DeepDPM: Deep Clustering With an Unknown Number of Clusters

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Abstract

*Deep Learning (DL) has shown great promise in the unsupervised task of clustering. That said, while in classical (*i.e.*, non-deep) clustering the benefits of the nonparametric approach are well known, most deep-clustering methods are parametric: namely, they require a predefined and fixed number of clusters, denoted by K. When K is unknown, however, using model-selection criteria to choose its optimal value might become computationally expensive, especially in DL as the training process would have to be repeated numerous times. In this work, we bridge this gap by introducing an effective deep-clustering method that does not require knowing the value of K as it infers it during the learning. Using a split/merge framework, a dynamic architecture that adapts to the changing K, and a novel loss, our proposed method outperforms existing nonparametric methods (both classical and deep ones). While the very few existing deep nonparametric methods lack scalability, we demonstrate ours by being the first to report the performance of such a method on ImageNet. We also demonstrate the importance of inferring K by showing how methods that fix it deteriorate in performance when their assumed K value gets further from the ground-truth one, especially on imbalanced datasets. Our code is available at* https://github.com/BGU-CS-VIL/DeepDPM.

1. Introduction

Clustering is an important unsupervised-learning task where, unlike in the supervised case of classification, class labels are unavailable. Moreover, in the purely-unsupervised (and more realistic) setting this work focuses on, the number of classes, denoted by K, and their relative sizes (*i.e.*, the class weights) are unknown too.

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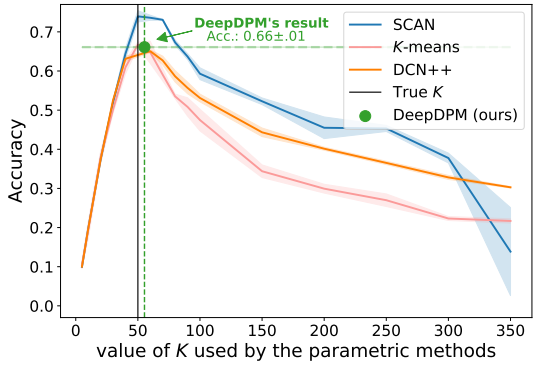
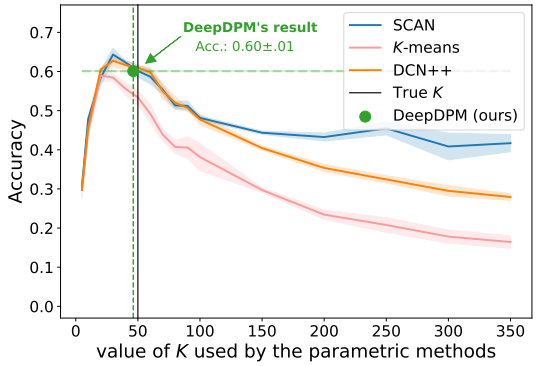


(a) ImageNet50: The original balanced dataset



(b) ImageNet50: An imbalanced dataset

Figure 1. Mean clustering accuracy of 3 runs ($\pm$ std. dev.) on ImageNet50. The Ground Truth K is 50. Parametric methods such as K-means, DCN++ (an improved variant of [71]) and SCAN [64], require knowing K. When given a poor estimate of K, they deteriorate in performance in a balanced dataset (a) and even more so in an imbalanced dataset (b). In contrast, the proposed DeepDPM does not require knowing K (it infers its value; *e.g.*, $K = 55.3 \pm 1.53$ in (a) and 46.3 ± 2.52 in (b)) and yet yields comparable results.

The emergence of Deep Learning (DL) has not skipped clustering tasks. DL methods usually cluster large and high-dimensional datasets better and more efficiently than classical (*i.e.*, non-deep) clustering methods [64, 71]. That said, while in classical clustering it is well understood that *nonparametric* methods (namely, methods that find K) have advantages over *parametric* ones (namely, methods that re-

quire a known K) [8,57], there are only a few nonparametric deep clustering methods. Unfortunately, the latter are neither scalable nor effective enough. *Our work bridges this gap by proposing an effective deep nonparametric method*, called DeepDPM. In fact, even when K is known, DeepDPM still achieves results comparable to leading parametric methods (especially in imbalanced cases) despite their "unfair" advantage; see, *e.g.*, Figure 1 or § 5.

More generally, the ability to infer the latent K has *practical* benefits, including the following ones. 1) Without a good estimate of K, parametric methods might suffer in performance. Figure 1 shows that using the wrong K can have a significant negative effect on parametric methods in both balanced and imbalanced datasets. When the value of K becomes more and more inaccurate, even a State-Of-The-Art (SOTA) parametric deep clustering method, SCAN [64], deteriorates in performance significantly. 2) Changing K during training has positive optimization-related implications; *e.g.*, by splitting a single cluster into two, multiple data labels are changed *simultaneously*. This often translates to large moves on the optimization surface which may lead to convergence to better local optima and performance gains [10]; *e.g.*, in § 5 we demonstrate cases where nonparametric methods, ours included, outperform parametric ones even when the latter are given the true K. 3) A common workaround to not knowing K is to use *model selection*: namely, run a parametric method numerous times, using different K values over a wide range, and then choose the "best" K via an unsupervised criterion. That approach, however, besides missing the aforementioned potential gains (not being able to make large moves), does not scale and is usually infeasible for large datasets, *especially in DL*. Moreover, *the negative societal impact of the model-selection approach must be noted as well*: training a deep net tens or hundreds of times on a large dataset consumes prohibitively-large amounts of energy. 4) K itself may be a sought-after quantity of importance.

Bayesian nonparametric (BNP) mixture models, exemplified by the Dirichlet Process Mixture (DPM) model, offer an elegant, data-adaptive, and mathematically-principled solution for clustering when K is unknown. However, the high computational cost typically associated with DPM inference is arguably why only a few works tried to use it in conjunction with deep clustering (*e.g.*, [11,66,74]). Here we propose to *combine the benefits of DL and the DPM effectively*. The proposed method, DeepDPM, uses splits and merges of clusters to change K together with a dynamic architecture to accommodate for such changes. It also uses a novel amortized inference for Expectation-Maximization (EM) algorithms in mixture models. DeepDPM can be incorporated in deep pipelines that rely on clustering (*e.g.*, for feature learning). Unlike an offline clustering step (*e.g.*, K-means), DeepDPM is differentiable during most of the training (the exception is during the discrete splits/merges) and thus supports gradient propagation through it. DeepDPM outperforms existing nonparametric clustering methods (both classical and deep ones) across several datasets and metrics. It also handles class imbalance gracefully and scales well to large datasets. While we focus on clustering and not feature learning, we also show examples of clustering on pretrained features as well as jointly learning features and clustering in an end-to-end fashion. To summarize, **our key contributions are:** 1) A deep clustering method that infers the number of clusters. 2) A novel loss that enables a new amortized inference in mixture models. 3) A demonstration of the importance, in deep clustering, of inferring K. 4) Our method outperforms existing nonparametric clustering methods and we are the first to report results of a deep nonparametric clustering method on a large dataset such as ImageNet [17].

2. Related Work

Parametric Deep Clustering methods. Recent such works can be divided into two types: two-step approaches and end-to-end ones. In the former, clustering is performed on features extracted in a pretext task. For instance, McConville *et al*. [47] run K-means on the embeddings, transformed by UMAP [48], of a pretrained Autoencoder (AE). While not scalable, [47] achieves competitive results when it is applicable. Another example is SCAN [64] which uses unsupervised pretrained feature extractors (*e.g.*, MoCo [13] and SimCLR [12]). While reaching SOTA results, SCAN, being parametric, depends on having an estimate of K and, as we show, deteriorates in performance when the estimate is too inaccurate. Moreover, SCAN assumes uniform class weights (*i.e.* a balanced dataset) and that is often unrealistic in purely-unsupervised cases.

End-to-end deep methods jointly learn features and clustering, possibly by alternation. Several works use an AE, or a Variational AE (VAE), with an additional clustering loss [40, 68, 70–72]; *e.g.*, DCN [71] runs K-means on the embeddings of a pretrained AE, and retrains it with a loss consisting of a reconstruction term and a clustering-based term, to simultaneously update the features, clusters' centers, and assignments. Other works, *e.g.* [5,6], use convolutional neural nets to alternately learn features and clustering.

While our work focuses on clustering, not feature learning, we demonstrate how it can also be incorporated with the two approaches above. Moreover, all the methods above assume a predefined and fixed K and, at least the more effective ones among them, take substantial time and resources to train (so searching for the "right" K using model selection is costly and/or inapplicable).

Nonparametric Classical Clustering. Closely related to our work is BNP clustering and, more specifically, the DPM model [1, 24]. While many computer-vision works rely on BNP clustering [4, 9, 14, 25–28, 30, 32, 33, 38, 39, 41, 44–46, 49, 53–59, 62], it has yet to become a mainstream

choice, partly due to the lack of efficient large-scale inference tools. Fortunately, this is starting to change; see, *e.g.*, the highly-effective DPM sampler from [21] (a modern and scalable implementation of the DPM sampler from [10]) or the scalable streaming DPM inference in [20]. Of note, an important alternative to sampling is variational DPM inference [3, 31, 34, 36, 42]. A non-Bayesian example of a popular nonparametric method is DBSCAN [23] which is density-based and groups together closely-packed points. While DBSCAN has efficient implementations, it is highly sensitive to its hyperparameters which are hard to tune.

Nonparametric Deep Clustering. Among the very few examples of deep methods that also find K are [11,52,66,74]. Some of them use an offline DPM inference for pseudo-labels for fine-tuning a deep belief network [11], or an AE [66] (similarly to the parametric methods in [5, 6, 71]). As the methods in [66] and [11] rely on slow DPM samplers, they do not scale to large datasets. AdapVAE [74] uses a DPM prior for a VAE. In DCC [52], feature learning and clustering are performed simultaneously like in [74]; however, instead of ELBO minimization, DCC uses a nearest-neighbor graph to group points that are close in the latent space of an AE. Our method is empirically more effective than [52, 74] and also scales much better. While not a clustering method per-se, and similarly to [47], [65] uses an AE and t-SNE [63] to find K. Like [47], however, [65] does not scale. In [22], a deep net is simultaneously trained on a family of losses instead of a single one. At least in theory, that approach may be adapted to nonparametric clustering but this direction has yet to be explored. Both [60] and [50] do not assume a known K, where the former focuses on clustering faces and the latter on generating posterior samples of cluster labels for any new dataset. Unlike our method, however, [50, 60] are supervised. Similarly, [2] iteratively forms clusters by sequentially examining each sample against the members of existing clusters. The clustering criterion is based on a supervised evaluation net. Lastly, while [73] relies on a BNP mixture, their method (and code) still uses a fixed K.

3. Preliminaries: DPGMM-based Clustering

Let $\mathcal{X} = (\boldsymbol{x}_i)_{i=1}^N$ denote N data points in $\mathbb{R}^d$. The clustering task aims to partition $\mathcal{X}$ into K disjoint groups, where z_i is the point-to-cluster assignment, known as the *cluster label*, of $\boldsymbol{x}_i$. *Cluster* k consists of all the points labeled as k; *i.e.*, $(\boldsymbol{x}_i)_{i:z_i=k}$. The number of clusters, $K \triangleq |\{k : k \in \boldsymbol{z}\}|$, is thus the number of unique elements in $\boldsymbol{z} = (z_i)_{i=1}^N$.

The classical Gaussian Mixture Model (GMM) has a BNP extension: the Dirichlet Process GMM (DPGMM) [1, 24]. Informally, the DPGMM (a specific case of the DPM) entertains the notion of a mixture with infinitely-many Gaussians:

$$p(\boldsymbol{x}|(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k)_{k=1}^\infty) = \sum\nolimits_{k=1}^\infty \pi_k \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \quad (1)$$

where $\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ is a Gaussian probability density function (pdf) (of mean $\boldsymbol{\mu}_k \in \mathbb{R}^d$ and a d-by-d covariance matrix $\boldsymbol{\Sigma}_k$) evaluated at $\boldsymbol{x} \in \mathbb{R}^d$, $\pi_k > 0\ \forall k$, and $\sum_{k=1}^\infty \pi_k = 1$. For a gentle introduction to the DPGMM with a computer-vision audience in mind, see [8, 57]. Let $\boldsymbol{\theta}_k = (\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ denote the parameters of Gaussian k. Note the distinction between *component* k (namely, the k-th Gaussian, identified with its parameter, $\boldsymbol{\theta}_k$) and cluster k. The components, $\boldsymbol{\theta} = (\boldsymbol{\theta}_k)_{k=1}^\infty$, and weights, $\boldsymbol{\pi} = (\pi_k)_{k=1}^\infty$, are assumed to be drawn (independently) from their own prior distributions: the weights, $\boldsymbol{\pi}$, are drawn using the Griffiths-Engen-McCloskey stick-breaking process (GEM) [51] with a concentration parameter $\alpha > 0$, while the parameters, $(\boldsymbol{\theta}_k)_{k=1}^\infty$, are independent and identically-distributed (i.i.d.) draws from their prior $p(\boldsymbol{\theta}_k)$, typically a Normal-Inverse Wishart (NIW) distribution. While there are infinitely-many *components*, note that there are still finitely-many *clusters* as the *latent random variable* K is bounded above by N. By possibly renaming cluster indices, we may assume without loss of generality that $\{k : k \in \boldsymbol{z}\} = \{1, 2, \ldots, K\}$.

The DPGMM is often used in clustering when K is unknown. DPGMM inference methods typically seek to find $\boldsymbol{z} = (z_i)_{i=1}^N$ (which implies K) and $(\boldsymbol{\theta}_k, \pi_k)_{k=1}^K$. As explained in our supplementary material (**Supmat**), the inferred value of K is affected by the following factors: $\mathcal{X}$, α, and the NIW hyperparameters. Our method (§ 4) is inspired in part by Chang and Fisher III's DPM sampler [10] which consists of a split/merge framework [37] (which we adopt) and a restricted sampler (which is less relevant to our work).

The split/merge framework augments the latent variables, $(\boldsymbol{\theta}_k)_{k=1}^\infty$, $\boldsymbol{\pi}$, and $(z_i)_{i=1}^N$, with auxiliary variables. To each z_i, an additional *subcluster label*, $\widetilde{z}_i \in \{1, 2\}$, is added. To each $\boldsymbol{\theta}_k$, two subcomponents are added, $\widetilde{\boldsymbol{\theta}}_{k,1}$, $\widetilde{\boldsymbol{\theta}}_{k,2}$, with nonnegative weights $\widetilde{\boldsymbol{\pi}}_k = (\widetilde{\pi}_{k,j})_{j\in\{1,2\}}$ (where $\widetilde{\pi}_{k,1} + \widetilde{\pi}_{k,2} = 1$), forming a 2-component GMM. Next, splits and merges allow changing K via the Metropolis-Hastings framework [29]. That is, during the inference, every certain amount of iterations the split of cluster k into its subclusters is proposed. That split is accepted with probability $\min(1, H_\mathrm{s})$ where

$$H_\mathrm{s} = \frac{\alpha\Gamma(N_{k,1}) f_{\boldsymbol{x}}(\mathcal{X}_{k,1}; \lambda)\Gamma(N_{k,2}) f_{\boldsymbol{x}}(\mathcal{X}_{k,2}; \lambda)}{\Gamma(N_k) f_{\boldsymbol{x}}(\mathcal{X}_k; \lambda)} \quad (2)$$

is the Hastings ratio, Γ is the Gamma function, $\mathcal{X}_k = (\boldsymbol{x}_i)_{i:z_i=k}$ stands for the points in cluster k, $N_k = |\mathcal{X}_k|$, $\mathcal{X}_{k,j} = (\boldsymbol{x}_i)_{i:(z_i,\widetilde{z}_i)=(k,j)}$ denotes the points in subcluster j ($j \in \{1, 2\}$), $N_{k,j} = |\mathcal{X}_{k,j}|$, and $f_{\boldsymbol{x}}(\cdot; \lambda)$ is the *marginal* likelihood where λ represents the NIW hyperparameters. See our **Supmat** for more details. Upon a split proposal acceptance, each of the newly-born clusters is augmented with two subclusters. This ratio, H_s, can be interpreted as comparing the marginal likelihood of the data under the two subclusters with its marginal likelihood under the cluster. Merge proposals are handled similarly (see **Supmat**).

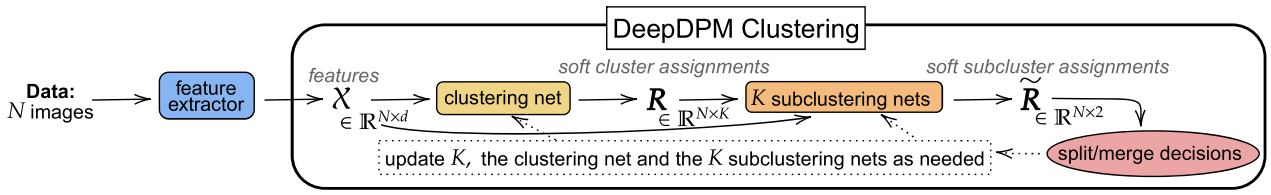


Figure 2. DeepDPM's pipeline: given features $\mathcal{X}$, the clustering net outputs cluster assignments, $\boldsymbol{R}$, while the subclustering nets generate subcluster assignments, $\widetilde{\boldsymbol{R}}$. Upon the acceptance of split/merge proposals, all those nets are updated during the learning.

4. The Proposed Method: DeepDPM

DeepDPM can be viewed as a DPM inference algorithm. Inspired by [10], we use splits and merges to change K where for every cluster we maintain a subcluster pair. For a nominal value of K, rather than resorting to sampling as in [10], we use a deep net trained by a novel amortized inference for EM [16] in a mixture model. DeepDPM has two main parts. The first is a clustering net, while the second consists of K subclustering nets (one for each cluster k, $k \in \{1,\dots,K\}$). In § 4.1 we describe how DeepDPM operates given a nominal value of K and in § 4.2 how K is changed and how our architecture adapts accordingly. We discuss the amortized-inference aspects of our approach in § 4.3, our weak prior in § 4.4, and how DeepDPM may be combined with feature learning in § 4.5. Figure 2 depicts the overall pipeline.

4.1. DeepDPM Under a Fixed K

We start by describing DeepDPM's forward pass during the training. Given a current value of K, the data is first passed to the clustering net, f_{cl}, which generates, for each data point $\boldsymbol{x}_i$, K soft cluster assignments:

$$f_{\text{cl}}(\mathcal{X}) = \boldsymbol{R} = (\boldsymbol{r}_i)_{i=1}^N \qquad \boldsymbol{r}_i = (r_{i,k})_{k=1}^K \tag{3}$$

where $r_{i,k} \in [0,1]$ is the soft assignment of $\boldsymbol{x}_i$ to cluster k (also called the responsibility of cluster k to data point $\boldsymbol{x}_i$) and $\sum_{k=1}^K r_{i,k} = 1$. From $(\boldsymbol{r}_i)_{i=1}^N$ we compute the hard assignments $\boldsymbol{z} = (z_i)_{i=1}^N$ by $z_i = \arg\max_k r_{i,k}$. Next, each subclustering net, f_{sub}^k (where $k \in \{1,\dots,K\}$), is fed with the data (hard-) assigned to its respective cluster (*i.e.*, f_{sub}^k is fed with $\mathcal{X}_k = (\boldsymbol{x}_i)_{i:z_i=k}$) and generates soft subcluster assignments:

$$f_{\text{sub}}^k(\mathcal{X}_k) = \widetilde{\boldsymbol{R}}_k = (\widetilde{\boldsymbol{r}}_i)_{i:z_i=k} \qquad \widetilde{\boldsymbol{r}}_i = (\widetilde{r}_{i,j})_{j=1}^2 \tag{4}$$

where $\widetilde{r}_{i,j} \in [0,1]$ is the soft assignment of $\boldsymbol{x}_i$ to subcluster j ($j \in \{1,2\}$), and $\widetilde{r}_{i,1} + \widetilde{r}_{i,2} = 1 \,\forall k \in \{1,\dots,K\}$. As detailed in § 4.2, the subclusters learned by $(f_{\text{sub}}^k)_{k=1}^K$ are used in split proposals. Each of the $K+1$ nets (f_{cl} and $(f_{\text{sub}}^k)_{k=1}^K$) is a simple multilayer perceptron with a single hidden layer. The last layer of f_{cl} has K neurons while the last layer of each f_{sub}^k has two.

We now introduce a new loss motivated by EM in the Bayesian GMM (though the idea, in fact, also holds in the non-Bayesian GMM case, as well as for EM in parametric mixtures with non-Gaussian components). Concretely, in each epoch, our clustering net is optimized to generate soft assignments that would resemble those obtained by an E step of the EM-GMM algorithm (recall that the E steps of the Bayesian and non-Bayesian EM-GMM coincide). Each E step is followed by a standard M step in a Bayesian GMM, except that the soft assignments used in the Maximum-a-Posterior (MAP) estimates are those produced by our clustering net. We now provide the details. For each $\boldsymbol{x}_i$ and each $k \in \{1,\dots,K\}$ we compute the (standard) E-step probabilities, $\boldsymbol{r}_i^{\text{E}} = (r_{i,k}^{\text{E}})_{k=1}^K$, where

$$r_{i,k}^{\text{E}} = \frac{\pi_k \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{k'=1}^K \pi_{k'} \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'})} \qquad k \in \{1,\dots,K\} \tag{5}$$

is computed using $(\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)_{k=1}^K$ from the previous epoch. Note that $\sum_{k=1}^K r_{i,k}^{\text{E}} = 1$. We then encourage f_{cl} to generate similar soft assignments using the following new loss:

$$\mathcal{L}_{\text{cl}} = \sum_{i=1}^N \text{KL}(\boldsymbol{r}_i \| \boldsymbol{r}_i^{\text{E}}) \tag{6}$$

where KL is the Kullback-Leibler divergence. Next, after every epoch we perform a Bayesian M step but with a twist. Recall that in this step, one uses the weighted versions of the MAP estimates of $(\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)_{k=1}^K$ (computed using standard formulas; see **Supmat**) where the weights are the $r_{i,k}^{\text{E}}$ values (Eq. (5)). We apply the same formulas but instead of $r_{i,k}^{\text{E}}$ we use the $r_{i,k}$ values (*i.e.*, the output of f_{cl}). Note that unlike methods (*e.g.* K-means or SCAN) that enforce/assume uniformity of the weights, our inferred cluster weights, $(\pi_k)_{k=1}^K$, are allowed to deviate from uniformity.

In principle, for $(f_{\text{sub}}^k)_{k=1}^K$ we could have used a loss similar to $\mathcal{L}_{\text{cl}}$. However, here we prefer an isotropic loss:

$$\mathcal{L}_{\text{sub}} = \sum_{k=1}^K \sum_{i=1}^{N_k} \sum_{j=1}^2 \widetilde{r}_{i,j} \|\boldsymbol{x}_i - \widetilde{\boldsymbol{\mu}}_{k,j}\|_{\ell_2}^2 \tag{7}$$

where $N_k = |\mathcal{X}_k|$ and $\widetilde{\boldsymbol{\mu}}_{k,j}$ is the mean of subcluster j of cluster k, computed after every epoch, alongside with subcluster weights and covariances, using weighted MAP estimates similarly to the clusters' case (see **Supmat**). This loss is more efficient than the KL loss while the latter (only in the subcluster case) did not yield improvement. The

iterative process described above needs to be initialized. We do this using K-means (using some initial value of K for the clustering and $K = 2$ for the subclustering). *DeepDPM is fairly robust to the initial K so the latter can be chosen arbitrarily* (see, *e.g.*, § 5.2).

4.2. Changing K via Splits and Merges

During training, we use splits and merges to change K (as in [10]). Every few epochs, we propose either splits or merges. Since K is changing, the architecture, and more specifically, the last layer of the clustering net and the number of subclustering nets, must change too. Of note, the splits/merges facilitate not only changing the value of K but also *large moves*, escaping many poor local optima [10].

Splits. In every split step, we propose to split each of the clusters into its two subclusters. A split proposal is accepted stochastically (as in [10]) with probability $\min(1, H_{\mathrm{s}})$; see Eq. (2). To accommodate for the increase in K, if a split proposal is accepted for cluster k, the k-th unit in the last layer of the clustering net, together with the weights connecting it to the previous hidden layer, is duplicated, and we initialize the parameters of the two new clusters using the parameters learned via the subcluster nets:

$$\begin{aligned} \boldsymbol{\mu}_{k_1} &\leftarrow \widetilde{\boldsymbol{\mu}}_{k,1}\,, \quad \boldsymbol{\Sigma}_{k_1} \leftarrow \widetilde{\boldsymbol{\Sigma}}_{k,1}\,, \quad \pi_{k_1} \leftarrow \pi_k \times \widetilde{\boldsymbol{\pi}}_{k,1} \\ \boldsymbol{\mu}_{k_2} &\leftarrow \widetilde{\boldsymbol{\mu}}_{k,2}\,, \quad \boldsymbol{\Sigma}_{k_2} \leftarrow \widetilde{\boldsymbol{\Sigma}}_{k,2}\,, \quad \pi_{k_2} \leftarrow \pi_k \times \widetilde{\boldsymbol{\pi}}_{k,2} \end{aligned} \tag{8}$$

where k_1 and k_2 denote the indices of the new clusters. We then also add, to each new cluster, a new subclustering net (dynamically allocating the memory).

Merges. When considering merges we must ensure we never simultaneously accept the proposals of, *e.g.*, merging clusters k_1 and k_2 and the merging of clusters k_2 and k_3, thereby mistakenly merging *three* clusters together. Thus, unlike split proposals which are done in parallel, not all possible merges can be considered simultaneously. To avoid sequentially considering all possible merges, we consider (sequentially) the merges of each cluster with only its 3 nearest neighbors. Merge proposals are accepted/rejected using a Hastings ratio, $H_{\mathrm{m}} = 1/H_{\mathrm{s}}$ (as in [10]). If a proposal is accepted, the two clusters are merged and a new subclustering network is initialized. Technically, one of the merged clusters' last layer's units, together with the net's weights connecting it to the previous hidden layer, is removed from f_{cl}, and the parameters and the weight of the newly-born cluster are initialized using the weighted MAP estimates.

4.3. Amortized EM Inference

Suppose we turn off splits/merges and use the Ground Truth (GT) K. Seemingly, this reduces each training epoch to mimicking a single EM iteration. Remarkably, however, and as shown in § 5, even then our method still yields results that are *usually better* than the standard EM. We hypothesize that this stems from the fact that we *amortize* the EM inference; by the virtue of the smoothness of the function learned by the deep net, we improve the prediction for the points in not only the current batch but also other batches. Moreover, the smoothness also serves as an inductive bias such that points which are close in the observation space should have similar labels.

In principle, instead of using our variational loss we could have also used the GMM negative log likelihood (or log posterior). However, empirically that led to unstable optimization and/or poor results. Moreover, basing our loss on matching soft labels rather than likelihood/posterior elegantly makes the method more general: f_{cl} and $\mathcal{L}_{\mathrm{cl}}$ can be used as they are for any component type, not just Gaussians.

4.4. A Weak Prior: Letting the Data Speak for Itself

Recall that the inferred K depends on $\mathcal{X}$, α, and the NIW hyperparameters. We intentionally choose the prior to be *very* weak. Meaning, we choose α as well as the so-called pseudocounts (two of the NIW hyperparameters) to be very low numbers, dwarfed by N, the number of points (see **Supmat** for details). Thus, we let the data, $\mathcal{X}$, to be the most dominant factor in determining K. The weak prior also means that the Bayesian EM-GMM nearly coincides with the non-Bayesian EM-GMM but still helps in the presence of a degenerate sample covariance or very small clusters.

4.5. Feature extraction

To show the effectiveness of our clustering method, we used two types of feature-extraction paradigms: an end-to-end approach, where features and clustering are learned jointly (using alternate optimization), and a two-step approach in which features are learned once (before the clustering) and then held fixed. For the two-step approach, we follow SCAN [64] and use MoCo [13] for (unsupervised) feature extraction. For more details, as well as the scheme we use for an end-to-end feature extraction, see **Supmat**.

5. Results

In this section we evaluate DeepDPM and compare it with several key methods on popular image and text datasets at varying scales. In our evaluations we use three common metrics: clustering accuracy (ACC); Normalized Mutual Information (NMI); Adjusted Rand Index (ARI). The higher the better in all three, and they can accommodate for differences between the inferred K and its GT value. See **Supmat** for more details on the experimental setup and the values of the hyperparameters that we used. Due to space limits, we omit here the NMI and ARI values in several comparisons but these appear in the **Supmat**. We round the results to 2 decimal places so, *e.g.*, a standard deviation (std. dev.) of .00 may still represent a positive (albeit small) number.

Comparing with Classical Methods. We compared DeepDPM with classical parametric methods (K-means;

	NMI	ARI	ACC	NMI	ARI	ACC	NMI	ARI	ACC
	MNIST [18]			USPS [35]			Fashion-MNIST [69]		
K-means^p	.90± .02	.84± .05	.85±.06	.86±.01	.79±.05	.80±.06	.67±.01	.50±.03	.60±.04
GMM^p	**.94±.00**	**.95±.00**	**.98±.00**	.86±.02	.79±.05	.81±.06	.66±.01	.49±.02	.58±.03
DBSCAN	.92±0	.86±0	.89±0	.72±0	.46±0	.57±0	.63±0	-.32±0	.39±0
DPM Sampler	.92±.01	.91±.04	.93±.05	.87±.01	.82±.02	.83±.03	.67±.01	.49± .02	.59±.03
moVB	.93±.00	.94±.00	.97±.00	.87±.02	**.86±.04**	**.90±.04**	.66±.02	.47±.03	.55±.03
DeepDPM (Ours)	**.94±.00**	**.95±.00**	**.98±.00**	**.88±.00**	**.86±.01**	.89±.2	**.68±.01**	**.51±.02**	**.62±.03**
	MNIST^{imb}			USPS^{imb}			Fashion-MNIST^{imb}		
K-means^p	.89± .03	.84± .06	.83±.06	.82±.02	.71±.05	.71±.05	.62±.01	.46±.02	.56±.03
GMM^p	.94±.02	.95±.03	.96±.04	.83±.01	.74±.05	.76±.05	.62±.01	.46±.02	.57±.03
DBSCAN	.93±0	.92±0	.94±0	.84±0	.79±0	.80±0	.62±0	.35±0	.46±0
DPM Sampler	.93±.01	.94±.02	.96±.02	.89±.02	.89±.06	.91±.04	**.66±.01**	**.50± .01**	**.61±.01**
moVB	.94±.00	.95±.00	.96±.00	.88±.01	.89±.02	.91±.02	.63±.01	.44±.02	.53±.02
DeepDPM (Ours)	**.95±.01**	**.97±.01**	**.98±.01**	**.90±.00**	**.92±.00**	**.94±.00**	.65±.00	**.50±.00**	**.61±.00**

Table 1. Comparing the mean results (±std. dev.) of DeepDPM with classical clustering methods. The results are the mean of 10 independent runs. Methods marked with ^{p} are parametric (require K). Datasets marked with ^{imb} are imbalanced ones.

Method	Inferred K		
	MNIST	USPS	Fashion-MNIST
DBSCAN	9.0±0.00	6.0±0.00	4.0±0.00
DPM Sampler	11.3±0.82	8.5±0.85	12.4±0.97
moVB	14±1.00	11.2±1.08	16.9±2.30
DeepDPM (Ours)	**10±0.00**	**9.2±0.42**	**10.2±0.79**

Table 2. Comparing the mean inferred value (±std. dev.) for K of 10 runs among nonparametric methods. GT $K = 10$.

GMM) and nonparametric ones (DBSCAN [23], moVB [34]; the SOTA DPM sampler from [21]). For feature extraction, we performed the process suggested in [47]. We performed the evaluation on the MNIST, USPS, and Fashion-MNIST datasets, as well their imbalanced versions (the latter are defined in the **Supmat**). All the methods used the same (and fixed) data embeddings as input, *and the parametric ones were given the GT K, given them an unfair advantage*. Table 1 shows that DeepDPM almost uniformly dominates across all datasets and metrics, and its performance gain only increases in the imbalanced cases. It is also observable that, compared with the parametric methods, the nonparametric ones (ours included) are less affected by the imbalance. Moreover, Table 2 shows that among the nonparametric methods, DeepDPM's inferred K is the closest to the GT K (see **Supmat** for similar results in the imbalanced case).

Comparing with Deep Nonparametric Methods. As there exist very few deep nonparametric methods, and some of them reported results only on *extremely-small* toy datasets [11, 66] (*e.g.*, one of them stated they could not process even MNIST's train dataset as it was too large for them), we compared DeepDPM with DCC [52] and AdapVAE [74], the only unsupervised deep nonparametric methods that can at least handle the MNIST [18], USPS [35], and STL-10 [15] datasets. As both those methods jointly learn features and clustering, and to show the flexible nature of DeepDPM, we demonstrate its integration with two feature-extraction techniques (described in § 4.5): an end-to-end pipeline (for MNIST and REUTERS-10k [43]) and a two-step approach using features pretrained by MoCo [13] (for STL-10). Unfortunately, we could not run AdapVAE's published code, and thus resort to including the results reported by them. For DCC, using their code we could reproduce their results only on MNIST, so we compare with both the results we managed to obtain using their code and the ones reported by them. Due to these reproducibility issues, we could compare with those methods only on the original (*i.e.*, balanced) datasets. Table 3 shows that DeepDPM outperforms both DCC and AdapVAE. Note we could not find other unsupervised deep nonparametric methods (let alone with available code) that scale to even these fairly-small datasets.

Clustering the Entire ImageNet Dataset. On ImageNet, we obtained the following results: ACC: 0.25, NMI: 0.65, ARI: 0.14. Our method was initialized with $K = 200$ and converged into 707 clusters (GT=1000). These are first results on ImageNet reported for deep nonparametric clustering. Figure 3 shows examples of images clustered together.

5.1. The Value of Deep Nonparametric Methods

When Parametric Methods Break. We study the effect of not knowing K on parametric methods, with and without

	MNIST [18]			STL-10 [15]			Reuters10k [43]		
Method	NMI	ARI	ACC	NMI	ARI	ACC	NMI	ARI	ACC
AdapVAE† [74] *avg*	.86±1.02	.84±2.35	N/A	.75±0.53	**.71±0.81**	N/A	.45±1.79	.43±5.73	N/A
DCC† [52] best	.912	N/A	.96	N/A	N/A	N/A	.59	N/A	.60
DCC‡ [52] *avg*	.90±.02	.89±.07	.91±.07	.22±.00	.01±.00	.04±.00	.25±.00	.00±.00	.00±.00
DeepDPM (ours) *avg*	.90±.01	.91±.02	.93±.03	.78±.004	.70±.01	.84±.01	.61±.00	.64±.01	.83±.00
DeepDPM (ours) best	**.92**	**.93**	**.96**	**.79**	**.71**	**.85**	**.61**	**.64**	**.83**

Table 3. Comparing deep nonparametric methods. †: reported in the papers. ‡: obtained using their code. *avg*: mean (±std. dev.) of 5 runs.

Figure 3. Examples of ImageNet images clustered together by DeepDPM. Each panel stands for a different cluster.

Method	NMI	ARI	ACC
	ImageNet-50: Balanced		
DBSCAN	.52±.00	.09±.00	.24±.00
moVB	.70±.01	.38±.01	.55±.02
DPM Sampler	.72±.00	.43±.01	.57±.01
DeepDPM (ours)	.75±.00	.49±.01	.64±.00
DeepDPM (ours)∗	**.77±.00**	**.54±.01**	**.66±.01**
	ImageNet-50: Imbalanced		
DBSCAN	.33±.00	.04±.00	.24±.00
moVB	.68±.01	.44±.03	.52±.03
DPM Sampler	.70±.00	.40±.01	.51±.00
DeepDPM (ours)	.74±.01	.48±.02	.58±.01
DeepDPM (ours)∗	**.75±.00**	**.51±.01**	**.60±.01**

Table 4. Comparison of nonparametric methods on ImageNet-50 and its imbalanced version. ∗ marks results with AE alternation.

Method	Final/best K: balanced	Final/best K: imbalanced
K-means^p	40	20
DCN++^{p}	60	40
SCAN^p	70	40
DBSCAN	16	13
moVB	46.2±1.3	**46.4±1.1**
DPM Sampler	72.0±2.6	70.3±4.6
DeepDPM (ours)	**52.0±1.0**	43.67±1.2
DeepDPM (ours)∗	55.3±1.5	46.3±2.5

Table 5. Comparing the mean (±std. dev.) value for K found on ImageNet-50 of 3 runs. For the parametric methods (marked with ^{p}) we use the K value with the best silhouette score. ∗ marks results obtained with AE alternation.

class imbalance. We evaluate each method with a wide range of different K values on ImageNet-50. The latter, curated in [64], consists of 50 randomly-selected classes of ImageNet [17]. To generate an imbalanced version of it, we sampled a normalized *nonuniform* histogram from a uniform distribution over the 50-dimensional probability simplex (*i.e.*, all histograms were equally probable) and then sampled examples from the 50 classes in proportions according to that nonuniform histogram. We compared with 3 parametric methods: 1) K-means; 2) the SOTA method SCAN [64]; 3) an improved version of DCN [71], self-coined DCN++, where instead of training an AE on the raw data, we trained it on top of the embeddings SCAN uses (MoCo [13]) where, following [64], we froze those embeddings during training. For DeepDPM, we used the same features.

Since SCAN requires large amounts of memory (*e.g.*, we could only run it on 2 RTX-3090 GPU cards with 24GB memory each, compared with DeepDPM for which a single RTX-2080 (or even GTX-1080) with 8GB sufficed), and due to resource constraints, we were limited in how many K values we could run SCAN with and in the number of times each experiment could run (this high computational cost is one of the problems with model selection in parametric methods). Thus, we collected the results of the parametric methods with K values ranging from 5 to 350. For both the balanced and imbalanced cases, we initialized DeepDPM with $K = 10$. Figure 1 summarizes the ACC results (see **Supmat** for ARI/NMI). As the K value used by the parametric methods diverges from the GT (*i.e.*, $K = 50$), their results deteriorate. Unsurprisingly, when using the GT K, or sufficiently close to it, the parametric methods outperform our

	ACC		
	K_{init}=3	K_{init}=10	K_{init}=30
No splits/merges	.29±.01	.59±.03	.46±.01
No splits	.29±.01	.59±.02	.45±.03
No merges	.46±.00	.58±.01	.47±.01
2-means instead of f_{sub}	.61±.00	.59±.02	.56±.02
No priors in the M step	.58±.01	.57±.02	.58±.01
Isotropic loss instead of $\mathcal{L}_{\text{cl}}$	.58±.00	.58±.00	.58±.02
DeepDPM (full method)	**.62±.03**	**.61±.00**	**.62±.01**

Table 6. DeepDPM's performance under different ablations.

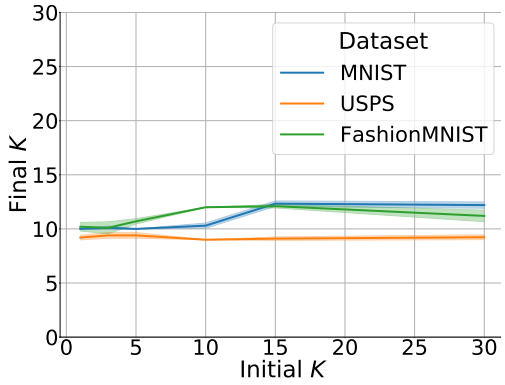


Figure 4. Robustness to the initial K. GT $K = 10$ in all datasets.

nonparametric one, confirming our claim that having a good estimate of K is important for good clustering. Figure 1a, however, shows that even with fairly-moderate deviates from the GT K, DeepDPM's result ($0.66 \pm .01$) surpasses the leading parametric method. Moreover, Figure 1 shows that the parametric SCAN is sensitive to class imbalance; *e.g.*, in Figure 1b, SCAN performs best when $K = 30$ suggesting it is due to ignoring many small classes. In contrast, DeepDPM (scoring $0.60 \pm .01$) is fairly robust to these changes and is comparable in results to SCAN when the latter was given the GT K. In addition, we also show in Table 4 the performance of other nonparametric methods (3 runs on the same features as ours: MoCo+AE). We include DeepDPM's results with alternation (between clustering and feature learning) and without (*i.e.*, holding the features frozen and training DeepDPM only once). Table 5 compares the K values found by the nonparametric methods. DeepDPM inferred a K value close to the GT in both the balanced and imbalanced cases. In the imbalanced case, moVB scored a *slightly* better K but its results (see Table 4) were worse. For the parametric methods, Table 5 also shows the K value of the best silhouette score. The *unsupervised* silhouette metric is commonly used for model selection (NMI/ACC/ARI are supervised, hence inapplicable for model selection). As Table 5 shows, DeepDPM yielded a more accurate K than that approach.

Running Times. Our running time is comparable with a *single* run of SCAN (the SOTA deep parametric method); *e.g.*, on ImageNet-50, SCAN (with 2 NVIDIA 3090 GPUs) trains for $\sim$8 [hr] while ours (with 1 weaker NVIDIA 2080 GPU) takes $\sim$11 [hr]. However, **training SCAN multiple times with a different K each time (as needed for model selection) took more than 3 days.** Thus, DeepDPM's value and positive environmental impact are clear.

5.2. Ablation Study and Robustness to the Initial K

Table 6 quantifies the performance gains due to the different parts of DeepDPM through an ablation study done on Fashion-MNIST (in the setting described earlier). It shows the effect of disabling splits, merges and both; *e.g.*, merges help even when initializing with $K = 3$. In fact, the large moves made by splits/merges help even when $K_{\text{init}} = 10$. Also, replacing the subclustering nets with K-means (using $K = 2$) results in deterioration. Likewise, either turning off the priors when computing the cluster parameters, or using an isotropic loss instead of $\mathcal{L}_{\text{cl}}$, hurts performance and (while not shown here) often destabilizes the optimization. Finally, Figure 4 demonstrates, on three different datasets, DeepDPM's robustness to the initial K.

6. Conclusion

Limitations. As with most clustering methods, if DeepDPM's input features are poor it would struggle to recover. Also, if K is known and the dataset is balanced, parametric methods (*e.g.*, SCAN) may be a slightly better choice.

Future work. An interesting direction is adapting DeepDPM to streaming data (*e.g.*, similarly to how [20] handled streaming DPM inference) or hierarchical settings [7, 19, 61]. Moreover, our results may improve given a more sophisticated framework for building split proposals (*e.g.*, see [67]).

Broader impact. We hope our work will inspire the deep-clustering community to adopt the nonparametric approach as well as raise awareness to issues with the parametric one. Nonparametrics also has an environmental positive impact: obviating the need to repeatedly train deep parametric methods for model selection drastically reduces resource usage.

Summary. We presented a deep nonparametric clustering method, a dynamic architecture that adapts to the varying K values, and a novel loss based on new amortized inference in mixture models. Our method outperforms deep and non-deep nonparametric methods and achieves SOTA results. We demonstrated the issues with parametric clustering, especially the sensitivity to the assumed K, and the added value the nonparametric approach brings to deep clustering. We showed the robustness of our method to both class imbalance and the initial K. Finally, we demonstrated the scalability of DeepDPM by being the first method of its kind to report results on ImageNet. Our code is publicly available.

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