified Literature | 0.0%    | -19.6%       | 2.8%        | -16785.0%     | -141.8%           | -221.6%     | 10.0%            |
| Evil Spiral      | 0.0%        | -11.8%       | 2.8%        | -1910.9%      | 1.2%              | 6.4%        | 9.1%             |
| High-Dimensional | 0.0%        | -6.5%        | 1.5%        | -23642.4%     | -335.2%           | -72.2%      | 4.3%             |
| Mean             | 0.0%        | -12.0%       | 2.8%        | -8475.6%      | -91.8%            | -53.6%      | 8.1%             |

Table 3: Standard deviations corresponding to the SSE improvements from Table 2. The values for \textit{breathing} \textit{k-means} are tiny, indicating a quite homogeneous quality of the solutions.

| problem group    | greedy km++ | vanilla km++ | better km++ | Hartigan-Wong | genetic algorithm | random swap | breathing k-means |
|------------------|-------------|--------------|-------------|---------------|-------------------|-------------|------------------|
| Known Optimum    | 5.7%        | 9.9%         | 2.5%        | 13.6%         | 0.2%              | 0.1%        | 0.0%             |
| Literature       | 2.1%        | 3.5%         | 1.8%        | 7.9%          | 0.6%              | 0.4%        | 0.9%             |
| Modified Literature | 3.5%    | 8.9%         | 2.8%        | 5606.9%       | 119.9%            | 38.3%       | 1.3%             |
| Evil Spiral      | 2.3%        | 4.6%         | 1.8%        | 828.5%        | 14.5%             | 1.2%        | 0.8%             |
| High-Dimensional | 2.1%        | 5.4%         | 1.3%        | 9395.0%       | 532.2%            | 248.2%      | 0.5%             |
| Mean             | 3.1%        | 6.5%         | 2.0%        | 3170.4%       | 133.5%            | 57.6%       | 0.7%             |

languages being used: Python, Fortran, and C. For algorithms with different implementation languages, the CPU time usage is not directly comparable. With this caveat, the observed CPU time usage is reported here to provide some efficiency indication.

Table 4 contains one row per problem group. It shows in the second column the mean CPU time in seconds used by the baseline algorithm, \textit{greedy} \textit{k-means}++, and in the following columns, the percentual CPU time usage relative to the baseline algorithm for all investigated approaches.

The algorithms implemented in Python (\textit{greedy} \textit{k-means}++, \textit{vanilla} \textit{k-means}++, \textit{better} \textit{k-means}++, \textit{breathing} \textit{k-means}) are all based on the \textit{scikit-learn} library, which makes
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| problem group          | t(greedy km++) | vanilla km++ | better km++ | Hartigan-Wong | genetic algorithm | random swap | breathing km++ |
|------------------------|---------------|--------------|-------------|---------------|------------------|-------------|---------------|
| Known Optimum          | 0.07s         | 83.8%        | 754.8%      | 18.2%         | 289.4%           | 4327.4%     | 382.4%        |
| Literature             | 0.06s         | 83.3%        | 568.2%      | 13.1%         | 237.1%           | 2439.9%     | 454.7%        |
| Modified Literature    | 0.07s         | 67.0%        | 1104.1%     | 44.5%         | 575.9%           | 36358.1%    | 523.2%        |
| Evil Spiral            | 0.10s         | 66.1%        | 1398.4%     | 26.3%         | 454.5%           | 38572.2%    | 605.3%        |
| High-Dimensional       | 0.10s         | 85.4%        | 903.1%      | 195.6%        | 1571.5%          | 69674.6%    | 523.2%        |
| Mean                   | 0.08s         | 77.1%        | 945.7%      | 59.5%         | 625.7%           | 23331.4%    | 555.6%        |

Table 4: CPU time relative to greedy k-means++. The column “t(greedy km++)” shows the mean CPU time used by the baseline algorithm. Green (red) background coloring indicates faster (slower) execution than the baseline algorithm.

The following observations can be made for CPU time usage of these algorithms:

- The fastest of these algorithms was vanilla k-means++. It was about 23% faster than the baseline algorithm, greedy k-means++, which, however, had a much better solution quality.

- Better k-means++ required about 9.5 times as much CPU time as the baseline algorithm.

- Breathing k-means required about 5.6 times as much CPU time as the baseline algorithm.

The only algorithm implemented in Fortran, Hartigan-Wong, was the fastest overall (about 40% faster than greedy k-means++). It is called from within R, but the implementation language is Fortran.

Among the two algorithms implemented in C, genetic algorithm was on average over 30 times faster than random swap, which was by far the most compute-heavy algorithm of all we investigated.

5.4 Effects of Multiple Runs and Running Breathing K-Means Only Once

Multiple runs is a technique to enhance algorithmic outcomes by running it several times and choosing the best result (Section 3.2.13). Table 5 shows the average improvements from ten runs of all algorithms, over the baseline. Using the same data as Table 2 (100 runs per problem-algorithm combo), results are grouped into ten clusters of ten, selecting the best from each. Percentage SSE difference from the baseline is calculated and averaged. Positive values in the greedy k-means++ column represent the improvement from ten runs.

Table 6 shows the SSE difference between single run and best-of-ten runs. The minimal improvements from multiple runs of breathing k-means suggest that it can be effectively
Table 5: Best of 10 runs: SSE improvements relative to greedy $k$-means++. The performed experimental results for each combination of problem and algorithm have been partitioned into groups of size ten, and the best result from each group was selected.

Table 6: Relative SSE difference between single run and best of 10 runs. This table compares the relative SSE difference between a single run and the best of ten runs, computed from Tables 5 and 2. The minor improvements for breathing $k$-means indicate that multiple runs are not required to achieve desirable results.

5.5 Effect of Varying the Breathing Depth Parameter $m$

The breathing depth parameter $m$ (default value: 5) serves as a means of balancing solution quality and computational resource demands. Higher values of $m$ typically result in
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Table 7: A single run of breathing k-means generally outperforms the best of ten runs for the analyzed competing algorithms, barring few exceptions like random swap and genetic algorithm. The figures represent the mean SSE improvements over the baseline algorithm from best-of-ten runs for competitors (Table 5) and a single run for breathing k-means (last column of Table 2). Breathing k-means (1 run) was the best overall, topping three individual problem groups, and ranking second and third in the remaining two.

| problem group      | greedy km++ (10 runs) | vanilla km++ (10 runs) | better km++ (10 runs) | Hartigan-Wong km++ (10 runs) | genetic algorithm km++ (10 runs) | random swap km++ (10 runs) | breathing k-means (1 run) |
|--------------------|------------------------|------------------------|-----------------------|----------------------------|----------------------------------|---------------------------|--------------------------|
| Known Optimum      | 5.6%                   | -3.1%                  | 7.8%                  | -12.5%                     | 9.3%                             | 9.6%                      | 9.7%                     |
| Literature         | 3.0%                   | -1.5%                  | 4.4%                  | 0.6%                       | 8.7%                             | 10.1%                     | 7.5%                     |
| Modified Literature| 5.0%                   | -7.2%                  | 6.9%                  | -9395.2%                   | -37.9%                           | -167.1%                   | 10.0%                    |
| Evil Spiral        | 3.4%                   | -5.0%                  | 5.4%                  | -967.2%                    | 8.6%                             | 8.1%                      | 9.1%                     |
| High-Dimensional   | 2.5%                   | -0.7%                  | 3.0%                  | -11848.1%                  | 0.5%                             | 4.7%                      | 4.3%                     |
| Mean               | 3.9%                   | -3.5%                  | 5.5%                  | -4444.5%                   | -2.1%                            | -26.9%                    | 8.1%                     |

Table 8: CPU time relative to greedy k-means++ when all algorithms including greedy k-means++ are run ten times, but breathing k-means is run only once. In this case breathing k-means is the fastest algorithm, requiring only 55.6% of the CPU time needed for ten runs of greedy k-means++.

| problem group      | t(greedy km++) (10 runs) | t(vanilla km++) (10 runs) | t(better km++) (10 runs) | t(Hartigan-Wong km++) (10 runs) | t(genetic algorithm km++) (10 runs) | t(random swap km++) (10 runs) | breathing k-means (1 run) |
|--------------------|----------------------------|---------------------------|--------------------------|----------------------------------|-------------------------------------|-----------------------------|--------------------------|
| Known Optimum      | 0.69s                      | 83.8%                     | 754.8%                   | 18.2%                            | 289.4%                              | 4327.4%                     | 38.2%                    |
| Literature         | 0.57s                      | 83.3%                     | 568.2%                   | 13.1%                            | 237.1%                              | 2439.9%                     | 45.5%                    |
| Modified Literature| 0.68s                      | 67.0%                     | 1104.1%                  | 44.5%                            | 575.9%                              | 36358.1%                    | 52.3%                    |
| Evil Spiral        | 0.98s                      | 66.1%                     | 1398.4%                  | 26.3%                            | 454.5%                              | 3857.2%                     | 60.5%                    |
| High-Dimensional   | 0.95s                      | 85.4%                     | 903.1%                   | 195.6%                           | 1571.5%                             | 69674.6%                    | 81.3%                    |
| Mean               | 0.77s                      | 77.1%                     | 945.7%                   | 59.5%                            | 625.7%                              | 23331.4%                    | 55.6%                    |

improved solutions, albeit at the expense of greater computation time, and vice versa. Figure 9 illustrates the average error improvement relative to the baseline algorithm across all test problems for varying values of m. Concurrently, Figure 10 presents the corresponding computation time relative to the baseline algorithm. For instance, replacing the default $m = 5$ with $m = 25$ improved the average solution quality by 0.9% for our test problems, but quadrupled the CPU time required.
Figure 9: Average error improvement across all test problems of breathing $k$-means over greedy $k$-means++, for varying values of the “breathing depth” parameter $m$. For the default value of $m = 5$, the average error improvement is 8.1% (see the lower-right value in Table 2).

Figure 10: Average computation time across all test problems of breathing $k$-means relative to greedy $k$-means++, for varying values of the “breathing depth” parameter $m$. For the default value of $m = 5$, the relative size of the CPU time is 555.6% (see the lower-right value in Table 4).
6. Conclusion

We introduced the novel breathing $k$-means algorithm which dynamically changes the size $k$ of the codebook to improve solutions found by the Generalized Lloyd Algorithm. We empirically compared breathing $k$-means (initialized by greedy $k$-means++) to the baseline greedy $k$-means++ (followed by the Generalized Lloyd Algorithm) and five other algorithms across diverse test problems. Our approach consistently outperformed all other methods in terms of solution quality, with only a few exceptions where it slightly lagged behind random swap or genetic algorithm. It also was the only approach able to find near-optimal solutions across all problems in the "Known Optimum" problem group. While random swap and genetic algorithm did outperform the baseline for most problems, they were dramatically inferior to the baseline in several cases, making them less suitable for unknown data. The comparison between greedy $k$-means++ and vanilla $k$-means++ underlined the improved solution quality offered by the former, validating its use as the present default $k$-means algorithm in scikit-learn.

Hartigan-Wong, the default algorithm in R’s stats package, consistently underperformed, suggesting its use should be limited to situations where low computational cost is a priority. Notably, breathing $k$-means maintained its superior performance even when other algorithms were run ten times and it was only run once. In this scenario, it continued to deliver significantly better solutions than greedy $k$-means++ while being nearly twice as fast.

Based on these findings, we recommend using breathing $k$-means over greedy $k$-means++ for improved solution quality and speed.

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Appendix A. Solution Quality Details

This section presents tables depicting solution quality per problem for all studied algorithms. The average SSE (Φ) for the baseline algorithm, greedy \( k\text{-means}++ \), is shown with a grey background. The percentages for non-baseline algorithms represent mean relative SSE improvement over the baseline, with negative values indicating worse performance. The color scheme corresponds to Figure 8. The best results in each row are boxed, including ties.

| data set     | n  | k  | Φ(greedy km++) | vanilla km++ | better km++ | Hartigan-Wong | genetic algorithm | random swap | breathing k-means |
|--------------|----|----|----------------|--------------|-------------|-----------------|-------------------|-------------|------------------|
| squares-3x3  | 225| 9  | 2.37e+00       | -22.4%       | 4.9%        | -27.2%         | 4.9%              | 4.9%        | 4.9%             |
| squares-5x5  | 625| 25 | 2.40e+00       | -19.8%       | 10.8%       | -30.5%         | 11.4%             | 11.5%       | 11.5%            |
| squares-7x7  | 1225| 49 | 2.36e+00       | -18.4%       | 9.5%        | -29.9%         | 12.0%             | 12.1%       | 12.1%            |
| angles-3x3   | 1728| 27 | 4.01e+00       | -14.3%       | 6.7%        | -34.3%         | 9.6%              | 10.2%       | 10.2%            |
| angles-5x5   | 2700| 75 | 2.22e+00       | -15.2%       | 4.1%        | -33.8%         | 9.8%              | 10.5%       | 10.6%            |
| angles-7x7   | 3675| 147| 1.52e+00       | -14.2%       | 2.9%        | -35.7%         | 10.2%             | 10.5%       | 10.8%            |
| 4squares-3x3 | 2304| 36 | 6.67e+00       | -10.9%       | 4.0%        | -25.4%         | 7.9%              | 8.7%        | 8.7%             |
| 4squares-5x5 | 3600| 100| 3.34e+00       | -12.3%       | 2.1%        | -28.2%         | 7.8%              | 8.8%        | 8.8%             |
| 4squares-7x7 | 4900| 196| 2.21e+00       | -12.0%       | 1.6%        | -28.2%         | 8.4%              | 9.0%        | 9.4%             |
| Mean         |     |    | -15.5%         | 5.2%         | -30.4%       | 9.1%           | 9.6%              | 9.7%        |                  |

Table A.1: Problems with known optimum: SSE improvements relative to greedy \( k\text{-means}++ \). Breathing \( k\text{-means} \) dominates, closely followed by random swap and less closely by genetic algorithm and better \( k\text{-means}++ \). Vanilla \( k\text{-means}++ \) and Hartigan-Wong are clearly inferior.
### Table A.2: Problems with known optimum: SSE deviations from the optimum. Green background marks cases where the optimum has been approached up to 0.001% tolerance. Only breathing k-means was able to consistently find such near-optimal solutions. Shades of blue indicate varying deviations from the optimum.

| data set       | n   | k   | greedy km++ | vanilla km++ | better km++ | Hartigan-Wong km++ | genetic algorithm km++ | random swap km++ | breathing k-means km++ |
|----------------|-----|-----|------------|--------------|-------------|---------------------|------------------------|-------------------|------------------------|
| squares-3x3    | 225 | 9   | 5.18%      | 28.77%       | 0.00%       | 33.82%              | 0.05%                  | 0.00%             | 0.00%                  |
| squares-5x5    | 625 | 25  | 12.96%     | 35.32%       | 0.81%       | 47.42%              | 0.08%                  | 0.00%             | 0.00%                  |
| squares-7x7    | 1225| 49  | 13.76%     | 34.67%       | 2.90%       | 47.79%              | 0.10%                  | 0.00%             | 0.00%                  |
| angles-3x3     | 1728| 27  | 11.31%     | 27.23%       | 3.80%       | 49.51%              | 0.56%                  | 0.00%             | 0.00%                  |
| angles-5x5     | 2700| 75  | 11.81%     | 28.75%       | 7.17%       | 49.63%              | 0.83%                  | 0.06%             | 0.00%                  |
| angles-7x7     | 3675| 147 | 12.05%     | 27.94%       | 8.80%       | 52.04%              | 0.67%                  | 0.28%             | 0.00%                  |
| 4squares-3x3   | 2304| 36  | 9.51%      | 21.44%       | 5.17%       | 37.35%              | 0.85%                  | 0.00%             | 0.00%                  |
| 4squares-5x5   | 3600| 100 | 9.67%      | 23.21%       | 7.32%       | 40.56%              | 1.09%                  | 0.07%             | 0.00%                  |
| 4squares-7x7   | 4900| 196 | 10.42%     | 23.70%       | 8.66%       | 41.58%              | 1.16%                  | 0.43%             | 0.00%                  |
| Mean           |     |     | 10.74%     | 27.89%       | 4.96%       | 44.41%              | 0.60%                  | 0.09%             | 0.00%                  |

### Table A.3: Literature problems: SSE improvements relative to greedy k-means++. For all problems in this group, random swap found the best solutions.

| data set       | n   | k   | Φ(greedy km++) | vanilla km++ | better km++ | Hartigan-Wong km++ | genetic algorithm km++ | random swap km++ | breathing km++ |
|----------------|-----|-----|----------------|--------------|-------------|---------------------|------------------------|-------------------|---------------|
| aggregation    | 788 | 200 | 2.55e+02       | -8.1%        | 1.1%        | 1.4%                | 10.9%                  | 11.8%            | 8.4%          |
| compound       | 399 | 50  | 4.08e+02       | -5.0%        | 0.9%        | -9.8%               | 8.2%                   | 10.5%            | 8.0%          |
| d31            | 3100| 100 | 1.39e+03       | -4.9%        | 1.2%        | -8.4%               | 3.8%                   | 5.6%             | 4.9%          |
| flame          | 240 | 80  | 4.99e+01       | -8.5%        | 1.8%        | 7.1%                | 13.2%                  | 14.5%            | 11.7%         |
| jain           | 373 | 30  | 6.31e+02       | -4.3%        | 2.7%        | -24.2%              | 7.2%                   | 9.0%             | 7.5%          |
| pathbased      | 300 | 50  | 3.00e+02       | -9.3%        | 3.3%        | -8.5%               | 11.5%                  | 12.8%            | 10.0%         |
| r15            | 600 | 30  | 7.04e+01       | -2.9%        | 3.1%        | -6.0%               | 6.3%                   | 7.7%             | 6.6%          |
| s2             | 5000| 100 | 2.70e+12       | -3.0%        | 0.7%        | -6.1%               | 2.3%                   | 4.5%             | 3.6%          |
| spiral         | 312 | 80  | 1.31e+02       | -12.8%       | 1.3%        | -28.5%              | 7.5%                   | 9.8%             | 7.0%          |
| Mean           |     |     | -6.5%          | 1.8%         | -9.2%       | 7.9%                | 9.6%                   | 7.5%             |               |
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Table A.4: Modified literature problems: SSE improvements relative to greedy \textit{k-means++}. For all problems, breathing \textit{k-means} found the best solutions. Also, better \textit{k-means++} was able to improve upon the baseline algorithm in all cases but by a considerably smaller margin. The other approaches produced worse solutions than the baseline algorithm for some or all problems.

| data set    | n   | k   | $\Phi$ (greedy km++) | vanilla km++ | better km++ | Hartigan-Wong | genetic algorithm | random swap | breathing km++ |
|-------------|-----|-----|----------------------|--------------|-------------|-----------------|-------------------|-------------|----------------|
| aggregation-* | 4200 | 200 | 1.93e+00             | -47.2%       | 1.3%        | -107733.9%     | -1170.0%          | -1877.7%   | 4.3%           |
| compound-*   | 4200 | 50  | 1.40e+02             | -11.5%       | 2.8%        | -1850.0%       | -2.9%             | 3.6%        | 10.8%          |
| d31-*        | 4200 | 100 | 2.72e+01             | -30.0%       | 3.5%        | -10598.7%      | -27.2%            | -56.1%      | 11.3%          |
| flame-*      | 4200 | 80  | 3.72e+01             | -10.4%       | 0.6%        | -1842.0%       | 10.8%             | -4.1%       | 13.4%          |
| jain-*       | 4200 | 30  | 3.29e+02             | -8.2%        | 2.8%        | -1514.9%       | -1.2%             | 8.1%        | 9.1%           |
| pathbased-*  | 4200 | 50  | 1.68e+02             | -15.2%       | 4.3%        | -1947.9%       | 5.9%              | 5.8%        | 11.7%          |
| r15-*        | 4200 | 30  | 1.99e+01             | -6.0%        | 4.7%        | -5888.4%       | -55.0%            | 8.8%        | 9.0%           |
| s2-*         | 4200 | 100 | 2.55e+10             | -28.9%       | 2.5%        | -13886.6%      | -32.3%            | -68.2%      | 9.2%           |
| spiral-*     | 4200 | 80  | 5.56e+01             | -19.0%       | 2.3%        | -5802.3%       | -4.1%             | -14.2%      | 11.0%          |
| Mean         |     |     |                      | -19.6%       | 2.8%        | -16785.0%      | -141.8%           | -221.6%     | 10.0%          |

Table A.5: "Evil Spiral" problems: SSE improvements relative to greedy \textit{k-means++}. Breathing \textit{k-means} is best apart from the first two problems.
Table A.6: High-dimensional problems: SSE improvements relative to greedy k-means++. The problem with the Norm25 data set and k = 25 seems to be so simple that all algorithms, except Hartigan-Wong, found the same solution (one centroid per cluster). The dimensionality of the data sets Norm25, Cloud, and Spam is 15, 10, and 58, respectively.
Appendix B. CPU Time Details

In this section, tables for each problem group illustrate the CPU time usage per problem for all investigated algorithms. The average CPU time in seconds for the baseline algorithm, greedy k-means++, is displayed with a blue background. Percentage values for non-baseline algorithms represent the CPU time relative to the baseline algorithm for each specific k-means problem. Values below 100% (faster than the baseline) are on green backgrounds, while values above 100% (slower than the baseline) are on red backgrounds.

Table B.1: Problems with known optimum: CPU time relative to greedy k-means++.

| data set     | n   | k   | t(greedy km++) | vanilla km++ | better km++ | Hartigan-Wong | genetic algorithm | random swap | breathing k-means |
|--------------|-----|-----|----------------|--------------|-------------|----------------|-------------------|-------------|------------------|
| squares-3x3  | 225 | 9   | 0.01s          | 91.0%        | 358.5%      | 32.8%         | 129.4%            | 2955.1%    | 298.7%           |
| squares-5x5  | 625 | 25  | 0.02s          | 102.8%       | 579.9%      | 21.9%         | 219.4%            | 3897.9%    | 339.3%           |
| squares-7x7  | 1225| 49  | 0.03s          | 86.3%        | 667.9%      | 14.8%         | 244.9%            | 3439.5%    | 271.7%           |
| angles-3x3   | 1728| 27  | 0.02s          | 92.9%        | 780.7%      | 20.1%         | 293.6%            | 7228.7%    | 514.2%           |
| angles-5x5   | 2700| 75  | 0.07s          | 74.0%        | 773.4%      | 14.0%         | 289.8%            | 3781.3%    | 351.9%           |
| angles-7x7   | 3675| 147 | 0.12s          | 74.2%        | 1030.7%     | 14.7%         | 393.8%            | 2839.7%    | 407.5%           |
| 4squares-3x3 | 2304| 36  | 0.04s          | 86.3%        | 743.4%      | 17.4%         | 288.8%            | 5177.4%    | 475.0%           |
| 4squares-5x5 | 3600| 100 | 0.10s          | 74.6%        | 883.3%      | 14.6%         | 339.7%            | 4454.3%    | 373.8%           |
| 4squares-7x7 | 4900| 196 | 0.22s          | 66.9%        | 975.6%      | 13.2%         | 404.9%            | 2772.7%    | 409.3%           |

Mean | 0.07s | 83.8% | 754.8% | 18.2% | 289.4% | 4327.4% | 382.4% |

Table B.2: Literature problems: CPU time relative to greedy k-means++.

| data set   | n     | k | t(greedy km++) | vanilla km++ | better km++ | Hartigan-Wong | genetic algorithm | random swap | breathing k-means |
|------------|-------|---|----------------|--------------|-------------|----------------|-------------------|-------------|------------------|
| aggregation| 788   | 200| 0.10s          | 75.8%        | 581.5%      | 7.0%          | 376.9%            | 681.7%     | 577.3%           |
| compound   | 399   | 50 | 0.03s          | 93.1%        | 530.7%      | 13.5%         | 213.7%            | 1842.7%    | 443.6%           |
| d31        | 3100  | 100| 0.11s          | 75.6%        | 727.5%      | 13.6%         | 307.5%            | 4342.1%    | 478.0%           |
| flame      | 240   | 80 | 0.04s          | 83.9%        | 493.9%      | 9.9%          | 189.3%            | 635.6%     | 439.2%           |
| jain       | 373   | 30 | 0.02s          | 82.7%        | 429.4%      | 15.6%         | 150.3%            | 2168.7%    | 425.9%           |
| pathbased  | 300   | 50 | 0.03s          | 89.6%        | 484.3%      | 13.2%         | 169.2%            | 1338.8%    | 374.4%           |
| r15        | 600   | 30 | 0.02s          | 81.7%        | 520.3%      | 16.4%         | 195.7%            | 2843.0%    | 462.0%           |
| s2         | 5000  | 100| 0.14s          | 83.3%        | 843.9%      | 19.3%         | 328.7%            | 7204.6%    | 551.5%           |
| spiral     | 312   | 80 | 0.04s          | 83.6%        | 502.3%      | 9.7%          | 202.7%            | 901.6%     | 340.1%           |

Mean | 0.06s | 83.3% | 568.2% | 13.1% | 237.1% | 2439.9% | 454.7% |
### Table B.3: Modified literature problems: CPU time relative to greedy k-means++.

| data set     | n    | k    | t(greedy km++) | vanilla km++ | better km++ | Hartigan-Wong algorithm | genetic algorithm | random swap | breathing k-means |
|--------------|------|------|----------------|--------------|-------------|-------------------------|-------------------|-------------|------------------|
| aggregation-*| 4200 | 200  | 0.15s          | 55.2%        | 1222.3%     | 28.0%                   | 569.8%           | 11926.3%    | 410.1%          |
| compound-*   | 4200 | 50   | 0.05s          | 72.2%        | 1052.4%     | 48.1%                   | 506.3%           | 39361.3%    | 560.5%          |
| d31-*        | 4200 | 100  | 0.09s          | 60.3%        | 1102.8%     | 37.8%                   | 528.9%           | 21590.9%    | 452.2%          |
| flame-*      | 4200 | 80   | 0.07s          | 65.5%        | 1113.7%     | 42.5%                   | 611.5%           | 24205.8%    | 624.7%          |
| jain-*       | 4200 | 30   | 0.03s          | 82.1%        | 1027.7%     | 55.6%                   | 579.2%           | 75741.6%    | 611.0%          |
| pathbased-*  | 4200 | 50   | 0.05s          | 69.7%        | 1080.7%     | 49.6%                   | 524.8%           | 37964.6%    | 498.0%          |
| r15-*        | 4200 | 30   | 0.03s          | 77.2%        | 1130.3%     | 61.1%                   | 722.7%           | 70939.1%    | 623.6%          |
| s2-*         | 4200 | 100  | 0.08s          | 61.1%        | 1126.0%     | 37.6%                   | 536.5%           | 21913.8%    | 468.0%          |
| spiral-*     | 4200 | 80   | 0.07s          | 60.0%        | 1080.8%     | 40.4%                   | 603.4%           | 23579.3%    | 460.5%          |
| Mean         |      |      | 0.07s          | 67.0%        | 1104.1%     | 44.5%                   | 575.9%           | 36358.1%    | 523.2%          |

### Table B.4: "Evil Spiral" problems: CPU time relative to greedy k-means++.

| data set     | n    | k    | t(greedy km++) | vanilla km++ | better km++ | Hartigan-Wong algorithm | genetic algorithm | random swap | breathing k-means |
|--------------|------|------|----------------|--------------|-------------|-------------------------|-------------------|-------------|------------------|
| espiral01    | 1000 | 100  | 0.05s          | 80.1%        | 678.5%      | 11.9%                   | 254.2%           | 1874.6%     | 428.9%          |
| espiral04    | 2500 | 100  | 0.08s          | 65.7%        | 838.6%      | 15.8%                   | 284.9%           | 2437.0%     | 457.7%          |
| espiral07    | 4000 | 100  | 0.09s          | 64.3%        | 1068.8%     | 21.3%                   | 351.3%           | 3077.9%     | 548.2%          |
| espiral10    | 5500 | 100  | 0.10s          | 61.1%        | 1243.7%     | 24.4%                   | 399.0%           | 3495.4%     | 561.7%          |
| espiral13    | 7000 | 100  | 0.10s          | 64.2%        | 1437.9%     | 28.2%                   | 465.0%           | 4046.0%     | 620.4%          |
| espiral16    | 8500 | 100  | 0.10s          | 68.6%        | 1707.7%     | 32.9%                   | 553.5%           | 4754.2%     | 678.7%          |
| espiral19    | 10000| 100  | 0.11s          | 63.4%        | 1787.6%     | 33.3%                   | 575.2%           | 4920.0%     | 679.0%          |
| espiral22    | 11500| 100  | 0.12s          | 65.0%        | 1885.9%     | 34.6%                   | 601.4%           | 5098.8%     | 748.0%          |
| espiral25    | 13000| 100  | 0.14s          | 62.4%        | 1936.9%     | 34.5%                   | 605.9%           | 5011.3%     | 725.1%          |
| Mean         |      |      | 0.10s          | 66.1%        | 1398.4%     | 26.3%                   | 454.5%           | 3857.2%     | 605.3%          |
Breathing $K$-Means

| data set | n  | k  | t(greedy km++) | vanilla km++ | better km++ | Hartigan-Wong algorithm | genetic swap | random swap | k-means breathing |
|----------|----|----|---------------|--------------|-------------|--------------------------|--------------|-------------|-------------------|
| Norm25   | 10000 | 10 | 0.02s         | 88.1%        | 1274.7%     | 76.0%                    | 2826.7%      | 96394.3%    | 1220.0%          |
| Norm25   | 10000 | 25 | 0.04s         | 73.7%        | 1523.8%     | 88.0%                    | 1470.6%      | 61781.7%    | 542.4%           |
| Norm25   | 10000 | 50 | 0.06s         | 73.4%        | 1679.4%     | 93.5%                    | 1126.8%      | 70495.7%    | 1206.8%          |
| Norm25   | 10000 | 100| 0.14s        | 68.4%        | 1593.3%     | 66.3%                    | 890.5%       | 53017.9%   | 953.9%           |
| Norm25   | 10000| 200| 0.33s        | 64.3%        | 1253.8%     | 42.5%                    | 837.6%       | 24060.5%   | 929.2%           |
| Cloud    | 1024 | 10 | 0.01s        | 117.2%       | 472.1%      | 51.1%                    | 363.7%       | 19053.3%   | 854.1%           |
| Cloud    | 1024 | 25 | 0.02s        | 97.8%        | 511.1%      | 31.3%                    | 307.3%       | 11720.1%   | 579.6%           |
| Cloud    | 1024 | 50 | 0.03s        | 87.8%        | 650.0%      | 26.5%                    | 374.5%       | 8589.4%    | 572.7%           |
| Cloud    | 1024 | 100| 0.07s       | 76.4%        | 576.7%      | 18.8%                    | 415.4%       | 1034.6%    | 508.4%           |
| Cloud    | 1024 | 200| 0.12s       | 73.7%        | 581.8%      | 15.5%                    | 557.8%       | 1966.7%    | 585.1%           |
| Spam     | 4601 | 10 | 0.03s        | 100.4%       | 534.5%      | 481.8%                    | 2835.9%      | 210704.4%  | 1076.4%          |
| Spam     | 4601 | 25 | 0.05s        | 112.4%       | 648.8%      | 760.3%                    | 2555.1%      | 156117.9%  | 797.9%           |
| Spam     | 4601 | 50 | 0.08s        | 90.8%        | 737.9%      | 594.0%                    | 2838.4%      | 149860.6%  | 760.4%           |
| Spam     | 4601 | 100| 0.14s       | 84.1%        | 801.3%      | 308.5%                    | 3115.1%      | 119787.8%  | 848.3%           |
| Spam     | 4601 | 200| 0.28s       | 72.8%        | 760.7%      | 279.3%                    | 3057.3%      | 57533.6%   | 754.5%           |
| Mean     |     |    | 0.10s        | 85.4%        | 903.1%      | 195.6%                    | 1571.5%      | 69674.6%   | 812.7%           |

Table B.5: High-dimensional problems: CPU time relative to greedy $k$-means++. The dimensionality of the data sets Norm25, Cloud, and Spam is 15, 10, and 58, respectively.