Accelerated Training of Large-Scale Gaussian Mixtures
by a Merger of Sublinear Approaches

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Abstract

We combine two recent lines of research on sublinear clustering to significantly increase the efficiency in the training of large-scale Gaussian mixture models (GMMs). First, we use a novel truncated variational EM approach for GMMs with isotropic Gaussians in order to increase clustering efficiency for large \( C \) (many clusters). Second, we use recent coreset approaches to increase clustering efficiency for large \( N \) (many data points). In order to derive a novel accelerated algorithm, we first show analytically how variational EM and coreset objectives can be merged to give rise to a new, combined clustering objective. Each iteration of the novel algorithm derived from this merged objective is then shown to have a run-time cost of \( O(N'G^2D) \) per iteration, where \( N' < N \) is the coreset size and \( G^2 < C \) is a constant related to the extent of local cluster neighborhoods. While the approach strongly reduces the number of distance evaluations per EM iteration, we observe the iterations to maintain a very effective increase of the clustering objective. In a series of numerical experiments, we use efficient seeding for initialization and measure the net computational demand of the merged approach in comparison to other recent approaches. For standard benchmarks which evaluate the trade-off between values of the clustering objective and clustering efficiency, the merged approach significantly improves the state-of-the-art. Depending on the data set and number of clusters, we observe several times (and up to an order of magnitude) faster execution times to reach the same quantization errors compared to the best recent approaches such as highly efficient coreset-based \( k \)-means.

1 Introduction

Efficiency demands for clustering algorithms are constantly increasing. As the volume of data and the number of data-driven tasks constantly grows, new algorithms for increasingly many clusters Pelleg and Moore [1999], Coates et al. [2011], Curtin [2017], Kobren et al. [2017] on increasingly large data sets Hilbert and López [2011] are required. The execution of standard clustering algorithms, such as \( k \)-means or expectation maximization (EM) for Gaussian mixture models (GMMs) McLachlan and Peel [2004], quickly becomes prohibitive at large scales as their run-time costs grow with \( O(NCD) \) per iteration (where \( N \) is the number of data points, \( C \) the number of clusters, and \( D \) the dimensionality of the data points). For any combination of large \( N, C, \) or \( D \), the execution of even just one iteration may exceed the limits of state-of-the-art computational hardware.

Related Work and Own Contribution. Newly developed methods have addressed the demand for more efficient clustering algorithms in different ways. Typically the focus is either on reducing the dependency on \( N, C, \) or \( D \) individually, or to reduce the required number of learning iterations Bachem et al. [2016a,b], Newling and Fleuret [2017]. The reduction of the dependency on \( D \) has been addressed relatively early. Run-time costs to compute metric distances have, for instance, been reduced by exploiting properties of the triangle inequality Elkan [2003] or by applying random projections Chan and Leung [2017]. Such reduction of computational costs for distance estimations are not the focus of this work but could potentially be used in addition. Instead, our main focus is a joint reduction of the linear scaling with \( N \) and \( C \). Decreasing the dependency on \( N \) is pursued by a line of research using coresets Har-Peled and Mazumdar [2004]. Most relevant for our work are
coresets for \(k\)-means and GMM-based clustering Feldman et al. [2011], Bachem et al. [2018], Lucic et al. [2018], more specifically the very recent approach of ‘lightweight’ coresets Bachem et al. [2018]. The central idea behind coresets is the use of efficient procedures to replace large data sets of size \(N\) with much smaller weighted data sets of size \(N'\). In parallel to this focus on \(N\), the dependency on \(C\) has also very recently been addressed, e.g., by using dual-tree approaches Curtin [2017] or variational approximations to exact EM Dai and Lücke [2014], Hughes and Sudderth [2016], Forster and Lücke [2018]. Dual-tree approaches can reproduce \(k\)-means (Lloyd’s algorithm) exactly with computational costs of \(O(N + C \log C)\) per iteration under some assumptions (where \(D\) is implicit). Additionally, tree construction of \(O(N \log N)\) is required at initialization. Variational EM methods follow another approach by first replacing the clustering objective by a lower bound (which is often referred to as free energy, e.g., by Neal and Hinton 1998 or Jordan et al. 1999, or by ELBO, e.g., Hoffman et al. 2013). Such variational lower bounds can then be optimized more efficiently. Here we use truncated variational approximations. Such approximations have been applied to scale different types of probabilistic data models, including sparse coding (e.g., Sheikh and Lücke [2016, topic models Hughes and Sudderth [2016], and mixture models Dai and Lücke [2014], Shelton et al. [2014], Hughes and Sudderth [2016], Lee et al. [2017]. Truncated approximations increase efficiency by neglecting latent values with low posterior probabilities. For clustering with isotropic clusters, this means neglecting distant clusters. Such neglect ideas were observed to reduce computational demands for probabilistic clustering approaches Dai and Lücke [2014], Hughes and Sudderth [2016], Forster and Lücke [2018] as well as for deterministic approaches such as \(k\)-means. For the latter, e.g. Phillips [2002], Agustsson et al. [2017] obtained algorithms scaling with \(O(NyD + C^2D)\) per iteration (where \(y < C\)). In contrast, other popular approaches for the acceleration of clustering Elkan [2003], Hamerly [2010] require at least one iteration which scales with \(O(NCD)\) (plus an \(O(C^2D)\) term to, e.g., keep track of boundary values for distances). Important for this work, efficiency of variational EM has recently been reduced still further by applying partial instead of full variational E-steps to GMMs Forster and Lücke [2018]. The most efficient such algorithms scaled with \(O(NG^2D)\) per iteration, where \(G\ll C\) is a small constant depending on cluster neighborhood relations.

The contribution of this work is a merger of fast coreset approximations Bachem et al. [2018] with fast variational EM approximations Forster and Lücke [2018] for GMMs. While data-specific, heuristic combinations of coresets and variational models have been successfully proposed before [e.g., Lee et al., 2017], we here follow a mathematically grounded approach and derive a single clustering objective which combines variational lower bounds with coreset likelihoods. We then show that recent approaches for efficient variational optimization Forster and Lücke [2018] can be generalized to the merged objective. The derived algorithm, for which we additionally use efficient seeding Bachem et al. [2016b,a], provably increases the merged objective and strongly reduces the run-time complexity per EM iteration to \(O(N'G^2D)\). A concrete realization of the algorithm is then used to show that theoretical complexity reductions translate into practically applicable algorithms with strongly reduced clustering times.

2 Merged Objective and Efficient Optimization

We approach the task of clustering by fitting a probabilistic data model in the form of Gaussian mixtures to a set of \(N\) data points \(\{\tilde{y}^{(1)}, \ldots, \tilde{y}^{(N)}\} \in \mathbb{R}^D\). We use the most elementary such mixture model with \(C\) isotropic clusters and equal mixing proportions. For a data point \(\tilde{y}\), the probability density is then given by

\[
 p(\tilde{y} | \Theta) = \frac{1}{C} (2\pi\sigma^2)^{-\frac{D}{2}} \sum_{c=1}^{C} \exp\left(-\frac{1}{2\sigma^2} \|\tilde{y} - \tilde{\mu}_c\|^2\right),
\]  

(1)

where \(\| \cdot \|\) denotes the standard Euclidean distance in \(\mathbb{R}^D\). Given this model, the clustering task takes the form of finding \(C\) cluster centers \(\tilde{\mu}_c\) and one cluster variance \(\sigma^2\), and we will use \(\Theta = \{\tilde{\mu}_1, \ldots, \tilde{\mu}_C, \sigma^2\}\) to denote these model parameters. The standard approach to finding parameters \(\Theta\) which fit a set of \(N\) data points well is to maximize the data log-likelihood \(L(\Theta) = \sum_{n=1}^{N} \log(p(\tilde{y}^{(n)} | \Theta))\). By inserting the GMM (1), the maximum likelihood solution \(\Theta^*\) for the clustering of \(N\) data points can formally be stated by:

\[
 \Theta^* = \arg\max_{\Theta} \left\{ L(\Theta) \right\}, \quad \text{with (2)}
\]

\[
 L(\Theta) = \sum_{n=1}^{N} \log \left( \sum_{c=1}^{C} \exp\left( -\frac{\|\tilde{y}^{(n)} - \tilde{\mu}_c\|^2}{2\sigma^2} \right) \right) + B(\sigma), \quad \text{(3)}
\]
where \( B(\sigma) = -N \log(C) - \frac{ND}{2} \log(2\pi\sigma^2) \). This likelihood objective requires the evaluation of \( NC \) distances; the total cost for computing the objective is therefore \( O(NCD) \).

Merging Coreset and Variational Objective. On a set of \( N \) data points, a coreset can be defined as a subset of \( N' < N \) data points with \( N' \) positive weights \( \gamma(n) \in \mathbb{R}^+ \) such that training on the approximates coreset training on the original data set. Given such a coreset \( \{\bar{y}^{(n)}, \gamma(n)\}_{n=1}^{N'} \) and GMM (1), we can, following Lucic et al. [2018], define a log-likelihood function of the following form:

\[
L^{\text{core}}(\Theta) = \sum_{n=1}^{N'} \gamma(n) \log(p(\bar{y}(n)|\Theta))
\]  

(4)

where \( p(\bar{y} | \Theta) \) denotes the GMM density (1). If coresets for GMMs are appropriately constructed, then the solutions for the optimization of (4) are close approximations to the solutions w.r.t. objective (3). For details see, e.g., Lucic et al. [2018].

An approximation of \( L(\Theta) \) alternative to a coreset likelihood (4) is provided by the application of variational EM (e.g., Jordan et al. 1999). Variational EM optimizes a lower bound of the likelihood. Such variational lower bounds (aka free energies or ELBOs) are defined (A) to be efficiently computable, and (B) to match the actual likelihood as closely as possible. Variational bounds (here denoted by \( \mathcal{F}(\Lambda, \Theta) \)) contain additional parameters (here \( \Lambda \)), which are optimized in a variational E-step that replaces the computation of full posterior probabilities in standard E-steps.

For our purposes, we now seek to combine the approximations \( L^{\text{core}}(\Theta) \) with efficiently computable variational bounds \( \mathcal{F}(\Lambda, \Theta) \). Variational bounds result from the introduction of variational approximations \( q^{(n)}(c; \Lambda) \) to exact posteriors \( p(c|\bar{y}^{(n)}, \Theta) \) via the application of Jensen’s inequality Jensen [1906], Bishop [2006]. Here, we first have to generalize the standard derivation in two ways: (A) in order to include the coreset weights, and (B) to allow for variational distributions \( q^{(n)}(c; \Lambda) \) with ‘hard’ zeros (which will be very important for efficiency). A detailed derivation is given in Suppl. A. Importantly, neither coreset weights nor ‘hard’ zeros interfere with the essential derivation steps. Variational bounds are consequently given in the form:

\[
\mathcal{F}(\Lambda, \Theta) = \sum_{n=1}^{N'} \gamma(n) \left\{ \log(p(c, \bar{y}^{(n)} | \Theta)) \right\}_{q^{(n)}} - \sum_{n=1}^{N'} \gamma(n) \left\{ \log(q^{(n)}(c; \Lambda)) \right\}_{q^{(n)}}.
\]  

(5)

where \( \langle \cdot \rangle_{q^{(n)}} \) denotes the expectation value w.r.t. the variational distribution \( q^{(n)}(c; \Lambda) \). We now choose variational distributions in a specific form using truncated posteriors:

\[
q^{(n)}(c; \mathcal{K}, \hat{\Theta}) = \frac{p(c, \bar{y}^{(n)}|\hat{\Theta})}{\sum_{\hat{c} \in \mathcal{K}^{(n)}} p(\hat{c}, \bar{y}^{(n)}|\hat{\Theta})} \delta(c \in \mathcal{K}^{(n)}),
\]  

(6)

where \( \hat{\Theta} \) are model parameters of the variational distribution, \( \mathcal{K}^{(n)} \) is a subset of the index set \( \{1, \ldots, C\} \), and \( \delta(c \in \mathcal{K}^{(n)}) = 1 \) if \( c \in \mathcal{K}^{(n)} \) and zero otherwise. Truncated posteriors are a natural choice to consider more than one ‘winning’ cluster while otherwise maintaining ‘hard’ zeros Forster and Lücke [2018]. The size of all \( \mathcal{K}^{(n)} \) we take to be constrained to \( |\mathcal{K}^{(n)}| = C' \) (i.e., \( C' \) ‘winning’ clusters). The variational parameters are then \( \Lambda = (\mathcal{K}, \hat{\Theta}) \). If full posteriors are dominated by few large values, variational distributions (6) approximate the full posteriors very well. For clustering and natural data sets, such a dominance of few values for posteriors \( p(c|\bar{y}^{(n)}, \Theta) \) (i.e., of few cluster responsibilities) is indeed very frequently observed. While being able to approximate true posteriors well, distributions (6) were indeed very frequently observed. While being able to approximate true posteriors well, distributions (6) were shown to reduce computational costs Dai and Lücke [2014], Sheikh and Lücke [2016], Hughes and Sudderth [2016]. Inserting the truncated distributions (6) into the variational bound for coresets (5), we obtain:

\[
\mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta) = \sum_{n=1}^{N'} \gamma(n) \sum_{c \in \mathcal{K}^{(n)}} s_c^{(n)} \log \left( \frac{p(c, \bar{y}^{(n)}|\Theta)}{s_c^{(n)}} \right).
\]  

(7)

where we have abbreviated distributions \( q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \) of (6) by \( s_c^{(n)} \). The total number of terms that have to be computed for objective (7) now grows with \( O(N'C') \), where \( C' \leq C \) is the number of clusters considered for each data point. The cost of each term in the sum remains \( O(D) \) because of the distance evaluations. The relation among the original, coreset and variational objective can be summarized as follows:

\[
L(\Theta) \approx L^{\text{core}}(\Theta) \geq \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta).
\]  

(8)
The cost to compute the objectives decreases from left to right but also the approximation quality decreases. However, while the computational cost strongly decreases, we can expect to maintain a relatively high approximation quality because of the way coresets and variational objectives can be defined. A number of results have shown that coresets give rise to very accurate clustering results compared to full data sets Lucic et al. [2018], Bachem et al. [2018], and truncated variational EM has been shown to result in tight lower bounds and to be advantageous in avoiding local optima Sheikh et al. [2014], Sheikh and Lücke [2016], Hughes and Sudderth [2016], Forster and Lücke [2018]. Furthermore, the degree of accuracy and efficiency can be traded off by choosing the approximation parameters \( C' \) and \( N' \). In their limits, the variational lower bound recovers the coreset likelihood (for \( C' \to C \)), and coreset likelihoods typically recover the original likelihood for \( N' \to N \).

The question now remains, how the objective (7) can be optimized efficiently.

**Optimization of Model Parameters: M-Step.** Although the number of summands in the merged objective (7) is strongly reduced, its basic analytical structure remains similar to the standard structure of variational lower bounds. The derivation of parameter update equations for (7) can therefore proceed essentially along the same lines as for standard EM for GMMs. By following Lucic et al. [2018] and by simultaneously replacing full posteriors \( p(c | \hat{y}^{(n)}, \Theta) \) with variational distributions \( q^{(n)}(c; \hat{K}, \hat{\Theta}) \), we obtain:

\[
\bar{\mu}^{\text{new}}_c = \frac{\sum_{n=1}^{N'} \gamma^{(n)} s_c^{(n)} \hat{y}^{(n)}}{\sum_{n=1}^{N'} \gamma^{(n)} s_c^{(n)}},
\]

\[
\sigma^2_{\text{new}} = \frac{1}{D} \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in K^{(n)}} \gamma^{(n)} s_c^{(n)} ||\tilde{y} - \bar{\mu}^{\text{new}}_c||^2.
\]

Because of the ‘hard’ zeros of \( s^{(n)}_c \) for \( c \not\in K^{(n)} \), the number of required computations for the M-step is of \( O(N'C'D) \).

**Optimization of Variational Parameters: E-Step.** A crucial and typically the computationally most demanding step in optimizations of probabilistic generative models is the E-step. In our case, we seek variational parameters \( \hat{K}, \hat{\Theta} \) that optimize the variational bound (7) while keeping \( \Theta \) fixed. A concern may be that this optimization w.r.t. \( K \) and \( \hat{\Theta} \) is much more demanding than the M-step optimization. This is because of the much larger search space consisting of all subsets \( \mathcal{K}^{(n)} \subseteq \{1, \ldots, C\} \) with size \( C' \). Therefore, while computation of the objective (7) is efficient, the size of the search space to find the best \( \mathcal{K}^{(n)} \) represents a combinatorial problem of size \( \binom{C}{C'} \), which for the whole \( \mathcal{K} = (\mathcal{K}^{(1)}, \ldots, \mathcal{K}^{(N')}) \) results in a total of \( \binom{C}{C'} \) to the power of \( N' \) combinations. In general, optimizations of functions depending on \( K \) can for this reason not be expected to be very efficient. For the merged objective (7), we can, however, make use of a number of theoretical results which can be derived for truncated variational distributions. More specifically:

(A) We use that \( \hat{\Theta} = \Theta \) maximizes \( \mathcal{F}(K, \hat{\Theta}, \Theta) \) w.r.t. \( K \) and \( \Theta \) are held fixed.

(B) We make use of a simplified functional form of \( \mathcal{F}(K, \hat{\Theta}, \Theta) \) for \( \hat{\Theta} = \Theta \).

(C) We define a partial E-step that increases instead of maximizes the variational bound.

To (A): Considering (7) we can generalize the proof by Lücke [2017] in order to show that \( \mathcal{F}(K, \Theta, \Theta) \) is an optimum of the lower bound \( \mathcal{F}(K, \hat{\Theta}, \Theta) \) if \( K \) and \( \Theta \) are held fixed (the coreset weights \( \gamma^{(n)} \) do not interfere with the main analytical steps, as shown in Suppl. B). The optimization problem that remains for the E-step is consequently the optimization of \( \mathcal{F}(K, \Theta, \Theta) =: \mathcal{F}(K, \Theta) \) w.r.t. sets \( \mathcal{K} \).

To (B): We can generalize a result for variational bounds with truncated distributions to the coreset-weighted variational bounds (7). Concretely, we obtain that the functional form of \( \mathcal{F}(K, \Theta) \) can be simplified to (see again Suppl. B):

\[
\mathcal{F}(K, \Theta) = \sum_{n=1}^{N'} \gamma^{(n)} \log \left( \sum_{c \in K^{(n)}} p(c, \hat{y}^{(n)}|\Theta) \right). \quad (10)
\]

The functional form of (10) is central in solving the optimization problem efficiently. In contrast to (5), the bound (10) shows no dependency on an entropy term for the approximate posteriors \( s^{(n)}_c \), and indeed no dependency on \( s^{(n)}_c \) at all. As \( \mathcal{F}(K, \Theta) \) now consists of a single sum with positive coreset weights \( \gamma^{(n)} \) and the strictly monotonic logarithm, it is sufficient to find for each \( n \) the \( C' \) clusters \( c \) with the largest joints \( p(c, \hat{y}^{(n)}|\Theta) \) to maximize (10). The optimization problem on the spaces of size \( \binom{C}{C'} \) for each \( n \) is consequently solvable with \( O(N'C) \) computations in total.
To (C): The above scaling is much more favorable than may have been expected at first. However, compared to the M-step with $O(N'C^2)$, such an E-step scaling is still not efficient enough. Therefore, we further improve efficiency by merely seeking to increase $\mathcal{T}(\mathcal{K}, \Theta)$ in each E-step instead of fully maximizing it. To do so, we generalize the result of Forster and Lücke [2018] for variational bounds with truncated distributions (6) to coreset-weighted truncated variational bounds, i.e., we show that pair-wise comparisons of distances are sufficient to warrant the variational bound to increase:

Proposition 1
Consider a coreset $(\tilde{y}^{(n)}(n), \gamma^{(n)})_{n=1,...,N'}$ for the GMM (1) with parameters $\Theta$, and the merged variational bound (10) with variational parameters $\mathcal{K}$. If we replace for an arbitrary $n$ a cluster $c \in \mathcal{K}(n)$ by a cluster $c^{\text{new}} \notin \mathcal{K}(n)$, then the variational bound increases if and only if:

$$\|\tilde{y}^{(n)}(n) - \bar{\mu}_{c,\text{new}}\| < \|\tilde{y}^{(n)}(n) - \bar{\mu}_c\|$$

(11)

The proof is given in Suppl. C.

The important observation for the proof is that the coreset weights $\gamma^{(n)}(n)$ do not change the criterion (11) compared to results for full data sets. This is because sets $\mathcal{K}(n)$ are optimized individually for each $n$, which means that the pair-wise comparison of distances is unaffected by the common positive multiplier $\gamma^{(n)}$. We can consequently apply the same efficient variational E-step as suggested by Forster and Lücke [2018] for the var-GMM-S algorithm.

3 Algorithmic Realization

In order to realize a concrete algorithm, we integrate the optimization of objective (7) with coreset construction. Additionally, we will use efficient seeding.

Constructing Lightweight Coresets. Algorithms for coreset construction come with different theoretical guarantees and different scaling properties. Coreset constructions that have been suggested previously Har-Peled and Mazumdar [2004] allow for relatively small coresets with still high guarantees for scaling. For our purposes, their construction is however computationally too demanding compared to the very efficient optimization of objective (7) itself. We therefore chose the recently suggested lightweight coresets Bachem et al. [2018] (LWCS), which are substantially faster to construct. They require only two passes through the data set with complexity $O(ND)$.

Efficient Seeding. Given an LWCS, we could start optimizing objective (7) by choosing initial cluster centers, e.g., randomly uniform. However, novel seeding techniques Bachem et al. [2016a,b], Newling and Fleuret [2017] offer improvements over random initializations. Proper seeding can improve the clustering quality and reduce the number of iterations until convergence. Here we adopt the AFK-MC² algorithm Bachem et al. [2016a], which has also been used for var-GMM-S in Forster and Lücke [2018]. For seeding, an initial single pass through the data with $O(N'D)$ is required to define a proposal distribution. The cluster centers are then computed using independent Markov chains of length $m$, resulting in a main seeding loop with complexity $O(mC^2D)$.

Initial Variance Estimation. In addition to the initialization of cluster centers $\mu_c$, efficient seeding methods, var-GMM-S and vc-GMM require an initial variance value to compute parameter updates in the M-step. To avoid having to specify this parameter value manually for each data set, we apply an efficient automated procedure to generate a coarse estimate for the initial variance: Since the optimization of the variational parameters $\mathcal{K}(n)$ during the E-step is independent of the variance, we first optimize these without computing $s_c^{(n)}(n)$ or performing M-steps. As the $\mathcal{K}(n)$ estimate the closest cluster centers for each data point, the distances of data points $\tilde{y}^{(n)}(n)$ with regard to clusters in $\mathcal{K}(n)$ then provide an estimate of the data variance:

$$\sigma^2_{\text{init}} = \frac{\sum_{n=1}^{N'} \gamma^{(n)}(n) \min_{c \in \mathcal{K}(n)} \|\bar{\mu}_{c,\text{init}} - \tilde{y}^{(n)}(n)\|^2}{D \sum_{n=1}^{N'} \gamma^{(n)}(n)}.$$  

(12)

In our experiments, the variational algorithms have been shown to be very robust to these initial values, with a coarse estimate of the approximate order of magnitude generally being sufficient. Thus, no additional $\mathcal{K}(n)$ optimization steps other than the first E-step (or initial E-steps as discussed in Suppl. F) were necessary for our experiments to gain sufficient initial values $\sigma^2$. Variational EM for the Merged Objective. After LWCS construction (which provides the weights $\gamma^{(n)}(n)$), seeding based on AFK-MC² (which provides the initial means $\bar{\mu}_c$) and initial variance estimation, we can now update the parameters to maximize the objective (7). To
Algorithm 1: The vc-GMM algorithm.

\begin{algorithm}
\begin{algorithmic}
\State construct LWCS ($\vec{y}^{(n)}$, $\gamma^{(n)})_{n=1...N'}$;
\State init $\mu_{1:C}$ (using AFK-MC$^2$) and $\sigma^2$;
\State init $\mathcal{G}_c$ randomly for all $c = 1, \ldots, C$;
\State init $\mathcal{K}^{(n)}$ randomly for all $n = 1, \ldots, N'$;
\Repeat
\For{$n = 1 : N'$}
\State $\mathcal{G}^{(n)} = \bigcup_{c \in \mathcal{K}^{(n)}} \mathcal{G}_c$;
\EndFor
\For{$c \in \mathcal{G}^{(n)}$}
\State $d_c^{(n)} = \|\vec{y}^{(n)} - \mu_c\|$;
\EndFor
\State update $\mathcal{K}^{(n)}$ to include $C'$ smallest $d_c^{(n)}$'s;
\EndFor
\For{$c = 1 : C$}
\State update $\mathcal{G}_c$ to include $G$ closest clusters to $c$;
\EndFor
\For{$n = 1 : N'$}
\EndFor
\For{$c \in \mathcal{K}^{(n)}$}
\State $s_c^{(n)} = \frac{\exp(-\frac{1}{2}(d_c^{(n)})/\sigma^2)}{\Sigma_{c' \in \mathcal{G}^{(n)}} \exp(-\frac{1}{2}(d_c^{(n)})/\sigma^2)}$;
\EndFor
\For{$n = 1 : N'$}
\For{$c \in \mathcal{K}^{(n)}$}
\State $\mu_c^{\text{new}} = \mu_c + \gamma(n) s_c^{(n)} \vec{y}^{(n)}$;
\State $\mu_c^{\text{tot}} = \mu_c^{\text{tot}} + \gamma(n) s_c^{(n)}$;
\EndFor
\State $\mu_c = \mu_c^{\text{new}} / \mu_c^{\text{tot}}$;
\EndFor
\For{$n = 1 : N'$}
\EndFor
\State $\sigma^2 = \sigma^2 + (\frac{\gamma(n) s_c^{(n)} \vec{y}^{(n)} - \mu_c\|^2}{\Sigma_{c' \in \mathcal{G}^{(n)}} \gamma(n)}$;
\EndFor
\Until $f(\mu_{1:C}, \sigma^2)$ has converged;
\end{algorithmic}
\end{algorithm}

\end{document}
Figure 1: Relative quantization error and speedup of vc-GMM, k-means on lightweight coresets (LWCS), var-GMM-S, AFK-MC² seeding, and k-means++. Each row refers to one benchmark (with increasing cluster numbers from top to bottom). The y-axes denote the relative quantization error with respect to k-means++, as given in Eq. (14). Different parameter settings of the algorithms show the trade-off between effectiveness (in terms of quantization error) and speed (in terms of distance evaluations, in the left column; and run time, in the middle column). Measurements for vc-GMM (with fixed G as given in the plot legends) and LWCS are given for five different coreset sizes N', denoted in the plots. The right column shows the performance trade-off due to decreasing coreset sizes of vc-GMM and LWCS. For vc-GMM and LWCS we also included the standard error of the mean (SEM), which is however very small except for one subplot (RNA). Measurements for var-GMM-S refer to configurations with G ∈ {3 +1, 5, 7} (+1' denotes one random additional cluster per G⁽ⁿ⁾), where settings with larger G lie to the right, as they require more distance evaluations and higher run times. Measurements for AFK-MC² seeding refers to Markov chains of lengths m = 2, 5, 10, 20 (from left to right). In addition to SONG with C = 4000, we provide SONG with C = 2000 in Suppl. Fig. S.1.
| Algorithm | G       | N'     | Relative Error $\eta$ | Speedup | Speedup | EM | Corest + Seeding |
|-----------|---------|--------|------------------------|---------|---------|----|------------------|
| KDD       | $k$-means++ | -      | $0.00\% \pm 0.04$     | 1.0x    | 1.0x    | 13.0 | 22%              |
|           | var-GMM-S | 5      | $0.94\% \pm 0.07$     | 6.4x    | 23.4x   | 17.0 | 1%               |
|           | LWCS     | 2\textsuperscript{13} | $11.73\% \pm 0.18$ | 27.8x   | 24.2x   | 10.2 | 3%               |
|           | vc-GMM   | 5       | $10.81\% \pm 0.08$    | 91.5x   | 361.0x  | 17.9 | 12%              |
| RNA       | $k$-means++ | -      | $0.00\% \pm 0.22$     | 1.0x    | 1.0x    | 18.0 | 15%              |
|           | var-GMM-S | 3 + 1  | $-1.59\% \pm 0.23$    | 1.6x    | 19.2x   | 72.3 | <1%              |
|           | LWCS     | 2\textsuperscript{15} | $11.24\% \pm 0.60$ | 21.2x   | 19.8x   | 14.2 | 3%               |
|           | vc-GMM   | 3 + 1\textsuperscript{2} | $7.28\% \pm 0.28$   | 33.3x   | 329.4x  | 47.8 | 5%               |
| CIFAR-10  | $k$-means++ | -      | $0.00\% \pm 0.02$     | 1.0x    | 1.0x    | 10.7 | 9%               |
|           | var-GMM-S | 5      | $-0.75\% \pm 0.02$    | 12.6x   | 16.4x   | 16.7 | 1%               |
|           | LWCS     | 2\textsuperscript{12} | $10.34\% \pm 0.03$  | 17.3x   | 17.6x   | 8.0  | 2%               |
|           | vc-GMM   | 5       | $8.98\% \pm 0.03$     | 166.4x  | 207.8x  | 13.4 | 20%              |
| SUSY      | $k$-means++ | -      | $0.00\% \pm 0.01$     | 1.0 x   | 1.0 x  | 47.5 | 7%               |
|           | var-GMM-S | 5      | $0.76\% \pm 0.01$     | 10.1x   | 83.8x   | 63.7 | <1%              |
|           | LWCS     | 2\textsuperscript{15} | $9.89\% \pm 0.02$   | 395.3x  | 381.8x  | 19.3 | 3%               |
|           | vc-GMM   | 5       | $9.55\% \pm 0.03$     | 1300.4x | 9964.3x | 62.8 | 11%              |
| SONG      | $k$-means++ | -      | $0.00\% \pm 0.01$     | 1.0x    | 1.0x    | 11.0 | 19%              |
|           | var-GMM-S | 5      | $0.99\% \pm 0.02$     | 24.9x   | 79.1x   | 26.2 | 1%               |
|           | LWCS     | 2\textsuperscript{16} | $10.42\% \pm 0.18$  | 10.5x   | 10.3x   | 9.1  | 1%               |
|           | vc-GMM   | 5       | $9.23\% \pm 0.07$     | 166.6x  | 513.9x  | 22.3 | 11%              |

Table 1: Relative quantization error (with SEM) and speedup of the algorithms in Fig. 1 with $k$-means++ as baseline. For vc-GMM and LWCS, we show values for coreset sizes that result in trade-offs that are closest to a maximal increase in error relative to $k$-means++ of around 10%. For var-GMM-S, we show values for the same $G$ parameter as used in vc-GMM. The last column shows the fraction of time spent on coreset construction and seeding.

where $Q$ denotes the quantization error for the considered approaches ($Q_{\text{algo}}$) and for $k$-means++ ($Q_{\text{kmpp}}$). Likelihood based measures would be more natural for vc-GMM but would hinder comparison. We additionally provide the normalized mutual information with respect to $k$-means++ solutions on the test data set (for CIFAR-10) or on the full data set (for all other benchmarks) in Suppl. Fig. S.2. The algorithms we compare to are: AFK-MC$^2$ seeding, $k$-means++, var-GMM-S, and LWCS followed by $k$-means updates. The latter is simply referred to as LWCS. var-GMM-S, LWCS and our vc-GMM use AFK-MC$^2$ for seeding. All algorithms were executed until the same convergence criterion was reached: We declared convergence if the relative change of the clustering objective fell below a threshold of $10^{-4}$ (Suppl. F for details). Fig. 1 shows clustering times and quantization errors for different settings of the algorithms at convergence. After convergence, quantization errors were for all algorithms computed on the standard test set (for CIFAR-10) or on the full data set (all other benchmarks), and are given relative to the quantization error of $k$-means++, which serves as baseline. Computational demand was measured in terms of executed distance evaluations until convergence (Fig. 1, left column) w.r.t. E-steps, seeding and coreset construction. Distance evaluations are often used for comparisons Bachem et al. [2016b], Forster and Lücke [2018] because they are implementation independent and align with the theoretically achievable optimum. In addition, we here also show the actual elapsed run time of the algorithms until convergence (middle column). Variational algorithms such as vc-GMM make use of more diverse updates than $k$-means. For vc-GMM and var-GMM-S overloads include updates of search spaces $G^{(n)}$, the computation of approximate posteriors $s^{(n)}_{c}$ from distances and more demanding M-step updates, as well as the update of index sets $\mathcal{K}^{(n)}$ and $\mathcal{G}_{c}$. We were therefore interested also in how much such overhead costs do impact actual execution times given a concrete implementation. To measure the elapsed time, we implemented all compared
algorithms, including seeding and LWCS construction, in C++ source code of equal structure.\footnote{Implementation available at https://bitbucket.org/fhirschberger/clustering/} The elapsed time until convergence was measured on a dual Xeon E5-2630 v4 system with 256GB of memory. For our measurements, elapsed time includes all computations required for each algorithm, including seeding, coreset construction and parameter optimization.

In order to investigate the trade-off between execution times and clustering quality, we use different values $G$ for vc-GMM and var-GMM-S, different values of $N'$ for LWCS and vc-GMM, and different values for $m$ for AFK-MC\textsuperscript{2}. In all cases other than $k$-means++ we used AFK-MC\textsuperscript{2} seeding for initialization with $m = 2$ for KDD, SONG, SUSY and CIFAR-10 and $m = 20$ for RNA. Fig. 1 shows results for the different settings as averages over 50 independent runs with new random seeds. Time measurements refer to the average time of one sequential execution of the algorithm with multiple independent seeds running in parallel. Tab. 1 shows more details on the average number of EM iterations until convergence and the time spent for coreset construction and seeding alone. The performance trade-off for LWCS and vc-GMM is compared for an error increase of \( \sim 10\% \).

By considering Fig. 1 and Tab. 1 it can be observed that vc-GMM (Alg. 1) can strongly reduce execution times in terms of distance evaluations as well as in terms of elapsed time. The overhead for auxiliary operations and M-steps does (as expected) impact the elapsed time measurements compared to the measured number of distance evaluations. However, like for distance evaluations, elapsed time speedups are very significant especially for large-scale clustering tasks. For CIFAR-10 with $C = 500$ and SONG with $C = 4000$, for instance, we observe up to one order of magnitude faster execution times than for (already highly efficient) LWCS-based clustering, with at the same time lower increases in clustering error. The results are discussed in a broader context below.

### 5 Discussion and Conclusion

How can we obtain as good as possible clustering results in as short times as possible? To address this question we have in this work combined efficient coreset construction with variational EM acceleration. The resulting algorithm, vc-GMM, can analytically be shown to scale with $O(N'G^2D)$ per iteration. Further numerical experiments revealed that the analytical complexity reduction translates into a concretely applicable algorithm with high efficiency. On standard benchmarks, we observed significant speedups while high clustering qualities were maintained. Fig. 1 illustrates the trade-off between clustering efficiency and quality for vc-GMM in comparison to clustering based on seeding, coresets, or variational EM alone. As can be observed, each approach trades off clustering efficiency and quality differently. The recent AFK-MC\textsuperscript{2} Bachem et al. [2016a] seeding is the fastest method, but clustering quality has clear limits (see Fig. 1). Variational acceleration with var-GMM-S Forster and Lücke [2018], on the other hand, maintains a high clustering quality, but speedups are finally limited (there is a lower limit on search space sizes). Furthermore, var-GMM-S has a high memory demand for large $N$.

The here investigated vc-GMM approach combines very fast clustering with high clustering quality by merging fast coresets Bachem et al. [2018] with variational EM Forster and Lücke [2018]. The speedup is most significant for large scale problems (large $N$, large $C$ and large $D$), i.e., when computational costs are highest. E.g., for SONG ($C = 4000$), we observed almost two orders of magnitude faster execution times compared to $k$-means++ with a decrease in quality of just $5\%$ (Fig. 1). And even compared to the already highly efficient LWCS based algorithm Bachem et al. [2018], we find that for same coreset sizes, error increases of vc-GMM are often comparable or lower, while achieving speedups of up to and over one order of magnitude on large scale data sets (e.g., SONG, CIFAR-10). For smaller scale clustering tasks, e.g., RNA, with relatively few features $D$, elapsed time speedups are less significant. But note that (considering Fig. 1), e.g., for a quality in the range of 10\% of $k$-means++, vc-GMM is still about 50\% faster than LWCS.

For the large-scale problems here considered, observe that seeding (and coreset construction) itself already makes up a large percentages of the total elapsed time (Tab. 1), i.e., the scaling of seeding with $C^2$ becomes an inadmissible factor for the total execution time. For problems with still larger $C$, future work on seeding or on efficient distance evaluations without $C^2$ scaling would therefore become more relevant. Further future work, which has not been the focus here, includes optimizations for parallel implementations and generalizations to GMMs with non-isotropic clusters.
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A Derivation of the Variational Bound for Coresets and Truncated Distributions

We provide detailed derivations for the main results used in the main text. Most of the derivations follow along similar lines as proofs in Lücke [2017]. The main observation is that the coreset weights do not interfere with the main analytical steps, such that results carry over when coresets are used.

We first derive a variational lower bound of the coreset likelihood (4) along the lines of standard variational EM Jordan et al. [1999]:

\[
L_{\text{core}}(\Theta) = \sum_{n=1}^{N'} \gamma(n) \log \left( p(\tilde{y}^{(n)}|\Theta) \right)
\]

\[
= \sum_{n=1}^{N'} \gamma(n) \log \left( \sum_{c=1}^{C} p(\tilde{y}^{(n)}, c|\Theta) \right)
\]

\[
= \sum_{n=1}^{N'} \gamma(n) \log \left( \sum_{c=1}^{C} q^{(n)}(c; \Lambda) \frac{p(\tilde{y}^{(n)}, c|\Theta)}{q^{(n)}(c; \Lambda)} \right),
\]

(15)

In the last step of (15), we introduced strictly positive variational distributions \( q^{(n)}(c; \Lambda) \). To derive a variational bound for truncated distributions \( q^{(n)}(c; \Lambda) = q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \) with hard zeros for all \( c \notin \mathcal{K}^{(n)} \), we consider the following reformulation:

\[
q^{(n)}(c; \mathcal{K}, \hat{\Theta}) = \frac{p(\tilde{y}^{(n)}, c|\hat{\Theta})}{\sum_{c' \in \mathcal{K}^{(n)}} p(\tilde{y}^{(n)}, c'|\hat{\Theta})} \delta(c \in \mathcal{K}^{(n)})
\]

\[
= \lim_{\epsilon_n \to 0} q^{(n)}(c; \mathcal{K}, \hat{\Theta}),
\]

(16)

with

\[
\tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) = \begin{cases} 
q^{(n)}(c; \mathcal{K}, \hat{\Theta}) - \epsilon_n^- & \forall c \in \mathcal{K}^{(n)} \\
q^{(n)}(c; \mathcal{K}, \hat{\Theta}) + \epsilon_n^+ & \forall c \notin \mathcal{K}^{(n)}
\end{cases}
\]

\[
= \begin{cases} 
q^{(n)}(c; \mathcal{K}, \hat{\Theta}) - \epsilon_n^- & \forall c \in \mathcal{K}^{(n)} \\
\epsilon_n^- & \forall c \notin \mathcal{K}^{(n)}
\end{cases},
\]

(17)

using

\[
0 < \epsilon_n^- < \min_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta})
\]

(18)

and

\[
\epsilon_n^+ := \frac{|\mathcal{K}^{(n)}|}{C - |\mathcal{K}^{(n)}|} \epsilon_n^- = \frac{C'}{C - C'} \epsilon_n^-.
\]

(19)

This reformulation leads to strictly positive variational distributions \( \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \) with \( \sum_c \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) = 1 \), that in the limit of \( \epsilon_n^- \to 0 \) recover the aimed at truncated distributions \( q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \). We now insert \( q^{(n)}(c; \Lambda) = \lim_{\epsilon_n \to 0} \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \) into Eq. (15) and use Jensen’s inequality to gain a lower bound for truncated distributions:

\[
L_{\text{core}}(\Theta) = \sum_{n=1}^{N'} \lim_{\epsilon_n \to 0} \gamma(n) \log \left( \sum_{c=1}^{C} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \frac{p(\tilde{y}^{(n)}, c|\Theta)}{q^{(n)}(c; \mathcal{K}, \hat{\Theta})} \right)
\]

\[
\geq \sum_{n=1}^{N'} \lim_{\epsilon_n \to 0} \gamma(n) \sum_{c=1}^{C} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( \frac{p(\tilde{y}^{(n)}, c|\Theta)}{q^{(n)}(c; \mathcal{K}, \hat{\Theta})} \right)
\]

\[
:= \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta)
\]

(20)

Splitting of the sums and evaluation of the limits \( \epsilon_n \to 0 \) then leads to:

\[
L_{\text{core}}(\Theta) \geq \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta)
\]

\[
= \sum_{n=1}^{N'} \gamma(n) \left[ \lim_{\epsilon_n \to 0} \sum_{c \in \mathcal{K}^{(n)}} \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( p(\tilde{y}^{(n)}, c|\Theta) \right) 
\]

\[
+ \lim_{\epsilon_n \to 0} \sum_{c \notin \mathcal{K}^{(n)}} \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( p(\tilde{y}^{(n)}, c|\Theta) \right) 
\]

\[
- \lim_{\epsilon_n \to 0} \sum_{c \in \mathcal{K}^{(n)}} \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \right) 
\]

\[
- \lim_{\epsilon_n \to 0} \sum_{c \notin \mathcal{K}^{(n)}} \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \right) \right]
\]

\[
= \sum_{n=1}^{N'} \gamma(n) \left[ \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( p(\tilde{y}^{(n)}, c|\Theta) \right) + 0 
\]

\[
- \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \right) 
\]

\[
- \lim_{\epsilon_n \to 0} \sum_{c \notin \mathcal{K}^{(n)}} \frac{C'}{C - C'} \epsilon_n^- \log \left( \frac{C'}{C - C'} \epsilon_n^- \right) \right].
\]

(21)

The second term, which only considers \( c \notin \mathcal{K}^{(n)} \), directly evaluates to zero by definition of the \( \tilde{q}^{(n)}(c; \mathcal{K}, \hat{\Theta}) \). With \( \lim_{\epsilon \to 0} \epsilon \log(\epsilon) = 0 \), the last term also disappears and we arrive at the truncated variational bound:

\[
\mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta) = \sum_{n=1}^{N'} \gamma(n) \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( p(c, \tilde{y}^{(n)}|\Theta) \right)
\]

\[
+ \sum_{n=1}^{N'} \gamma(n) H(q^{(n)}(c; \mathcal{K}, \hat{\Theta})),
\]

(22)
with
\[ H(q^{(n)}(c; \mathcal{K}, \hat{\Theta})) = -\sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log(q^{(n)}(c; \mathcal{K}, \hat{\Theta})). \]

The derivation above generalizes the derivation for standard likelihoods Lücke [2017] to coreset likelihoods (4).

Based on the lower bound (22), the M-step equations (9) are derived following the standard procedure: We first take derivatives of \( F(\mathcal{K}, \hat{\Theta}, \Theta) \) in (22) w.r.t. \( \mu_c \) and \( \sigma^2 \). For the derivatives, \( \hat{\Theta} \) can be held fixed (which implies that the entropy term can be neglected). If we demand the derivatives to be zero, we obtain the M-steps (9).

**B Derivation of Variational E-Step**

We here show, that the simplified variational bound \( F(\mathcal{K}, \Theta) \) in Eq. (10) is indeed a lower bound of the coreset likelihood \( L^{\text{core}}(\Theta) \) (4) and an upper bound of \( F(\mathcal{K}, \hat{\Theta}, \Theta) \) (7), such that
\[
L^{\text{core}}(\Theta) \geq F(\mathcal{K}, \Theta) \geq F(\mathcal{K}, \hat{\Theta}, \Theta). \tag{23}
\]

Due to the truncated formulation of \( F(\mathcal{K}, \Theta) \) and the monotonicity of the logarithm, it is immediately clear, that \( F(\mathcal{K}, \Theta) \) is a lower bound of the coreset likelihood:
\[
L^{\text{core}}(\Theta) = \sum_{n=1}^{N'} \gamma^{(n)} \log \left( \sum_{c=1}^{C} p(c, \tilde{\gamma}^{(n)} | \Theta) \right) \geq \sum_{n=1}^{N'} \gamma^{(n)} \log \left( \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{\gamma}^{(n)} | \Theta) \right) =: F(\mathcal{K}, \Theta), \tag{24}
\]
which becomes tighter, the more probability mass of \( p(c, \tilde{\gamma}^{(n)} | \Theta) \) is covered in the subspace \( \mathcal{K}^{(n)} \).

For the relation between \( F(\mathcal{K}, \Theta) \) and \( F(\mathcal{K}, \hat{\Theta}, \Theta) \), we apply Jensen’s inequality to \( F(\mathcal{K}, \Theta) \) while using truncated distributions \( q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \) as in (6):
\[
F(\mathcal{K}, \Theta) := \sum_{n=1}^{N'} \gamma^{(n)} \log \left( \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{\gamma}^{(n)} | \Theta) \right) = \sum_{n=1}^{N'} \gamma^{(n)} \log \left( \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \frac{p(c, \tilde{\gamma}^{(n)} | \Theta)}{q^{(n)}(c; \mathcal{K}, \hat{\Theta})} \right) \geq \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( \frac{p(c, \tilde{\gamma}^{(n)} | \Theta)}{q^{(n)}(c; \mathcal{K}, \hat{\Theta})} \right) = F(\mathcal{K}, \hat{\Theta}, \Theta) \tag{25}
\]

The combination of (24) and (25) proves (23) and generalizes the proofs of Lücke [2017] to coreset-weighted data.

To show, that the variational bound \( F(\mathcal{K}, \Theta) \) (7) is identical to the simplified form \( F(\mathcal{K}, \Theta) \) (10) for \( \hat{\Theta} = \Theta \), i.e., \( F(\mathcal{K}, \Theta) \equiv F(\mathcal{K}, \Theta, \Theta) \), we proceed as follows: We insert \( s_{c}^{(n)} = q^{(n)}(c; \mathcal{K}, \Theta) \) of Eq. (6) into the variational lower bound Eq. (7), while making sure that \( \hat{\Theta} \) is set to \( \Theta \). We then derive:
\[
F(\mathcal{K}, \Theta, \Theta) = \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{\gamma}^{(n)} | \Theta) \log \left( \frac{p(c, \tilde{\gamma}^{(n)} | \Theta)}{q^{(n)}(c; \mathcal{K}, \Theta)} \right) = \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{\gamma}^{(n)} | \Theta) \log \left( \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{\gamma}^{(n)} | \Theta) \right) = F(\mathcal{K}) \tag{26}
\]

The combination of the equivalence (26) for \( \hat{\Theta} = \Theta \) and the relation (25) show that \( \hat{\Theta} = \Theta \) is a maximum of \( F(\mathcal{K}, \hat{\Theta}, \Theta) \) holding \( \mathcal{K} \) and \( \Theta \) fixed, which is again a generalization of the proofs of Lücke [2017] to coreset-weighted data.

For further analytical investigations of the properties of these bounds, we now regard the difference between \( L^{\text{core}}(\Theta) \) and \( F(\mathcal{K}, \hat{\Theta}, \Theta) \):
\[
L^{\text{core}}(\Theta) - F(\mathcal{K}, \hat{\Theta}, \Theta) = \sum_{n=1}^{N'} \gamma^{(n)} \log \left( p(\tilde{\gamma}^{(n)} | \Theta) \right) - \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( \frac{p(c, \tilde{\gamma}^{(n)} | \Theta)}{q^{(n)}(c; \mathcal{K}, \hat{\Theta})} \right) = \sum_{n=1}^{N'} \gamma^{(n)} \log \left( p(\tilde{\gamma}^{(n)} | \Theta) \right) - \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( \frac{p(c, \tilde{\gamma}^{(n)} | \Theta)}{q^{(n)}(c; \mathcal{K}, \hat{\Theta})} \right) + \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \log \left( q^{(n)}(c; \mathcal{K}, \hat{\Theta}) \right). \tag{27}
\]
Because of the definition of \(q^{(n)}(c; \mathcal{K}, \Theta)\), the summation over \(c\) of the second term directly evaluates to \(\sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \Theta) = 1\) and therefore the first and second term cancel out. Combination of the third and fourth term then recover coreset-weighted sums of Kullback-Leibler divergences between the distributions \(q^{(n)}(c; \mathcal{K}, \Theta)\) and \(p(c \mid \tilde{y}^{(n)}, \Theta)\):

\[
L_{\text{core}}(\Theta) - \mathcal{F}(\mathcal{K}, \Theta, \Theta) = - \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \Theta) \log \left( \frac{p(c \mid \tilde{y}^{(n)}, \Theta)}{q^{(n)}(c; \mathcal{K}, \Theta)} \right) - \sum_{n=1}^{N'} \gamma^{(n)} \sum_{c \in \mathcal{K}^{(n)}} q^{(n)}(c; \mathcal{K}, \Theta) \log \left( \frac{q^{(n)}(c; \mathcal{K}, \Theta)}{p(c \mid y^{(n)}, \Theta)} \right)
\]

\[
= \sum_{n=1}^{N'} \gamma^{(n)} D_{\text{KL}} \left( q^{(n)}(c; \mathcal{K}, \Theta), p(c \mid \tilde{y}^{(n)}, \Theta) \right) \geq 0, \quad (28)
\]

where for the identification with the KL-divergence, we again used that \(\lim_{\epsilon \to 0} \epsilon \log(\epsilon) = 0\), which allows to expand the sum over all \(c\).

The here used M-step for parameter updates (9) is derived such that \(\mathcal{F}(\mathcal{K}, \Theta, \Theta)\) is increased, and the variational E-step is defined to monotonically increase the lower bound \(\mathcal{F}(\mathcal{K}, \Theta)\) (see below). The used algorithm consequently provably increases the bound \(\mathcal{F}(\mathcal{K}, \Theta)\) in each EM iteration.

### C Proof of Proposition 1 for Coresets

To prove Prop. 1, we make use of the simplified form of the variational bound for \(\tilde{\Theta} = \Theta\):

\[
\mathcal{F}(\mathcal{K}, \Theta) = \sum_{n} \gamma^{(n)} \log \left( \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{y}^{(n)} \mid \Theta) \right). \quad (29)
\]

We now seek for those \(\mathcal{K} = (\mathcal{K}^{(1)}, \ldots, \mathcal{K}^{(N')})\) that maximize \(\mathcal{F}(\mathcal{K}, \Theta)\):

\[
\mathcal{F}(\tilde{\mathcal{K}}, \Theta) \geq \mathcal{F}(\mathcal{K}, \Theta) \iff \sum_{n} \gamma^{(n)} \log \left( \sum_{c \in \tilde{\mathcal{K}}^{(n)}} p(c, \tilde{y}^{(n)} \mid \Theta) \right) \geq \sum_{n} \gamma^{(n)} \log \left( \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{y}^{(n)} \mid \Theta) \right). \quad (30)
\]

For this maximization, it is sufficient to consider the case where \(\forall n:\)

\[
\log \left( \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{y}^{(n)} \mid \Theta) \right) \geq \log \left( \sum_{c \in \mathcal{K}^{(n)}} p(c, \tilde{y}^{(n)} \mid \Theta) \right),
\]

since for all \(n\) where this inequality does not hold, \(\tilde{\mathcal{K}}^{(n)}\) can directly be replaced by \(\mathcal{K}^{(n)}\) for these \(n\)-th summands in \(\mathcal{F}(\tilde{\mathcal{K}}, \Theta)\), which leads to a new increased variational bound, where the inequality (31) holds for all \(n\).

The optimization w.r.t. \(\mathcal{K}\) can therefore be regarded as individual optimization of the variational bound w.r.t. the \(\mathcal{K}^{(n)}\) for each individual corset-weighted data point. Consequently, this optimization is independent of the individual corset weights \(\gamma^{(n)}\). Considering the monotonicity of the logarithm, this problem then reduces to finding those \(\mathcal{K}^{(n)}\) for each data point \(\tilde{y}^{(n)}\) that have clusters \(c \in \mathcal{K}^{(n)}\) with highest cumulative joint probabilities \(p(c, \tilde{y}^{(n)} \mid \Theta)\). If we now consider replacement of one \(c \in \mathcal{K}^{(n)}\) by a new \(c^{\text{new}}\) previously not in \(\mathcal{K}^{(n)}\), then this increases the variational bound if and only if the joint probability for this replaced cluster \(p(c, \tilde{y}^{(n)} \mid \Theta) \rightarrow p(c^{\text{new}}, \tilde{y}^{(n)} \mid \Theta)\) increases:

\[
p(c^{\text{new}}, \tilde{y} \mid \Theta) > p(c, \tilde{y} \mid \Theta) \\
\iff \exp \left( -\frac{1}{2\sigma^2} \| \tilde{y} - \tilde{\mu}_{c^{\text{new}}} \|^2 \right) > \exp \left( -\frac{1}{2\sigma^2} \| \tilde{y} - \tilde{\mu}_c \|^2 \right) \\
\iff -\frac{1}{2\sigma^2} \| \tilde{y} - \tilde{\mu}_{c^{\text{new}}} \|^2 > -\frac{1}{2\sigma^2} \| \tilde{y} - \tilde{\mu}_c \|^2 \\
\iff \| \tilde{y} - \tilde{\mu}_{c^{\text{new}}} \| < \| \tilde{y} - \tilde{\mu}_c \|, \quad (32)
\]

which recovers Prop. 1.

### D Details of the Variational Loop of vc-GMM

Because of Prop. 1, the variational loop can be realized for each \(n\) of the coreset by using any of the algorithms investigated in Forster and Lücke [2018]. Here we choose the var-GMM-S which scales independently of \(C\) per iteration and considers more than one ‘winning’ cluster. As the variational loop only has to be executed for the \(N\) data points of the coreset, the run time of the variational E-step of vc-GMM has a run-time cost of \(O(N'G^2D)\) and memory requirement of \(O(CD + N'G^2 + CG + N)\). Tab. S.1 summarizes the computational complexities of vc-GMM as well as the complexities of the approaches.
we compare to in the numerical experiments. The pseudo-code of the variational loop is given in Alg. 2. The nested loops over $c$ and $n$ in the last computational block can (because of the if-condition) be rewritten to scale with $O(N'G^2)$ (using $C' = G$) Forster and Lücke [2018].

**Algorithm 2:** The $vc$-GMM variational loop.

\[
\begin{align*}
&\text{for } n = 1 : N' \text{ do} & O(N'C'GD) \\
&\quad G^{(n)} = \bigcup_{c \in \mathcal{K}^{(n)}} G_c; & O(C'G) \\
&\quad \text{for } c \in G^{(n)} \text{ do} & O(C'GD) \\
&\quad \quad d_{c^n} = \|y^{(n)}_c - \bar{\mu}_c\|; & O(D) \\
&\quad \quad \mathcal{K}^{(n)} = \{ c | d_{c^n} \text{ is among the} \\
&\quad \quad \quad C' \text{ smallest distances} \}; & O(C'G) \\
&\text{for } n = 1 : N' \text{ do} & O(N'C'G) \\
&\quad c_o^{(n)} = \arg\min_{c \in G^{(n)}} \{ d_{c^n} \}; & O(C'G) \\
&\quad I_{c_o^{(n)}} = I_{c_o^{(n)}} \cup \{ n \}; & O(1) \\
&\text{for } c = 1 : C \text{ do} & O(N'C'G) \\
&\quad \text{for } n \in I_c \text{ do} & O((N'/C)C'G) \\
&\quad \quad \text{for } c' \in G^{(n)} \text{ do} & O(C'G) \\
&\quad \quad \quad d_{c'c} = d_{c^n} + d_{c'c}; & O(1) \\
&\quad \quad \quad b_{c'c} = b_{c'c} + 1; & O(1) \\
&\text{for } c = 1 : C \text{ do} & O(N'C'G) \\
&\quad \text{for } n \in I_c \text{ do} & O((N'/C)C'G) \\
&\quad \quad \text{for } c' \in G^{(n)} \text{ do} & O(C'G) \\
&\quad \quad \quad \text{if } \text{normalized}_{c} \neq 1 \text{ then} \\
&\quad \quad \quad \quad d_{c'c} = d_{c'c}/b_{c'c}; & O(1) \\
&\quad \quad \quad \quad \text{normalized}_{c} = 1; & O(1) \\
&\quad \quad d_{cc} = 0; & O(1) \\
&\quad G_c = \{ c' | d_{c'c} \text{ is among the} \\
&\quad \quad \quad C' \text{ smallest distances } d_{cc} \}; & O((N'/C)C'G) \\
\end{align*}
\]

For the variational loop, we introduce cluster-neighborhoods $G_c$ (with $c \in G_c$) of constant size $G = |G_c|$. Search spaces to find closer clusters for each data point $y^{(n)}_c$ are given by $G^{(n)} = \bigcup_{c \in \mathcal{K}^{(n)}} G_c$. The variational loop then consists of two parts: First, for each data point $y^{(n)}_c$ we compute distances to all clusters $c \in G^{(n)}$ and select the $C'$ closest clusters to define new $\mathcal{K}^{(n)}$. Second, we construct sets $I_c$ for each cluster $c = \{1, \ldots, C\}$ that hold the indices $n$ of those data points $y^{(n)}_n$ for which $c$ is the closest found cluster in this iteration. The sets $I_c$ can therefore be thought of as an estimated partition of the data set. If we assume already well converged cluster centers and search spaces that indeed include the closest clusters, then the average data-to-cluster distances of data points in sets $I_c$

\[
d_{cc} = \frac{1}{|I_c|} \sum_{n \in I_c} d_{c^n}^{(n)}
\]

represent a good estimate for the distances between cluster $c$ and close-by clusters $c'$. In other words: We estimate the distance $d_{c,c'}$ between clusters $c$ and $c'$ by averaging over distances $d_{c^n}^{(n)}$ of clusters $c'$ to data points $y^{(n)}_n$ which lie in close proximity to cluster $c$. The distance $d_{c,c}$ between a cluster $c$ to itself is afterwards manually set to zero. For more distant clusters $c'$, where no distance $d_{c^n}^{(n)}$ was calculated in this iteration, $d_{c,c'}$ is here treated as infinite. However, since only the distances to the closest clusters are relevant for the update of $G_c$, a good estimate of close-by cluster distances is sufficient. And even if the cluster-to-cluster estimates are very coarse, e.g. in the beginning of clustering, the definition of the $\mathcal{K}^{(n)}$ updates in Alg. 2 always warrants that the merged objective (10) monotonically increases. For more details, see Forster and Lücke [2018].

## E Implementation Details

Measurements of run times of different algorithms can depend greatly on choices regarding the actual implementation (realization of update rules and used memory structures, programming language, libraries for numerical subroutines, etc.). We therefore chose to use our own C++ implementations of Lloyd’s algorithm, $D^2$-seeding, AFK-MC$^2$-seeding, and lightweight coreset construction in addition to our C++ implementations of $vc$-GMM. $var$-GMM-S is trivially realized by $vc$-GMM when no coresets are used (using all data points, and setting all weights $\gamma^{(n)} = 1$). For AFK-MC$^2$ our code follows the published Cython implementation provided by Bachem et al. [2016a]. To achieve high throughput of vector operations, i.e., distance computations and reductions, we selected the blaze library, a high performance C++ math library Igberger [2012]. We used double precision in all cases.
F Details of the Numerical Experiments

For comparisons of the computational cost of different algorithms, we need to define after how many EM iterations parameter updates have converged sufficiently. In general, we declare convergence of an iterative algorithm when the relative change of the objective it optimizes falls below a predefined threshold. For \textit{vc-GMM} and \textit{var-GMM-S} these objectives take the form of variational lower bounds (that can be computed efficiently). Also \textit{k-means} can be interpreted as a variational algorithm Lücke and Forster [2017] for which a variational lower bound of the likelihood can be defined Lücke and Forster [2017]. For consistency, we use this bound (which is closely related to the quantization error) for \textit{k-means}. In the case of \textit{k-means}, the computation of the bound requires additional computations, which we exclude from the measurements of elapsed time.

For all algorithms, we chose a threshold of $\epsilon = 10^{-4}$, i.e., the algorithm stops when the relative change of the objective falls below this value. We observed that a stricter criterion in form of a substantially smaller $\epsilon$, conflicts with the tradeoff between clustering quality and computational cost. Linear increases in cost with each additional EM iteration would then only yield a marginal improvement in clustering quality. For example, the difference of the quantization error between a threshold of $10^{-4}$ and $10^{-5}$ for \textit{k-means} on the KDD dataset is approximately 0.8%. The number of EM iterations until convergence, however, increases from an average of approx. 13 to 38. A smaller threshold of $10^{-3}$ would, on the other hand, result in substantially lower clustering qualities (note the already relatively low number of EM iterations of \textit{k-means} for $10^{-4}$).

Other than the stopping criterion, the number of iterations required for \textit{vc-GMM} (and the other used algorithms) until convergence highly depends on the data set and potentially the seeding. Most iterations were required for variational approaches (\textit{vc-GMM} and \textit{var-GMM-S}) with small search spaces (small $G$). Given the strong computational gains per iteration, \textit{vc-GMM} with small search spaces were still finally the most efficient approaches.

Regarding the choice for $G$ in our experiments, $G = 2$ represents the limit of small search spaces, see e.g. Forster and Lücke [2018]. For increasingly large $G$ we, in general, observed an increasingly effective increase of the merged objective per iteration but also the computational cost per iteration increases. Slightly larger than the minimally possible search spaces (i.e., values of $G = 3$ to $G = 5$) were consistently found to result in the most favorable efficiency vs. clustering quality trade-off. As also observed by Forster and Lücke [2018], the small
search spaces of $G = 3$ significantly profited from the addition of one random cluster. The inclusion of this additional random cluster helps to more quickly improve the initial search space $G^{(n)}$, as the initial $G_c$ might be unfavorably scattered over far away groups of clusters, with large gaps in between that can not (or only with many iterations) be overcome by regarding immediate cluster neighborhoods alone.

Considering Fig. 1, the RNA dataset is the data set with the least speedups in elapsed time. This is mainly due to the low data dimensionality $D$. A further difference of the RNA dataset compared to the other benchmarks is the in general slower convergence. Bachem et al. [2016a], for instance, report that relatively long Markov chains are required for seeding for RNA (while short chain lengths were observed to be sufficient KDD, SONG and SUSY, CIFAR-10). We here verified this observation (see results for AFK-MC$^2$-seeding). For the RNA and CIFAR-10 datasets we observed that variational var-GMM-S algorithm resulted in on average better quantization errors than $k$-means++. This is presumably the case because of the general tendency of truncated approximations to avoid local optima more effectively Hughes and Sudderth [2016], Forster et al. [2018].

When it was first suggested, var-GMM-S used initial E-steps before the model parameters were update for the first time Forster and Lücke [2018]. In the benchmarks considered here, such E-steps did in general not reliably result in any or in significant performance gains. The exception was again the RNA dataset. Here, initial E-steps were observed to be favorable. For var-GMM-S we find that for $G = 3 + 1$, initial E-steps improve the average quantization error from $1.73 \cdot 10^6$ to $1.65 \cdot 10^6$ (four E-steps), and for $G = 5$ from $1.73 \cdot 10^6$ to $1.67 \cdot 10^6$ (two E-steps).

G Additional Numerical Results

Fig. S.1 provides further results on the SONG data set for the standard setting of $C = 2000$ clusters additional to the higher scale setting of $C = 4000$ that we already showed in Fig. 1. To better evaluate the trade-off between clustering quality and speedup, Fig. S.2 furthermore shows for all data sets the normalized mutual information (NMI) of the hard partitions of vc-GMM (given by the MAP estimate) and LWCS with respect to the partitions found by standard $k$-means++. For all coreset sizes vc-GMM shows to better reproduce the $k$-means++ partitions than the LWCS version of $k$-means. The respective speedups of vc-GMM and LWCS are the same as in Fig. 1 (left and middle column), which again shows the superior trade-off between speed and clustering quality (now in terms of NMI) given by vc-GMM.