CPU- and GPU-based Distributed Sampling in Dirichlet Process Mixtures for Large-scale Analysis

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Abstract

In the realm of unsupervised learning, Bayesian nonparametric mixture models, exemplified by the Dirichlet Process Mixture Model (DPMM), provide a principled approach for adapting the complexity of the model to the data. Such models are particularly useful in clustering tasks where the number of clusters is unknown. Despite their potential and mathematical elegance, however, DPMMs have yet to become a mainstream tool widely adopted by practitioners. This is arguably due to a misconception that these models scale poorly as well as the lack of high-performance (and user-friendly) software tools that can handle large datasets efficiently. In this paper we bridge this practical gap by proposing a new, easy-to-use, statistical software package for scalable DPMM inference. More concretely, we provide efficient and easily-modifiable implementations for high-performance distributed sampling-based inference in DPMMs where the user is free to choose between either a multiple-machine, multi-core, CPU implementation (written in Julia) and a multiple-stream GPU implementation (written in CUDA/C++). Both the CPU and GPU implementations come with a common (and optional) python wrapper, providing the user with a single point of entry with the same interface. On the algorithmic side, our implementations leverage a
leading DPMM sampler from [1]. While Chang and Fisher III’s implementa-
tion (written in MATLAB/C++) used only CPU and was designed
for a single multi-core machine, the packages we proposed here dis-
tribute the computations efficiently across either multiple multi-core
machines or across multiple GPU streams. This leads to speedups,
alleviates memory and storage limitations, and lets us fit DPMMs to
significantly larger datasets and of higher dimensionality than was
possible previously by either [1] or other DPMM methods. Our open-
source code (GPLv2 licensed) is publicly available on github.com.

1 Introduction

In unsupervised learning, Bayesian Nonparametric (BNP) mixture mod-
els, exemplified by the Dirichlet-Process Mixture Model (DPMM), provide
a principled approach for Bayesian modeling while adapting the model
complexity to the data. This contrasts with finite mixture models whose
complexity is determined manually or via model-selection methods. To fix
ideas, an important DPMM example is the Dirichlet-Process Gaussian Mix-
ture Model (DPGMM), a Bayesian $\infty$-dimensional extension of the classical
Gaussian Mixture Model (GMM). Despite their potential, however, and al-
though researchers have used them successfully in numerous applications
during the last two decades, DPMMs still do not enjoy wide popularity
among practitioners, largely due to computational bottlenecks that exist
in current algorithms and/or implementations. In particular, one of the
missing pieces is the availability of software tools that: 1) can efficiently
handle DPMM inference in large datasets; 2) are user-friendly and can also
be easily modified.

We argue that in order for DPMMs to become a practical choice for large-scale
data analysis, implementations of DPMM inference must leverage parallel- and
distributed-computing resources (in an analogy, consider how advances in
GPU computing and GPU software contributed to the success of deep
learning). This is because of not only potential speedups but also memory
and storage considerations. For example, this is especially true in dis-
tributed mobile robotic sensing applications where multiple autonomous
agents working together have limited computational and communication
resources. As another motivating example, consider unsupervised data-
analysis tasks in large and high-dimensional computer-vision datasets.

In other words, while DPMMs are theoretically ideal for handling unlabeled
datasets, current implementations of DPMM inference do not scale well
Table 1: Overview of the proposed packages

| Package   | Processor       | Description                                                                 |
|-----------|-----------------|-----------------------------------------------------------------------------|
| CUDA/C++  | GPU             | The fastest package for high $N$ (number of data points) and $d$ (data dimensions) on a single machine; supports multiple GPU streams. |
| Julia     | CPU             | Supports both multiple cores and multiple machines.                         |
| Python    | Either CPU or GPU| Wrapper to the CUDA/C++ and Julia packages                                    |

with the size of the dataset and/or the dimensionality.

This is partly since most existing implementations are serial and they do not harness the power of distributed computing. This does not mean that there do not exist distributed algorithms for DPMM inference. There is, however, a large practical gap between designing such an algorithm and having it implemented efficiently in a way that fully utilizes the available computing resources. Thus, the very few publicly-available implementations of such distributed algorithms are fairly limited in their capabilities (as well as their expressiveness; e.g., some support only isotropic Gaussians [2], etc.). Our work closes this gap by providing effective and scalable statistical software for typical large-scale inference.

Concretely, we propose two solutions from which the users can choose according to their needs, constraints, and available computing resources. The first proposed solution, implemented purely in CPU, is based on distributing computations across multiple cores as well as multiple machines. The second proposed solution, based mostly on GPU, relies on distributing computations across multiple GPU streams in a single machine. See Table 1 for more details.

More generally (than the topic of DPMM inference), distributed implementations, at least in traditional programming languages used for such implementations, tend to be hard to debug, read, and modify. This clashes with the usual workflow of algorithm development. As a remedy, in our recent workshop paper [3], which constitutes a preliminary and partial version of this paper, we proposed a Julia implementation for distributed sampling-based DPMM inference. Since the publication of [3] we have improved the performance of our Julia implementation, have added its GPU counterpart in CUDA/C++, and added an optional Python wrapper for
both the CPU and GPU implementations.

To summarize, in this paper we explain how to use, via either Julia or CUDA/C++, an efficient distributed DPMM inference for large-scale analysis. Particularly, based on a leading parallel Markov Chain Monte Carlo (MCMC) inference algorithm [1] (to be discussed in section 2) – originally implemented in C++ for a single multi-core CPU single machine in a highly-specialized fashion using a shared-memory model – we provide novel, more scalable, and easier-to-use-or-modify implementations that leverage either the latest Nvidia’s asynch memory allocation API for GPU or Julia’s capabilities for distributing CPU computations efficiently across multiple multi-core machines using a distributed memory model. This leads to speedups, alleviates memory and storage limitations, and lets us infer DPMMs from significantly larger and higher-dimensional datasets than was previously possible by either [1] or other DPMM inference methods. Our Julia and CUDA/C++ implementations are also accompanied by an optional Python wrapper which hides the Julia & CUDA/C++ code from the user and provides a single point of entry that lets the user employ, in the same settings and with the same code, either one of our CPU and GPU packages.

2 Models and the Inference Algorithm

2.1 Preliminaries: Finite Mixture Models and Clustering

Let $d$ and $K$ be two positive integers and let $x$ be a generic point in $\mathbb{R}^d$. A $K$-component Finite Mixture Model (FMM), also known as a parametric mixture model, is a probabilistic model whose associated $d$-dimensional probability density function (pdf) is

$$p(x; \theta) = \sum_{k=1}^{K} \pi_k f(x; \theta_k)$$

where $\theta = (\pi_k, \theta_k)_{k=1}^{K}$, $(\pi_k)_{k=1}^{K}$ form a convex combination (namely, $\sum_{k=1}^{K} \pi_k = 1$ and $\pi_k \geq 0 \forall k$), and $f(x; \theta_k)$ is a $d$-dimensional pdf parameterized by $\theta_k$. The $(f(\cdot; \theta_k))_{k=1}^{K}$ functions are called the mixture components while $(\pi_k)_{k=1}^{K}$ are called the mixture proportions (or weights).

**Example 1** In the (finite) Gaussian Mixture Model (GMM), $\theta_k = (\mu_k, \Sigma_k)$ and $f(x; \theta_k) = \mathcal{N}(x; \mu_k, \Sigma_k)$ where the latter is a multivariate Gaussian pdf evaluated at $x$ and parameterized by a mean vector, $\mu_k \in \mathbb{R}^d$, and a Symmetric Positive-
Definite (SPD) $d \times d$ covariance matrix, $\Sigma_k$. In other words, in this example

$$f(x; \theta_k) = \mathcal{N}(x; \mu_k, \Sigma_k) \triangleq (2\pi)^{-d/2} \det(\Sigma_k)^{-1/2} \exp\left(-\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k)\right).$$

The case where $x$ takes values in a discrete set is similar, except that each component is a probability mass function (pmf), not a pdf. A popular example is a mixture of categorical distributions or, more generally, multinomial distributions.

Let $X = (x_i)_{i=1}^N$ stand for $N$ data points and again let $K > 0$ be an integer. Clustering is the task of partitioning $X$ into $K$ parts, called clusters and denoted by $C = (C_k)_{k=1}^K$. Let $z_i$ denote the latent point-to-cluster assignment of $x_i$; i.e., cluster $k$ is defined as $C_k = \{x_i : z_i = k\}$. In the standard formulation of FMM-based clustering, the data points are assumed to be independent and identically-distributed (i.i.d.) draws from an FMM and one typically tries to maximize the corresponding likelihood function, $p(X | \theta)$, over $\theta$. The most popular approach for (locally-) maximizing that likelihood is via an Expectation-Maximization (EM) algorithm [4]. As the time-honored Bayesian formulation helps avoiding problems such as over-fitting and enables encoding prior knowledge, the FMM also has a Bayesian (but still finite) variant, where $\theta$ is assumed to be random and drawn from a suitable prior [5] (specifically, the prior over $(\pi_k)_{k=1}^K$ is usually a Dirichlet distribution, not to be confused with a Dirichlet process). In which case, one targets the posterior distribution, $p(\theta | X)$, rather than the likelihood; e.g., one can try to maximize $p(\theta | X)$ over $\theta$, sample $\theta$ from it, compute posterior expectations, etc.

### 2.2 The Dirichlet Process Mixture Model (DPMM)

Below we provide a brief and informal introduction to the DPMM, focusing only on the essentials required for understanding this manuscript and make it self-contained as possible. For a comprehensive and formal mathematical treatment, see [6]. For an applied data-analysis perspective, see [7]. For a gentle introduction with machine-learning and/or computer-vision readers in mind, see the theses by [8] or [9].

The DPMM is a BNP extension of the FMM [10]. Loosely speaking, a DPMM entertains the notion of a mixture of infinitely-many components.

The weights, $\pi = (\pi_k)_{k=1}^\infty$, are drawn from a Griffiths-Engen-McCloskey (GEM) stick-breaking process with a concentration parameter $\alpha > 0$ [11],
while the components, \((\theta_k)_{k=1}^\infty\), are drawn from a prior as in the Bayesian FMM case.

**Example 2** The Dirichlet Process GMM (DPGMM) is a GMM with infinitely-many Gaussians.

Like the FMM, the DPMM is often used for clustering. With a DPMM, however, the number of clusters, \(K\), is not assumed to be known; rather, it is viewed as a latent random variable whose value is inferred with the rest of the model.

While in an FMM the number of clusters and the number of components are typically equal, and are thus both denoted by a single symbol, \(K\), with a DPMM the situation is different: although there are infinitely-many components, the (latent and random) number of clusters, \(K\), is finite (particularly, \(K \leq N\)). The inferred value of \(K\) depends on \(\alpha\) (the higher \(\alpha\) is, the more clusters are expected), on the complexity of the data, and on the (hyper-parameters of the) prior over the components (that said, when \(N\) is large, the last two factors are usually more influential than \(\alpha\)).

**Example 3** Recall that the standard prior for Gaussian components is a Normal Inverse-Wishart (NIW) distribution [5]. If the NIW’s hyper-parameters are set to strongly favor small covariances (hence small clusters), then this will implicitly favor a large \(K\). Likewise, if the NIW prior strongly favors larger covariances (hence large clusters), then \(K\) will tend to be small. In the lack of prior knowledge, however, the NIW prior can be set to be very weak (i.e., high uncertainty), letting the data speak for itself.

For simplicity, our text below implicitly assumes that all the random vectors involved have either a pdf or a pmf. One known mathematical construction of the DPMM uses the following distributions:

\[
\begin{align*}
\pi \mid \alpha & \sim \text{GEM} (\pi; \alpha), \quad (3) \\
\theta_k \mid \lambda & \overset{i.i.d.}\sim f_\theta (\theta_k; \lambda), \quad \forall k \in \{1, 2, \ldots\}, \quad (4) \\
z_i \mid \pi & \overset{i.i.d.}\sim \text{Cat} (z_i; \pi), \quad \forall i \in \{1, 2, \ldots, N\}, \quad (5) \\
x_i \mid z_i, \theta_{z_i} & \sim f_x (x_i; \theta_{z_i}), \quad \forall i \in \{1, 2, \ldots, N\}. \quad (6)
\end{align*}
\]

Here, \(f_\theta (\cdot; \lambda)\) is the pdf or pmf (associated with some base measure) parameterized by \(\lambda\), the infinite-length vector \(\pi = (\pi_k)_{k=1}^\infty\) is drawn from a GEM stick-breaking process with a concentration parameter \(\alpha > 0\) (particularly, \(\pi_k > 0\) for every \(k\) and \(\sum_{k=1}^\infty \pi_k = 1\)) while \(\theta_k\) is drawn from \(f_\theta\). Each of the
$N$ i.i.d. observations $(x_i)_{i=1}^N$ is generated by first drawing a label, $z_i \in \mathbb{Z}^+$, from $\pi$ (i.e., Cat is the categorical distribution), and then $x_i$ is drawn from (a pdf or a pmf) $f_x$ parameterized by $\theta_{z_i}$. Informally, $x_i \sim \sum_{k=1}^{\infty} \pi_k f(x_i; \theta_k)$.

Here too, each $f_x(\cdot; \theta_k)$ is called a component and we make no distinction between a component, $f_x(\cdot, \theta_k)$, and its parameter, $\theta_k$. The so-called labels $(z_i)_{i=1}^N$ encode the observation-to-component assignments. A cluster is a collection of points sharing a label; i.e., $x_i$ is in cluster $k$, denoted by $C_k$, if and only if $z_i = k$. Let (the random variable) $K$ be the number of unique labels: $K = |\{k : z_i = k \text{ for some } i \in \{1, \ldots, N\}\}|$; i.e., $K$ is also the number of clusters and is bounded above by $N$. Typically, and as assumed in this manuscript, $f_\theta$ is chosen to be a conjugate prior [5] to $f_x$. The latent variables here are $K$, $(\theta_k)_{k=1}^{\infty}$, $\pi$, and $(z_i)_{i=1}^N$. For more details (and other constructions), see [8].

**Example 4** In the case of Gaussian components, where $f_\theta(\cdot; \lambda)$ is an NIW pdf, we have

$$f_\theta(\mu_k, \Sigma_k; \kappa, m, v, \Psi) = \text{NIW}(\mu, \Sigma; \kappa, m, v, \Psi) \triangleq \mathcal{N}(\mu; m, \frac{1}{\kappa} \Sigma) \mathcal{W}^{-1}(\Sigma; v, \Psi)$$

where $\mathcal{W}^{-1}(\Sigma; v, \Psi)$ is the Inverse-Wishart distribution (over $d \times d$ SPD matrices), the hyperparameters are

$$\lambda = (m, \Psi, \kappa, v)$$

where $m \in \mathbb{R}^d$, the $d \times d$ matrix $\Psi$ is SPD, and the two real numbers $\kappa$ and $v$ satisfy $\kappa > 0$ and $v > d - 1$ (do not confuse $\kappa$ ("kappa") with $k$, the index of the component).

### 2.3 Inference via Chang and Fisher III’s DPMM Sampler

We now briefly review a DPMM sampler proposed by [1]. That sampler consists of a restricted Gibbs sampler [12] and a split/merge framework [13] which together form an ergodic Markov chain. The operations in each step of that sampler are highly parallelizable. Importantly, the splits and merges let the sampler make large moves along the (posterior) probability surface as in such operations multiple labels change their label simultaneously to the same different label. This is unlike what happens, e.g., in methods that
must change each label separately from the others. We now describe the essential details.

The augmented space. The latent variables, \((\theta_k)_{k=1}^{\infty}, \pi,\) and \((z_i)_{i=1}^{N}\), are augmented with auxiliary variables. For each component \(\theta_k\) two subcomponents (conceptually thought of as \(l=\text{“left”}\) and \(r=\text{“right”}\)) are added, \(\bar{\theta}_{k,l}, \bar{\theta}_{k,r}\), with subcomponent weights \(\bar{\pi}_k = (\bar{\pi}_{k,l}, \bar{\pi}_{k,r})\). Implicitly, this means that every cluster \(C_k\) is augmented with two subclusters, \(\bar{C}_{k,l}\) and \(\bar{C}_{k,r}\). For each cluster label \(z_i\), an additional subcluster label, \(\bar{z}_i \in \{l, r\}\), is added; i.e., subcluster \(\bar{C}_{k,l} \subset C_k\) consists of all the points in \(C_k\) whose subcluster label is \(l\) (the other subcluster, \(\bar{C}_{k,r}\), is defined similarly).

The restricted Gibbs sampler. This restricted sampler is not allowed to change (the current estimate of) \(K\); rather, it can change only the parameters of the existing clusters and subclusters, and when sampling the labels, it can assign an observation only to an existing cluster. For each instantiated component \(k\), changing \(\theta_k, \bar{\theta}_{k,l}, \text{and} \bar{\theta}_{k,r}\) is done using

\[
p(\theta_k|C_k; \lambda), p(\bar{\theta}_{k,l}|\bar{C}_{k,l}; \lambda), \text{and} p(\bar{\theta}_{k,r}|\bar{C}_{k,r}; \lambda),
\]

respectively, where the latter three are the conditional distributions of the cluster or subcluster parameters given the cluster or subclusters (and the prior hyperparameters, \(\lambda\)). In section 4, we will dive deeper into the details of the restricted Gibbs sampler.

The split/merge framework. Splits and merges allow the sampler to change \(K\) using the Metropolis-Hastings framework [14]. Particularly, the auxiliary variables are used to propose splitting an existing cluster or merging two exiting ones. When a split is accepted, each of the newly-born clusters is augmented with two new subclusters. The Hastings ratio of a split is [1]:

\[
H_{\text{split}} = \frac{\alpha \Gamma(N_{k,l})f_x(\bar{C}_{k,l}; \lambda) \Gamma(N_{k,r})f_x(\bar{C}_{k,r}; \lambda)}{\Gamma(N_k)f_x(C_k; \lambda)}
\]

where \(\Gamma\) is the Gamma function, \(N_k, N_{k,l}\) and \(N_{k,r}\) are the numbers of points in \(C_k, \bar{C}_{k,l}\) and \(\bar{C}_{k,r}\), respectively, while

\[
f_x(C_k; \lambda), f_x(\bar{C}_{k,l}; \lambda), \text{and} f_x(\bar{C}_{k,r}; \lambda)
\]
Figure 1: 20 clusters detected by DPMMSubClusters

represent the marginal likelihood of $C_k, \tilde{C}_{k,l}$ and $\tilde{C}_{k,r}$ respectively. Concrete expressions for the marginal likelihood, in the case of Gaussian or Multinomial components (the component types considered in our experiments) appear in [9].

Finally, a merge proposal is based on taking two existing clusters and proposing merging them into one. The corresponding Hastings ratio is $H_{merge} = 1/H_{split}$ where $\tilde{C}_{k,l}$ and $\tilde{C}_{k,r}$ are replaced with the two clusters, and $C_k$ is replaced with the result of the merge. For the derivation behind $H_{split}$ and $H_{merge}$, see [1].

Importantly, and as any successful DPMM inference method, Chang and Fisher III’s sampler can detect different numbers of clusters according to the complexity of the dataset. For example, in Figure 1 we demonstrate unlabeled data with 20 clusters while in Figure 2 we show data consisting of 6 clusters. Using our implementation (the topic of the next section), the sampler correctly detected the different numbers of clusters in each dataset, while using the same code and the same hyperparameters.

3 Software

The proposed software supports three different software languages (Julia, CUDA/C++, Python), two operating systems (Windows & Linux) as well as multiple interface options. In terms of performance, the proposed software is faster than other publicly-available packages that exist today and that we were able to test. Particularly, as long as the product of $N$ (number of data points) times $d$ (the dimension of the data) is not too low, then our GPU version is consistently at least a few times faster than any other
3.1 Installation

Our software (licensed under GPLv2) is available on GitHub. The URLs for our packages appear in Table 2. In order to compile the CUDA/C++ package the user will need C++14 (or higher) and CUDA 11.2 (or higher). For visualization purposes (i.e., plotting points in 2D), the CUDA/C++ windows version also requires OpenCV. However, this visualization is used only for debugging purposes so the installation of OpenCV is not mandatory for using our implementation. For the CPU package the user will need Julia 1.5 (or higher). For Python we used 3.8. The installation steps below were tested successfully on Windows 10 (Visual Studio 2019), Ubuntu 18.04, and Ubuntu 21.04.

1. Install CUDA version 11.2 (or higher) from https://developer.nvidia.com/CUDA-downloads
2. git clone https://github.com/BGU-CS-VIL/DPMMSubClusters_GPU
3. Install Julia from: https://julialang.org/downloads/platform
4. Add our DPMMSubCluster package from within a Julia terminal via Julia package manager:
   ] add DPMMSubClusters
5. Add our dpmmmpython package in python:
   pip install dpmmmpython
(6) Add Environment Variables:

- On Linux:
  (a) Add "CUDA_VERSION" with the value of the version of your CUDA installation (e.g., 11.5).
  (b) Add to the "PATH" environment variable the path to the Julia executable (e.g., in .bashrc add: export PATH =$PATH:$HOME/julia/julia-1.6.0/bin).
  (c) Make sure that CUDA_PATH exist. If it is missing add it with a path to CUDA (e.g., export CUDA_PATH=/usr/local/cuda-11.6/).
  (d) Make sure that the relevant CUDA paths are included in $PATH and $LD_LIBRARY_PATH (e.g., export PATH=/usr/local/cuda-11.6/bin:$PATH, export LD_LIBRARY_PATH=/usr/local/cuda-11.6/lib64:$LD_LIBRARY_PATH).

- On Windows:
  (a) Add "CUDA_VERSION" with the value of the version of your CUDA installation (e.g., 11.5).
  (b) Add to the "PATH" environment variable the path to the Julia executable (e.g., C:\Users\USER\AppData\Local\Programs\Julia\Julia-1.6.0\bin).
  (c) Make sure that CUDA_PATH exists. If it is missing add it with a path to CUDA (e.g., C:\Program Files\NVIDIA GPU Computing Toolkit\CUDA\v11.6).

(7) Install cmake if necessary.

(8) Install PyJulia from within a Python terminal:
  ```python
  import julia; julia.install();
  ```

(9) For Windows only (optional, used on for debugging purposes): Install OpenCV
  (a) run Git Bash
  (b) cd \YOUR_PATH_TO_DPMMSUBCLUSTERS\GPU\DPMMSUBCLUSTERS
  (c) ./installOCV.sh
Table 2: GitHub URL for each package.

| Package     | GitHub URL                                                                 |
|-------------|---------------------------------------------------------------------------|
| CUDA/C++    | https://github.com/BGU-CS-VIL/DPMMSubClusters_GPU                         |
| Julia       | https://github.com/BGU-CS-VIL/DPMMSubClusters.jl                          |
| Python      | https://github.com/BGU-CS-VIL/dpmmpython                                   |

### 3.2 Building

For Windows for the CUDA/C++ package both of the build options below are viable. For Linux use Option 2.

**Option 1:** DPMMSubClusters.sln - Solution file for Visual Studio 2019

**Option 2:** CMakeLists.txt

1. Run in the terminal:
   ```
   cd <YOUR_PATH_TO_DPMMSubClusters_GPU>/DPMMSubClusters
   mkdir build
   cd build
   cmake -S ../
   ```

2. Build:
   - **Windows:**
     ```
     cmake --build . --config Release --target ALL_BUILD
     ```
   - **Linux:**
     ```
     cmake --build . --config Release --target all
     ```

### 3.3 Post Build

Add Environment Variable:

- **On Linux:**
  Add "DPMM_GPU_FULL_PATH_TO_PACKAGE_IN_LINUX" with the value of the path to the binary of the package DPMMSubClusters_GPU.
  The path is: `<YOUR_PATH_TO_DPMMSubClusters_GPU>/DPMMSubClusters/DPMMSubClusters`.

- **On Windows:**
  Add "DPMM_GPU_FULL_PATH_TO_PACKAGE_IN_WINDOWS" with the value of the path to the exe of the package DPMMSubClusters_GPU.
The path is: `<YOUR_PATH_TO_DPMMSubClusters_GPU>\DPMMSubClusters\build\Release\DPMMSubClusters.exe`.

### 3.4 Executing

Below are listed several options to run DPMM inference using our software. Usually the best performance will be achieved by running the CUDA/C++ version which uses the GPU (when available).

#### 3.4.1 From Julia code - CPU

The following sample code generates a synthetic GMM dataset with $N = 10^5$ points, dimension $d = 2$ and $K = 10$ clusters, and then fits a DPMM to the data (without knowing $K$ or the other parameters of the GMM) using the sampler.

```julia
using DPMMSubClusters

x, labels, clusters =
    DPMMSubClusters.generate_gaussian_data(10^5, 2, 10, 100.0)

hyper_params =
    DPMMSubClusters.niw_hyperparams(Float32(1.0),
                                      zeros(Float32, 2),
                                      Float32(5),
                                      Matrix{Float32}(I, 2, 2)*1)

DPMMSubClusters.dp_parallel(x, hyper_params, Float32(100000.0),
                             100, 1, nothing, true, false, 15,
                             labels)
```

#### 3.4.2 From a C++ code – GPU

`dp_parallel()` in ‘dp_parallel_sampling_class’ is the function that should be called in order to run the program. The sample code below will first generate a synthetic random dataset and will then run the sampler to fit a DPMM to it.

```cpp
srand(12345);
data_generators.data_generators;
MatrixXd x;
std::shared_ptr<LabelsType> labels =
    std::make_shared<LabelsType>();
double** tmean;
```
double** tcov;
int N = (int)pow(10, 5);
int D = 2;
int numClusters = 2;
int numIters = 100;

data_generators.generate_gaussian_data(N, D, numClusters, 100.0,
x, labels, tmean, tcov);

std::shared_ptr<hyperparams> hyper_params =
    std::make_shared<niw_hyperparams>(1.0, VectorXd::Zero(D), 5,
    MatrixXd::Identity(D, D));
dp_parallel_sampling_class dps(N, x, 0, prior_type::Gaussian);
ModelInfo dp = dps.dp_parallel(hyper_params, N, numIters, 1, true,
false, false, 15, labels);

3.4.3 From the command line – GPU

Running the CUDA/C++ program can be done from the command line (in
both Linux and Windows). There are a few parameters that can be used
to run the program. In order to set the hyperparams the params_path
parameter can be used. The value of the parameter should be a path for a
Json file which includes the hyperparams (i.e. alpha or hyper_params for
the prior). In order to use this parameter follow this syntax:

    --params_path=<PATH_TO_JSON_FILE_WITH_MODEL_PARAMS>

There are few more parameters like model_path for the path to a npy
file which include the model and result_path for the path of the output
results.

Our code has support for both Gaussian and Multinomial distributions. It
can be easily adapted to other component distributions, e.g., Poisson, as
long as they belong to an exponential family. The default distribution is
Gaussian. To specify a distribution other than a Gaussian, use the prior_type
parameter. For example:

    --prior_type="Multinomial"

The Json file containing the model parameters can contain many parameters
that can be controlled by the user. A few examples are: alpha, prior, number
of iterations, burn_out and kernel. The full list of parameters can be seen
in the function init() in ‘global.params’. The result file is a Json file
which by default contains the predicted labels, the weights, the Normalized
Mutual Information (NMI) score and the running time per iteration. A few other parameters can be added to the result file. Samples for these additional parameters are commented out in the main.cpp file.

### 3.4.4 From Python code – CPU and GPU

The dpmmwrapper.py file contains an example for how to run either the GPU or CPU packages from Python (look for the code in the function `main`). In the following example we are generating a GMM synthetic dataset for $10^5$ point, 2 dimensions and 10 clusters. We are running it on the GPU.

```python
from julia.api import Julia
jl = Julia(compiled_modules=False)
from dpmmpython.dpmmwrapper import DPMMPython
from dpmmpython.priors import niw

data, gt = DPMMPython.generate_gaussian_data(sample_count=10000, dim=2, k=10, var=100.0)
prior = niw(kappa = 1, mu = np.zeros(2), nu = 3, psi = np.eye(2))
labels, clusters, results = DPMMPython.fit(data = data, alpha = 100,
prior = prior, verbose = True,
   gt = gt,
gpu = True)
```

Here, the variable “results” depends on the backend: for the CUDA/C++ backend it will be ‘null’, while for the Julia backbone “results” will contain other information (see the documentation of our Julia ‘fit’ function). The “gt” variable stands for the ground-truth labels.

### 3.4.5 From a Jupiter notebook – CPU and GPU

The notebook dpmmwrapper.ipynb can be executed to test different packages including our GPU and CPU packages on multiple datasets.

### 3.5 Test

Our CUDA/C++ package was built with the Test Development Driven (TDD) methodology. The Windows version comes with 53 unit tests which cover more than 60% of the code. Usually it takes less than 3 minutes to run all
tests. Those tests are for both Gaussian and Multinomial distributions, and include the different CUDA kernels (for matrix multiplication) mentioned in section 4 below. We used the GoogleTest framework to write those tests and they were validated with a Visual Studio 2019 test engine.

4 The Proposed Implementation

4.1 Design and Implementation

In our implementation(s) after we initialize all the required objects, we start running the iterations of the sampler. For each iteration in group_step() we execute the algorithm which is described below in detail. For concreteness, below we will refer to the CUDA/C++ code during the algorithm’s description and not to the Julia code. However, the structure of the code in both packages is similar enough to be followed as long as the reader is familiar with any of those languages.

We use the same notation as in [1] where $N$ is the number of data points and $K$ is the (current estimate of the) number of clusters.

- For each iteration of the restricted Gibbs sampling:
  
  (a) Sample cluster weights $\pi_1, \pi_2, \ldots, \pi_K$:

  \[
  (\pi_1, \ldots, \pi_K, \tilde{\pi}_{K+1}) \sim \text{Dir}(N_1, \ldots, N_K, \alpha). \tag{14}
  \]

  In our code we built a vector points_count that holds the number of points for each cluster and apply a Dirichlet-distribution sampling at once for all clusters:

  \[
  \text{dirichlet_distribution<\text{std::mt19937}> d(points_count);}
  \text{std::vector<double> dirichlet = d(*globalParams->gen);}
  \]

  (b) Sample sub-cluster weights from a 2D Dirichlet distribution:

  \[
  (\tilde{\pi}_{kl}, \tilde{\pi}_{kr}) \sim \text{Dir}(N_{kl} + \alpha/2, N_{kr} + \alpha/2), \quad \forall k \in \{1, \ldots, K\}. \tag{15}
  \]

  In order to propose meaningful splits that are likely to be accepted, the algorithm uses auxiliary variables such that each cluster consists of 2 sub-clusters (conceptually thought of as “left” and “right”). $\tilde{\pi}_k = \{\tilde{\pi}_{kl}, \tilde{\pi}_{kr}\}$ denote the weights of the sub-clusters of cluster $k$. The code is implemented in sample_cluster_params() in ‘shared_actions’.
(c) Sample cluster parameters:

$$\theta_k \sim f_x(x_{I_k}; \theta_k)f_\theta(\theta_k; \lambda), \quad \forall k \in \{1, \ldots, K\}.$$  \hspace{1cm} (16)

Here, $f_x(X; \theta_k)$ is the likelihood of a set of data points under the parameter $\theta_k$, $f_\theta(\theta; \lambda)$ is the likelihood of the parameter $\theta$ under the prior $f_\theta(\cdot; \lambda)$, $\sim$ denotes sampling proportional to the right-hand side of the equation, and $I_k = \{i: z_i = k\}$ is the set of indices of that points labels as belonging to cluster $k$. Each distribution (e.g., a Gaussian or a Multinomial) has its own `sample_distribution()` function which calculates the cluster’s parameters. The prior classes for the Gaussian and Multinomial distributions are ‘niw’ and the ‘multinomial_prior’ respectively which inherit from the ‘prior’ class. The likelihood is calculated in each class within the function `log_marginal_likelihood()`. In order to extend and support to more distributions new classes which inherit from ‘prior’ may be added.

(d) Sample sub-cluster parameters:

$$\bar{\theta}_{kh} \sim f_x(x_{I_{kh}}; \bar{\theta}_{kh})f_\theta(\bar{\theta}_{kh}; \lambda), \quad \forall k \in \{1, \ldots, K\} \quad , \quad h \in \{l, r\}.$$  \hspace{1cm} (17)

$\bar{\theta}_k = \{\bar{\theta}_{kl}, \bar{\theta}_{kr}\}$ denotes the parameters of the sub-clusters of cluster $k$. In the code we used the same functions that we used for the calculation the cluster’s parameters. We maintain the following objects in memory: a `std::vector` of `local_cluster` type where each item in that vector holds the cluster and sub-cluster parameters (e.g., $\bar{\theta}_k$, $\mu_k$, $\Sigma_k$, $\bar{\theta}_{kl}$, $\bar{\theta}_{kr}$, $\pi_{kl}$ and $\pi_{kr}$ for the $k$th Gaussian), the point counts (i.e., $N_k$, $N_{kl}$, $N_{kr}$) and the sufficient statistics as well as the cluster weights (i.e., $\pi_1$, $\pi_2$, $\ldots$, $\pi_K$).

(e) Sample cluster assignments for each point:

$$z_i \sim \sum_{k=1}^{K} \pi_k f_x(x_i; \theta_k)1(z_i = k), \quad \forall i \in \{1, \ldots, N\}.$$  \hspace{1cm} (18)

To sample from a probability distribution efficiently we implemented a GPU kernel in `sample_by_probability()` based on a C algorithm [15]. To summarize all $k$ of a point we wrote the `dcolwise_dot_all_kernel()` kernel. These kernels are working in parallel on all components. Each component is working in a different GPU
stream while in each stream the points are aggregated to blocks that are running in parallel. We set a number of 512 threads per block. This parameter can be fine-tuned to optimize the performance based on the GPU hardware being used.

(f) Sample sub-cluster assignments for each point:

\[ \bar{z}_i \sim \sum_{h \in \{l, r\}} \pi_{z_i|h}f_x(x_i; \tilde{\theta}_{z_i|h})1(\bar{z}_i = h), \quad \forall i \in \{1, \ldots, N\}. \]  

\[ \bar{z}_i \in \{l, r\} \] variables are (conceptually thought of as “left” and “right”) indicate which of the sub-cluster the \(i^{th}\) point is assigned to. We have a thin version of the cluster and sub-cluster parameters thin_cluster.params. For a single machine this structure is unneeded since the data already exists in ‘local_cluster’. However, we maintain it not only for consistency with the Julia package but also because this option may be valuable in the future to scale our CUDA/C++ implementation to multiple machines.

For efficiency we are not copying the data; rather, we use std::shared_ptr between the structures. We have also chunks of the data per GPU in the device memory as part of the ‘gpuCapability’ structure. The structure contains the following 3 properties: List of points \(x_i\) (d_points), chunks of the cluster assignments \(z_i\) (d_labels) and sub-cluster assignments \(\bar{z}_i\) (d_sub_labels).

```cpp
struct gpuCapability {
    int* d_labels;
    int* d_sub_labels;
    double* d_points;
};
```

```cpp
class cudaKernel {
protected:
    std::map<int, gpuCapability> gpuCapabilities;
};
```

• Propose and Accept Splits:
  By sampling the sub-clusters, one is able to propose and accept meaningful splits that divide a cluster into its 2 sub-clusters.

  (a) Propose to split cluster \(k\) into its 2 sub-clusters for all \(k \in \{1, 2, \ldots, K\}\).
(b) Calculate the Hastings ratio $H$ and accept the split with probability $\min(1, H)$:

$$H_{\text{split}} = \frac{\alpha \Gamma(N_{kl}) f_x(x_{T_{kl}}; \lambda) \cdot \Gamma(N_{kr}) f_x(x_{T_{kr}}; \lambda)}{\Gamma(N_k) f_x(x_{T_k}; \lambda)}$$

The proposal is done in the function `should_split_local()` and the split itself is done in the kernel `split_cluster_local_worker()`.

- Propose and Accept Merges:
  Merges are proposed by merging 2 sub-clusters into one with each of the original clusters becoming a sub-cluster of the new merged cluster.
  
  (a) Propose to merge clusters $k_1, k_2$ for all pairs $k_1, k_2 \in \{1, 2, \ldots, K\}$.

(b) Calculate the Hastings ratio $H_{\text{merge}}$,

$$H_{\text{merge}} = \frac{\Gamma(N_{k_1} + N_{k_2})}{\alpha \Gamma(N_{k_1}) \Gamma(N_{k_2})} \frac{p(x|\hat{z})}{p(x|z)} \times \frac{\Gamma(\alpha)}{\Gamma(\alpha + N_{k_1} + N_{k_2})} \times \frac{\Gamma(\frac{\alpha}{2} + N_{k_1}) \Gamma(\frac{\alpha}{2} + N_{k_2})}{\Gamma(\frac{\alpha}{2}) \Gamma(\frac{\alpha}{2})}$$

and accept the merge with probability $\min(1, H_{\text{merge}})$. The proposal is done in function `should_merge()` and the merge itself is done in the kernel `merge_clusters_worker()`.

### 4.2 Optimizing Processing

**Two kernels for optimization**

In order to optimize the performance of the matrix multiplication which is required in our algorithm we used two different CUDA kernels and decide which one to use based on the size of the $d \times N$ matrix (where $d$ is the dimension of the data and $N$ is the number of points). We added a built-in capability to automatically select, at run-time, the best kernel automatically based on $d$, $N$ and the GPU capabilities. For more optimization in case that the best kernel is known we provide an option to set the kernel which can save some time at the beginning of the run (especially with a high $N$ and a high $d$). We measured the optimal kernel on an NVidia Quadro RTX 4000 card. On matrices whose size was below 640,000 size ($d \times N$), Kernel #1 is optimized and above this number Kernel #2 is optimized. Kernel #1 was written in a native way for CUDA to multiply two matrices. Kernel #2 was written with cublas API which is more optimal for big matrices.
Data Structure
To optimize the operations that needed to be done on the matrices and in the device, all the data in the GPU and in Eigen’s structure are stored in a column-major order. In general, in places where we needed to perform operations on all data points, we iterate on the dimensions and run (in parallel) each point calculation on a different GPU core.

4.3 Parallelism
The sampler from [1] was designed with massive parallelization in mind. Thus, most of its operations are parallelizable. Particularly, sampling cluster parameters is parallelizable over the clusters, sampling assignments can be computed independently for each point, and cluster splits can be proposed in parallel. Thus, a multi-core implementation is quite straightforward, with the caveat that one needs to be careful with merges; i.e., to prevent more than 2 clusters merge into the same single cluster; e.g., if clusters 1 and 2 are merged at the same time when clusters 2 and 3 are merged, this would imply the three clusters (1, 2, and 3) would be merged into a single one. However, this would be inconsistent with the underlying model. Recall that [1] released a multi-core single-machine C++ implementation (for CPU). The nature of the algorithm, however, let us build an implementation that goes beyond their original implementation, by allowing parallelization across multiple machines, not just multiple CPU cores. In turn, this enables us to not only leverage more computing power and gain speedups but also provide practical benefits in terms of memory and storage. For example, our Julia implementation can be used within a distributed network of weak agents (e.g., small robots collecting data). It also never transfers data (which is expensive and slow); rather, we transfer only sufficient statistics and parameters. Thus, the proposed implementation is also well suited for a network of low-bandwidth communication. Likewise, on a single machine, we are able to use the GPU’s cores powers and Nvidia streams and asynchronous calls.

4.3.1 Multiple GPU Streams
Most of the code was written as separated individual streams. Each stream contains sequences of operations that execute in issue-order on the GPU. CUDA operations in different streams may run concurrently. In many places we tied the stream to a specific cluster. Thus, we could run close to $O(1)$ instead of $O(K)$. We took advantage of CUDA’s asynchronous memory allocation API which was exposed lately in version 11. We were able to
allocate and deallocate the parameters as part of the sequence of operations and in this way to improve the concurrency of other kernels that were running on other streams. In Figure 3 we show an example of memory allocation operations that were performed on the GPU in parallel and at the same time that the kernel operation was running.

4.3.2 Multiple GPU Cards

We tested the performance of our implementation by parallelizing the processing across multiple GPUs. The logic that we adopt was to parallelize the parts that we were running with multi-streams on multi-GPUs. We implemented a container with all available GPUs: std::map<int, gpuCapability> gpuCapabilities. In the places that we sample the cluster and sub-cluster parameters and where the sufficient statistics are been calculated, instead of creating a stream on the same GPU we took the next available GPU by calling to the function pick any device and created a stream on the current selected device. Our hypothesis was that in places which $K$ is large there should be more impact. Our observation when we tested 2 GPUs (of type Quadro RTX 4000) was that the performance is not better. Consequently, we disabled that option by default in the cudaKernel::init function using the following line: numGPU = 1. On a different hardware and different GPU types, however, it is possible that this option will yield better results. Thus, the user may want to experiment with codenumGPU ≥ 1, depending on the available hardware.

4.4 Runtime Complexity

We now go throughout the CUDA/C++ runtime complexity step by step based on the algorithm. The symbol $G$ below denotes the number of GPU cores.

For each iteration of a restricted Gibbs sampling: Sampling the cluster and sub-cluster parameters (including weights) takes constant time for
each cluster. In Julia it is parallelized over \( P \) processes on the master.

This takes \( O(K \times d/P) \) time. In CUDA/C++ we observed that using `omp parallel for` (for \( K \)) when sampling the cluster parameters is slower than performing it sequentially. The root cause is the fact that Eigen (which we rely on for matrix manipulation) already uses multiple CPU cores and it also uses the GPU efficiently in each one of its threads. Thus, running over the \( K \) clusters in parallel is slower than sequentially. Therefore the complexity of CUDA/C++ is \( O(K \times d) \). Sampling the cluster weights is also done in constant time. Copying cluster and sub-cluster weights and parameters from host to device is parallelized over CUDA streams over \( K \) clusters. The process is parallelized over \( K \) clusters and over \( G \) GPU cores so it takes \( O(K \times d/G) \). Sampling the cluster assignments takes \( O(N \times K \times T/G) \) time, where \( T \) depends on the observation model, e.g. for multivariate Gaussian observation model with NIW prior \( T = d^2 \), wherein for a multinomial observation model with Dirichlet prior \( T = d \). Sampling the sub-cluster assignments takes \( O(N \times T/G) \). Updating the cluster and sub-cluster sufficient statistics can be split up into 3 steps. The first step is for all streams to calculate the sufficient statistics for the data it is in charge of which is common to all kinds of distributions. This step takes \( O(N/G) \) time. The second step is to calculate the sufficient statistics which is unique per the distribution. It is done in parallel to each sub-cluster \((l, r)\) and to the cluster. This step takes \( O(N \times T/G) \) time. The third step is to aggregate across all streams. This step takes \( O(K \times d) \) time. Overall, this takes \( O(N \times K \times T/G) + O(N \times T/G) + O(K) \) time. So total: \( O(N \times K \times T/G) \).

**Splits:** Proposing splits by looking at each cluster is \( O(K) \), noting that we can drop the \( T \) here as we use previously calculated values. Processing all the accepted splits requires updating the sufficient statistics which could take at the worst case \( O(N/G) + O(K) \) if all clusters are split.

**Merges:** Proposing merges by inspecting each cluster pair is \( O(K^2) \), as in the splits, we can drop the \( T \), by using the previously calculated values. Processing all the accepted merges also requires updating sufficient statistics. The worst case (i.e., if all clusters are merged) is thus \( O(N) + O(K) \).

To summarize, the total runtime complexity is \( O(K) + O(N \times K \times T/G) = O(N \times K \times T/G) \).
4.5 Memory Complexity

We now look at the amount of memory used on the GPU. The data is stored as one array, so we have $O(d \times N)$ on the GPU. The amount of data for the labels and sub labels is $O(N)$. Each stream also has a copy of the cluster and sub-cluster parameters which takes $O(K)$ space. We also have to aggregate sufficient statistics for each cluster after sampling the assignments, taking $O(K \times T)$. Hence, we have a total memory usage of $O(d \times N)$. Since usually $N \gg K$, the memory overhead is insignificant in comparison to the data itself.

5 Illustrations

5.1 Synthetic Data: Dirichlet Process Gaussian Mixture Model (DPGMM)

We tested our implementation on small and large synthetic GMM datasets. We wrote a class `data_generators` to generate the synthetic datasets. We ran 112 tests with different parameters: $N (10^3,10^4,10^5,10^6)$, $d (2,4,8,16,32,64,128)$ and $K (4,8,16,32)$. For each test we ran 100 iterations (sufficed for convergence in all methods). We repeated each test 10 times with the same random Gaussian synthetic data that we generated and then averaged the resulting NMI scores and running times. In each test we compared CUDA/C++, Julia, and a Bayesian Gaussian Mixture from sklearn. The latter, like our implementations, infers $K$ with the rest of the model. However, unlike our implementations, this sklearn’s model requires an upper bound on $K$.

During our testing we observed that, on a single machine, our CUDA/C++ implementation is faster than our Julia implementation in most of the cases. The cases in which Julia was faster were when running with a low $N$ (up to 10K) and a low $d$ (up to 32). When the data is larger (e.g., when $N = 10^6$ or $d = 128$) the CUDA/C++ solution is 2.5 times faster than Julia on average. In general, when $N \times d \times K$ is high the CUDA/C++ solution is faster than the Julia solution. Both Julia and CUDA/C++ are faster on average than sklearn solution: on average, Julia was 2.6 times faster and the CUDA/C++ was 5.3 times faster. Moreover, in a few cases the CUDA/C++ was 35 times faster than sklearn.

In Figure 4 we demonstrated the time comparison for $N = 10^6$. In the left side when $d \leq 4$ we see that our solutions were faster than sklearn. Due to the slowness of sklearn for the cases when $d > 4$ we set in the right side...
Figure 4: DPGMM synthetic data, time, $N = 10^6$. In the right panel, due to sklearn’s slowness, we had to give it the unfair advantage of using the true $K$ as the upper bound of the number of clusters.

of the figure an easier target for sklearn and set sklearn’s upper bound for $K$ to the true $K$ (without doing it, sklearn’s running time for a high $d$ was impractically slow, many orders of magnitude slower than our implementations). It is obvious from the figure than even when we gave a big advantage to sklearn, our implementations still beat it. For accuracy we measured the NMI for each case. NMI comparison is displayed in Figure 5. Again we split the test into two parts. The left side of the figure describes a fair comparison where all the methods were given the same conditions. The right side describes the case sklearn enjoyed the advantage of a reduced complexity achieved by using the true $K$ as the upper bound. Despite that advantage, our solutions still yielded better results almost in all cases. All tests can be reproduced by running the dpmmwrapper.ipynb Jupiter Notebook from https://github.com/BGU-CS-VIL/dpmmpython. Because of the slowness of sklearn, the notebook as is might take many days. You can consider to reduce the number of permutations that we tested for $N$, $d$ and $K$ or to reduce the number of repeats.
Figure 5: DPGMM synthetic data, NMI, $N = 10^6$. In the right panel, due to sklearn’s slowness, we had to give it the unfair advantage of using the true $K$ as the upper bound of the number of clusters.

5.2 Synthetic Data: Dirichlet Process Multinomial Mixture Model (DPMNMM)

We ran 72 tests with different parameters: $N (10^3,10^4,10^5,10^6)$, $d (4,8,16,32,64,128)$ and $K (4,8,16,32)$ while $d \geq K$. For each test we ran 100 iterations (sufficed for convergence). We repeated 10 times each test with the same random multinomial synthetic data and then averaged the NMI results and running times. In each test we compared our CUDA/C++ and Julia solutions to each other (sklearn does not support multinomial components when the number of components is unknown). Unlike in the case of Gaussian components, here, with multinomials, we observed that our CUDA/C++ solution was uniformly faster than our Julia solution. On average the former was 5 times faster than the latter. The results (using $N = 10^6$) are displayed in Figure 6. The corresponding NMI scores appear in Figure 7.
Figure 6: DPMNMM synthetic data, time, $N = 10^6$.

Figure 7: DPMNMM synthetic data, NMI, $N = 10^6$. 
5.3 Real Data

We also tested our solution on real datasets, where, as pre-processing, we used Principal Component Analysis (PCA) to reduce the dimensionality. For DPGMM we used the following datasets: \textbf{mnist} \((N = 60000, d = 32, K = 10)\); \textbf{fashion mnist} \((N = 60000, d = 32, K = 10)\) and \textbf{ImageNet-100} \((N = 125000, d = 64, K = 100)\). We compared our CUDA/C++ and Julia implementations with sklearn BayesianGaussianMixture. For DPMNMM we used \textbf{20newsgroups} \((N = 11314, d = 20000, K = 20)\), and compared our CUDA/C++ and Julia implementations to each other (sklearn does not support multinomial components when the number of components is unknown). In the DPMNMM case, when the dimension was very high \((d = 20,000)\) the CUDA/C++ package was 188 times faster than Julia. In Figure 8 we compared the running times on each dataset between the different packages. It is clear from the figure that our CUDA/C++ package is much faster from the two others, and that our Julia package is much faster than sklearn. In Figure 9 we displayed the NMI comparison the different packages. On \textbf{ImageNet-100}, our CUDA/C++ and Julia packages are almost equal sklearn (with a minor difference of 0.013). In all other cases, our solutions were more accurate than sklearn. Moreover, even though, on \textbf{ImageNet-100}, our solutions did not score higher NMI values than sklearn, the \(K\) value that we predicted was much more accurate. That is, while the true \(K\) was 100, sklearn predicted \(K = 500\) (which was the value of the upper bound it was given). In contrast we predicted on average \(K = 96.8\) (with a standard deviation of 17.78).

6 Summary and Discussion

We extended the DPMM inference method from [1] by efficient and easily-modifiable implementations for high-performance distributed sampling-based inference. Our software can be adopted by practitioners in an easy way where the user is free to choose between either a multiple-machine, multiple-core, CPU implementation (written in Julia) and a multiple-stream GPU implementation (written in CUDA/C++). We also provide an optional Python wrapper which hides the CPU and GPU implementations as a single package with one interface. The proposed implementation supports both Gaussian and Multinomial components. However, it is also easy to extent the code to support other exponential families. We also tested the proposed implementation for learning models from real datasets as mnist, fashion mnist, ImageNet-100 and 20newsgroups. We compared our solution
Figure 8: DPMM on real data: running times. In the 20newsgroup dataset (where the data dtype is discrete) the components are Multinomials. In the other datasets the components are Gaussians.

to sklearn and showed that for large and high dimensions our solution achieves the same, or better, accuracy while being much faster. Empirically, we found that when using high-dimensional Gaussians on a single machine our GPU package is faster than any other solution that is currently publicly available. For Multinomial components, our GPU package showed even better results which are by at least two order of magnitude faster than any other existing solution. We provided a solution for cross operating systems platforms (Windows & Linux). Our tests can be easily reproduced via a Jupiter Notebook included with our Python package.

7 Computational details

We ran our tests on two different hardware. One with strong CPU, more RAM and GPU from GTX family: i7-6800K CPU, 3.40GHz with 12 cores, 64GB RAM, GeForce GTX 1070. Second configuration with slower CPU, less RAM and GPU from RTX family: E5-2620 v3 CPU, 2.40GHz with 12 cores, 32GB RAM, Quadro RTX 4000. In both cases we used the same code. We used CUDA driver version 11. We tested on Windows 10 and Linux.
Figure 9: DPMM on real data: NMI scores. In the 20newsgroup dataset (where the data dtype is discrete) the components are Multinomials. In the other datasets the components are Gaussians.

Ubuntu 18.04 and 21.04. The Python version that we used for the wrapper was 3.8. In the CUDA/C++ package for windows we used OpenCV version 4.5.2 to demonstrate visualization in 2D of the clustering process iteration by iteration.

8 Open Sources

In Table 3 we specify all the open sources that we use in the CUDA/C++ package. In Table 4 we specify all the open sources that we use in the Julia package.
| Open Source       | Usage                                           | Link                                                                 |
|------------------|-------------------------------------------------|----------------------------------------------------------------------|
| cnpy             | Read and write models from npy format           | https://github.com/rogersce/cnpy                                     |
| zlib             | Required by cnpy                                | https://github.com/madler/zlib                                       |
| dirichlet_distribution | Dirichlet distribution                       | https://github.com/gcant/dirichlet-cpp                               |
| logdet           | Log determinant for Eigen using Cholesky        | https://gist.github.com/redpony/ftc8a0db6b20f7b1a3f23                 |
| vcflib           | Log(gamma) and multinormal sampling             | https://github.com/vcflib/vcflib                                     |
| eigen            | Matrix and vector operations                    | https://eigen.tuxfamily.org                                          |
| stats            | Sampling from an inverse-Wishart                | https://www.kthohr.com/statslib.html                                |
| gcem             | Required by stats                               | https://github.com/kthohr/gcem                                      |
| jsoncpp          | Read and write Json files                       | https://github.com/open-source-parsers/jsoncpp                      |
| MIToolbox        | Calculates NMI                                  | https://github.com/Craigacp/MIToolbox                               |
| opencv           | Drawing (for debugging)                         | https://opencv.org/                                                 |

Table 3: C++ open-source packages used in the proposed implementation
| Open Source        | Usage                                | Link                                      |
|-------------------|--------------------------------------|-------------------------------------------|
| Clustering.jl     | Evaluation metrics                   | https://github.com/JuliaStats/Clustering.jl |
| DistributedArrays.jl | Distribute Computations              | https://github.com/JuliaParallel/DistributedArrays.jl |
| Distributions.jl  | Probability Distributions            | https://github.com/JuliaStats/Distributions.jl |
| JLD2.jl           | Saving and restoring checkpoints     | https://github.com/JuliaIO/JLD2.jl        |
| NPZ.jl            | Compatibility with Numpy data        | https://github.com/fhs/NPZ.jl             |
| SpecialFunctions.jl | Log Gamma function                   | https://github.com/JuliaMath/SpecialFunctions.jl |

Table 4: Julia open-source packages used in the proposed implementation
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