

Image Modeling with Deep Convolutional Gaussian Mixture Models

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Abstract—In this conceptual work, we present Deep Convolutional Gaussian Mixture Models (DCGMMs): a new formulation of deep hierarchical Gaussian Mixture Models (GMMs) that is particularly suitable for describing and generating images. Vanilla (i.e., flat) GMMs require a very large number of components to describe images well, leading to long training times and memory issues. DCGMMs avoid this by a stacked architecture of multiple GMM layers, linked by convolution and pooling operations. This allows to exploit the compositionality of images in a similar way as deep CNNs do. DCGMMs can be trained end-to-end by Stochastic Gradient Descent. This sets them apart from vanilla GMMs which are trained by Expectation-Maximization, requiring a prior k-means initialization which is infeasible in a layered structure. For generating sharp images with DCGMMs, we introduce a new gradient-based technique for sampling through non-invertible operations like convolution and pooling. Based on the MNIST and FashionMNIST datasets, we validate the DCGMMs model by demonstrating its superiority over flat GMMs for clustering, sampling and outlier detection.

Index Terms—Deep Learning, Gaussian Mixture Models, Deep Learning, Deep Convolutional Gaussian Mixture Models, Stochastic Gradient Descent

I. INTRODUCTION

This conceptual work is in the context of probabilistic image modeling, whose main objectives are both, density estimation and image generation (sampling). Since images usually do not precisely follow a Gaussian mixture distribution, such a treatment is inherently approximative in nature. Image generation is currently a very active research topic, and similar techniques are being investigated for generating videos [9], [25].

An issue with many recent approaches is the lack of density estimation capacity, i.e., explicitly expressing the learned probability-under-the-model $p(\mathbf{x})$ of an image \mathbf{x} .

In contrast, GMMs explicitly describe the distribution $p(\mathbf{X})$, given by a set of training data $\mathbf{X} = \{\mathbf{x}_n\}$, as a weighted mixture of K Gaussian component densities $\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \equiv \mathcal{N}_k(\mathbf{x})$:

$$p(\mathbf{x}) = \sum_k^K \pi_k \mathcal{N}_k(\mathbf{x}). \quad (1)$$

Conceptually, GMMs are latent-variable models: it is assumed that the unobservable (latent) variable z determines from

which component a data vector \mathbf{x} has been sampled, which is expressed as

$$p(\mathbf{x}, z) = \pi_z \mathcal{N}_z(\mathbf{x}) \quad (2)$$

Marginalizing the latent variable in Eq. (2), we obtain Eq. (1).

GMMs require the mixture weights to be normalized: $\sum_k \pi_k = 1$ and the covariance matrices to be positive definite: $\mathbf{x}^T \boldsymbol{\Sigma}_k \mathbf{x} > 0 \ \forall \mathbf{x}$. The quality of the current fit-to-data is expressed by the (incomplete) log-likelihood

$$\mathcal{L}(\mathbf{X}) = \mathbb{E}_n \left[\log \sum_k \pi_k \mathcal{N}_k(\mathbf{x}_n) \right], \quad (3)$$

which is what GMM training optimizes, usually by variants of Expectation-Maximization (EM) [4]. It is shown that any distributions can be approximated by mixtures of Gaussians given enough components [11]. Thus, GMMs are guaranteed to model the complete data distribution, but only to the extent allowed by the number of components K .

In this respect, GMMs are similar to flat neural networks with a single hidden layer. Although, by the universal approximation theorem of [26] and [14], they *can* approximate arbitrary functions (from certain rather broad function classes), they fail to do so in practice. The reason for this is that the number of required hidden layer elements is unknown, and usually beyond the reach of any reasonable computational capacity. For images, this problem was largely solved by introducing deep Convolutional Neural Networks (CNNs). CNNs model the statistical structure of images (hierarchical organization and translation invariance) by chaining multiple convolution and pooling layers. Thus, the number of parameters can be reduced without compromising accuracy.

A. Objective, Contribution and Novelty

The objective of this article is to introduce a GMM architecture which exploits the same principles that led to the performance explosion of CNNs. In particular, the genuinely novel characteristics are:

- conceptually new formulation of deep GMMs, including convolution and pooling operations
- scalable end-to-end training by SGD from random initial conditions (no k-means initialization)
- efficient large-scale training on high-demensional images

- realistic sampling despite non-invertible operations (pooling, convolutions)
- better empirical performance than vanilla GMMs on images for sampling, clustering and outlier detection

In addition, we provide a publicly TensorFlow implementation which supports a Keras-like construction of DCGMMs.

B. Related Work

GANs and VAEs The currently most widely used models of image modeling and generation are Generative Adversarial Networks (GANs) [1], [12], [22] and Variational AutoEncoders (VAEs). GANs are capable of sampling photo-realistic images [28], but are unable to perform density estimation since there is no way to obtain $p(\mathbf{x})$ for a given sample \mathbf{x} . Furthermore, their probabilistic interpretation remains unclear since they do not possess a differentiable loss function that is minimized by training. They may suffer from what is termed *mode collapse*, which is hard to detect automatically due to the absence of a loss function [28]. VAEs show similar performance when it comes to sampling, in addition to minimizing a differentiable loss function. Moreover, density estimation with VAEs is problematic. Similar approaches, with similar strengths in sampling but a lack of density estimation, are realized by the PixelCNN architecture [23], GLOW [18] and their variants.

Hierarchical GMMs A hierarchical extension of GMMs is presented by [20] with the goal of unsupervised clustering: responsibilities of one GMM are treated as inputs to a subsequent GMM, together with an adaptive mechanism that determines the depth of the hierarchy. [6] present a comparable, more information-theoretic approach but not targeting sampling either. The closest related work to the model we present here is described in [30]–[32]. All of these models perceive hierarchical GMMs as modular decompositions of GMMs that are flat. The conceptual foundation is that sampling from a GMM implies the transformation of a normally distributed latent variable \mathbf{z} by a single GMM component k , with weight π_k , \mathbf{z} as $\mathbf{y} = \mathbf{A}_k \mathbf{z} + \boldsymbol{\beta}_k + \boldsymbol{\epsilon}_k$. This leads to a distribution $\mathbf{y} \sim \mathcal{N}(\boldsymbol{\beta}_k, \mathbf{A}_k \mathbf{A}_k^\top + \boldsymbol{\epsilon}_k)$. The choice which GMM component is allowed to transform the latent variable is based on component weights π_k . Hierarchical GMMs are now realized by *several* sampling steps (layers), and the sampling results of the previous layer representing the latent variable to be transformed by the next one. None of these models consider convolutional or max-pooling operations which have been proven to be important for modeling the statistical structure of images.

Mixture of Factor Analyzers (MFAs) MFAs models [8], [21] can be considered as hierarchical GMMs because they are formulated in terms of a lower-dimensional latent-variable representation, which is mapped to a higher-dimensional space. The use of MFAs for describing natural images is discussed in detail in [28], showing that the MFA model alone, without further hierarchical structure, compares quite favorably to GANs when considering image generation.

Hierarchical Mixture Models An interesting overview of the current research landscape in terms of hierarchical generative mixture models is given in [16]. All of these models are, in principle, capable of sampling and density estimation although the quality of sampling, and the data they can be trained on, vary considerably. Principal competitors in this domain are Sum-Product Networks (SPNs, see, e.g., [27]), which are tree structures of arbitrary depth, with leaves that represent tractable distribution families (typically multi-variate normal, binomial or student-t distributions). SPN nodes perform either weighted summation or multiplication, and with appropriate constraints on the tree structure it can be shown that sampling, inference and density estimation remain tractable. Problems include finding a suitable SPN structure, and dealing with complex and high-dimensional data. Convolutional extensions of the SPN model exist, although they have been applied to very small images only [2]. A similar approach is represented by probabilistic circuits (PCs, see, e.g., [24]) or Tensorial Mixture Models (TMMs, see, e.g., [29]).

Convolutional GMMs The only work we could identify proposing hierarchical convolutional GMMs is [10]. This work describes a hybrid model combining a CNN and a GMM.

SGD and End-To-End Training for GMMs Training GMMs by Stochastic Gradient Descent (SGD) is challenging due to local optima and the need to enforce model constraints, most notably the constraint of positive-definite covariance matrices. At the same time, SGD is attractive in deep architectures due to its simplicity, which is facilitated even further by modern machine learning packages that perform automatic differentiation. SGD for GMMs has recently been discussed in [15], although the proposed solution requires parameter initialization by k-means and introduces several new hyperparameters. Thus, it is unlikely to work as-is in a hierarchical structure. An SGD approach that achieves robust convergence even without k-means-based parameter initialization is presented by [7]. Undesirable local optima caused by random parameter initialization are circumvented by an adaptive annealing strategy. SPNs and PCs can be trained end-to-end by SGD as well, although no article describes this in detail. It is presumable that data-driven initialization is required, as well. Previous hierarchical GMM proposals [30]–[32] use (quite complex) extensions of the EM algorithm initialized by k-means for training. In [28], training is performed using SGD, although with a k-means initialization.

II. DCGMM: MODEL OVERVIEW

The Deep Convolutional Gaussian Mixture Model (DCGMM) is a hierarchical model consisting of *layers* in analogy to CNNs.¹ Each layer with index L expects an input tensor $\mathbf{A}^{(L-1)} \in \mathbb{R}^4$ of the dimensions $N, H^{(L-1)}, W^{(L-1)}, C^{(L-1)}$ and produces an output tensor $\mathbf{A}^{(L)} \in \mathbb{R}^4$ of dimensions the $N, H^{(L)}, W^{(L)}, C^{(L)}$. Layers can have internal variables $\theta^{(L)}$ that are adapted during SGD training.

¹Repository: <https://gitlab.cs.hs-fulda.de/ML-Projects/dcgmm>

A DCGMM layer L has two basic operating modes (see Fig. 1): for (density) *estimation*, an input tensor $\mathbf{A}^{(L-1)}$ from layer $L-1$ is transformed into an output tensor $\mathbf{A}^{(L)}$. For *sampling*, the direction is reversed: each layer receives a control signal $\mathbf{T}^{(L+1)}$ from layer $L+1$ (same dimensions as $\mathbf{A}^{(L)}$), which is transformed into a control signal $\mathbf{T}^{(L)}$ to layer $L-1$ (same dimensions as $\mathbf{A}^{(L-1)}$).

A. Layer Types

We define four layer types: Folding (F), Pooling (P), Linear Classifier (C) and GMM (G). Each implements distinct operations for both modes, i.e., estimation and sampling.

1) *Folding Layer*: For density estimation, this layer performs a part of the convolution operation well-known from CNNs. Based on the filter sizes $f_X^{(L)}$, $f_Y^{(L)}$ and the filter strides $\Delta_X^{(L)}$, $\Delta_Y^{(L)}$, all entries of the input tensor inside the range of the sliding filter window are dumped into the channel dimension of the output tensor. We thus obtain an output tensor of dimensions $N, H^{(L)} = 1 + \frac{H^{(L-1)} - f_Y^{(L)}}{\Delta_Y^{(L)}}, W^{(L)} = 1 + \frac{W^{(L-1)} - f_X^{(L)}}{\Delta_X^{(L)}}$ and $C^{(L)} = C^{(L)} f_X^{(L)} f_Y^{(L)}$, whose entries are computed as $\mathbf{A}_{nhwc}^{(L)} = \mathbf{A}_{nh'w'c'}^{(L-1)}$ with $h = h'/f_Y^{(L)}$, $w = w'/f_X^{(L)}$ and $c = c' + ((h' - h\Delta_Y^{(L)})f_X^{(L)} + w' - w\Delta_X^{(L)})C^{(L-1)} + c'$.

When sampling, the inverse mapping is performed which is not a one-to-one correspondence: input tensor elements which receive several contributions are averaged over all these.

2) *Pooling Layer*: For density estimation, pooling layers perform the same operations as standard (max-)pooling layers in CNNs based on the kernel sizes $k_Y^{(L)}$, $k_X^{(L)}$ and strides $\Delta_X^{(L)}$, $\Delta_Y^{(L)}$. When sampling, pooling layers perform a simple nearest-neighbor up-sampling by a factor indicated by the kernel sizes and strides.

3) *GMM Layer*: This layer type contains K GMM components, each of which is associated with trainable parameters π_k , μ_k and Σ_k , $k=1\dots K$, representing the GMM *weights*, *centroids* and *covariances*. What makes GMM layers convolutional is that they do not model single input vectors, but the channel content at *all* positions h, w of the input $\mathbf{A}_{n,w,h,:}^{(L-1)}$, using a shared set of parameters. This is analogue to the way a CNN layer models image content at all sliding window positions using the same filters. A GMM layer maps the input tensor $\mathbf{A}^{(L-1)} \in \mathbb{R}^{N,H^{(L-1)},W^{(L-1)},C^{(L-1)}}$ to $\mathbf{A}^{(L)} \in \mathbb{R}^{N,H^{(L-1)},W^{(L-1)},K}$, each GMM component $k \in \{1, \dots, K\}$ contributing the likelihood $\mathcal{N}_k(\mathbf{A}_{nhw,:}^{(L-1)}; \mu_k, \Sigma_k)$ of having generated the channel content at position h, w (for sample n in the mini-batch). This likelihood is often referred to as *responsibility* and is computed as

$$p_{nhw,:}(\mathbf{A}^{(L-1)}) = \mathcal{N}_k(\mathbf{A}_{nhw,:}^{(L-1)}; \mu_k, \Sigma_k) \quad (4)$$

$$\mathbf{A}_{nhw,:}^{(L)} \equiv \frac{p_{nhw,:}}{\sum_{c'} p_{nhw,c'}}.$$

For training the GMM layer, we optimize the GMM log-likelihood $\mathcal{L}^{(L)}$ for each layer L :

$$\begin{aligned} \mathcal{L}_{hw}^{(L)} &= \sum_n \log \sum_k \pi_k p_{nhw,:}(\mathbf{A}^{(L-1)}) \\ \mathcal{L}^{(L)} &= \frac{\sum_{hw} \mathcal{L}_{hw}^{(L)}}{H^{(L-1)} W^{(L-1)}} \end{aligned} \quad (5)$$

Training is performed by SGD according to the technique, and with the recommended parameters, presented by [7], which uses a max-component approximation to $\mathcal{L}^{(L)}$. In sampling mode, a control signal $\mathbf{T}^{(L)}$ is produced by standard GMM sampling, performed separately for all positions h, w . GMM sampling at position h, w first selects a component by drawing from a multinomial distribution. If the GMM layer is the last layer of a DCGMM instance, the multinomial's parameters are the mixing weights π_k for each position h, w . Otherwise, the control signal $\mathbf{T}_{nhw,:}^{(L+1)}$ received from layer $L+1$ is used. It is consistent to use the control signal for component selection in layer L , since it was sampled by layer $L+1$, which was in turn trained on the component responsibilities of layer L , see Sec. V. The selected component (still at position h, w) then samples $\mathbf{T}_{nhw,:}^{(L)}$. It is often beneficial for sampling to restrict the selected number to the S components with the highest control signal (top- S sampling). This reduces the diversity of sampling as fewer components can participate, but improves its quality since selection is restricted to the most likely components.

4) *Linear Classifier Layer*: This layer type implements a linear classifier, trained in a supervised manner by cross-entropy loss. Logits are obtained via an affine transformation $\mathbf{A}^{(L)} = \hat{\mathbf{A}}^{(L-1)} \mathbf{W}^{(L)} + \mathbf{b}^{(L)}$ from the flattened input activities $\hat{\mathbf{A}}^{(L-1)} \in \mathbb{R}^{N \times HWC}$. The logits have the dimension $N \times K$, with K representing the number of classes or categories. For sampling, a control signal is generated by approximately inverting this transformation: $\mathbf{T}^{(L-1)} = \mathbf{W}^{(L)} \hat{\mathbf{T}}^{(L)} - \mathbf{b}^{(L)}$, where $\hat{\mathbf{T}}^{(L)} \in \mathbb{R}^{N \times K}$ contains the one-hot coded classes for each sample to be generated.

B. Architecture-Level Functionalities

1) *End-to-End Training*: To train an DCGMM instance, we optimize $\mathcal{L}^{(L)}$ for each GMM layer L by vanilla SGD², using learning rates $\epsilon^{(L)}$. This is different from a standard CNN classifier, where only a single loss function is minimized. Usually a cross-entropy loss is computed from the last layer's outputs. Learning is *not* conducted layer-wise but end-to-end. Parameter initialization for GMM layers selects the initial values for the mixing weights as $\pi_k = K^{-1}$. Centroid elements sampled from $\mu_{kl} \sim \mathcal{U}_{[-0.01, 0.01]}$ and diagonal covariances are initialized to unit entries. Training is conducted in two steps to ensure convergence. First, only centroids are adapted, whereas both centroids and precisions are adapted in the second step.

²Advanced SGD strategies like RMSProp [13] or Adam [17] seem incompatible with GMM optimization.

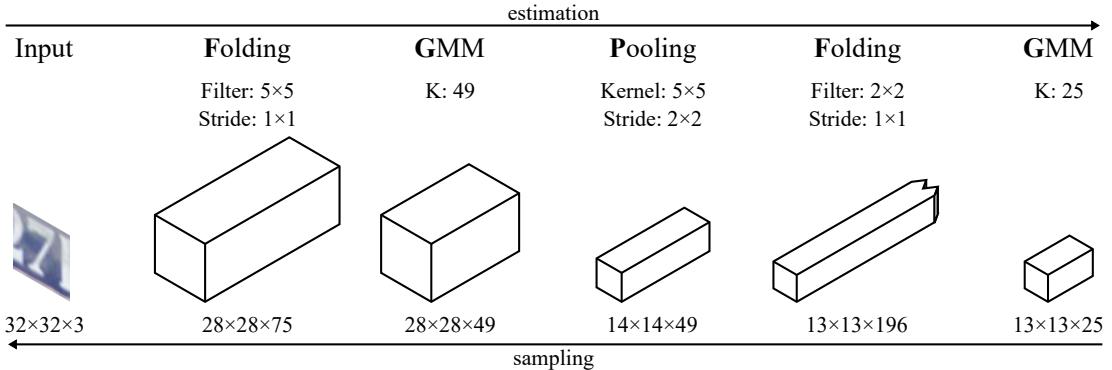


Fig. 1: Illustration of a DCGMM instance, with exemplary dimensionalities and parameters for each layer.

2) *Density Estimation and Outlier Detection*: Outlier detection requires the computation of long-term averages in all layers and positions, $\mathbb{E}_n \mathcal{L}_{nhw}^{(L)}$ and variances $\text{Var}_n(\mathcal{L}_{nhw}^{(L)})$ over the training set, preferably during a later, stable part of training. Thus, for every layer and position h, w , inliers are characterized by

$$\mathcal{L}_{hw}^{(L)} \geq \mathcal{B}_{hw}^{(L)} \equiv \mathbb{E}_n \mathcal{L}_{nhw}^{(L)} - c \sqrt{\text{Var}_n(\mathcal{L}_{nhw}^{(L)})}. \quad (6)$$

A larger c implies a less restrictive identification of inliers.

Assuming that the topmost GMM layer is global ($h = w = 1$), Eq. (6) reduces to a single condition that determines whether the sample as a whole is an inlier. However, we can also localize inlier/outlier image parts by evaluating Eq. (6) in lower GMM layers.

3) *Sampling and Sharpening*: Sampling starts in the highest layer L , assumed to be a GMM layer, and propagates control signals downwards (see Fig. 1 and Sec. II-A3), with control signal $\mathbf{T}^{(L)}$ constituting the sampling result. Sampling suffers from information loss due to the non-invertible mappings effected by Pooling and Folding layers. To counteract this, a Folding or Pooling layer at $L - 1$ performs *sharpening* on the control signal $\mathbf{T}^{(L-1)}$ it generates from $\mathbf{T}^{(L)}$. This involves computing $\mathcal{L}^{(L)}(\mathbf{T}^{(L-1)})$ for the GMM layer at level L and performing G gradient ascent steps $\mathbf{T}_{nhwc}^{(L-1)} \rightarrow \mathbf{T}_{nhwc}^{(L-1)} + \epsilon_s \partial \mathcal{L}^{(L)} / \partial \mathbf{T}_{nhwc}^{(L-1)}$. The reason for sharpening is that filters in Folding layers usually overlap, and neighboring filter results are correlated. This correlation is captured by all higher GMM layers, and most prominently by the next-highest one. Therefore, modifying $\mathbf{T}^{(L-1)}$ by gradient ascent will recover some of the information lost by pooling or folding. After sharpening, the tensor $\mathbf{T}^{(L-1)}$ is passed as control signal to $L - 2$.

4) *Conditional Sampling*: By conditional sampling we understand the ability to selectively produce samples from a certain class. Obviously, this is only possible when the DCGMM instance has a top-level linear classifier layer. We proceed as in Sec. II-B3, except for the component selection in the top-level GMM layer. For conditional sampling, we simply train a linear classifier in the last layer L on the outputs $\mathbf{A}^{(L-1)}$ of the previous layer, and then approximately invert

this mapping given a certain class label to obtain a control signal $\mathbf{T}^{(L)}$ for sampling in layer $L - 1$.

5) *In-Painting*: This is a functionality where a corrupted image, from which a part has been deleted, is supplied to a trained DCGMM instance, which then *completes* the missing parts. Here, we add a twist by not informing the model on which parts of the image have been deleted. Rather, a DCGMM should infer this on its own using its outlier detection capability, see Sec. II-B2.

Mathematically, in-painting requires that we perform *posterior inference* from a trained DCGMM. We shall consider this kind of inference for a flat GMM first, and subsequently generalize to DCGMMs.

Assuming that an image \mathbf{x} is composed of two parts \mathbf{x}_1 and \mathbf{x}_2 , where \mathbf{x}_2 is corrupted. To recover it, we wish to draw samples from the distribution $p(\mathbf{x}_2|\mathbf{x}_1)$. A simple computation yield an expression that can be evaluated by re-introducing the latent variable z of the GMM, see Eq. (2):

$$\begin{aligned} p(\mathbf{x}_2|\mathbf{x}_1) &= \frac{p(\mathbf{x}_1\mathbf{x}_2)}{p(\mathbf{x}_1)} = \sum_z \frac{p(\mathbf{x}_1, z)}{p(\mathbf{x}_1, z)} \frac{p(\mathbf{x}_2|\mathbf{x}_1, z)}{p(\mathbf{x}_1)} = \\ &= \sum_z p(\mathbf{x}_2|\mathbf{x}_1, z)p(z|\mathbf{x}_1) \equiv \sum_z \gamma_z p(\mathbf{x}_2|\mathbf{x}_1, z). \end{aligned} \quad (7)$$

This shows that the distribution we wish to sample from is again a Gaussian mixture. The mixture coefficients are given by the *responsibilities* $\gamma_z = p(z|\mathbf{x}_1)$, whereas the component densities can be simplified as $p(\mathbf{x}_2|\mathbf{x}_1, z) \sim p(\mathbf{x}_2|\mathbf{x}_1, z)$. We first draw a value z^* from a multi-nomial distribution defined by γ_i , and then generate a sample \mathbf{x} from component probability $p(\mathbf{x}_2|\mathbf{x}_1, z^*)$ of the Gaussian mixture. The part of \mathbf{x} that belongs to \mathbf{x}_1 is simply limited when sampling.

In a DCGMM, we implement this procedure for every position (h, w) in all GMM layers. We start at the top of the hierarchy (layer O), where responsibilities are simply the activities $\mathbf{A}^{(O)}$ computed by forward-propagating the corrupted input in estimation mode. The responsibilities are used to draw $z^*(h, w)$ for each position (h, w) as detailed above. Using z^* , we obtain a control signal for layer $O - 1$ as

$$\mathbf{T}_{hw:}^{(O)} \sim \mathcal{N}_{z^*(h, w)}(\cdot), \quad (8)$$

which propagated downwards through pooling and folding layers to the next-deeper GMM layer.

As for each GMM layer $L < O$, we want to in-paint only those parts which are not corrupted. We combine the raw control signal $\mathbf{T}^{(L)}$ and the activities $\mathbf{A}^{(L)}$ obtained in the forward pass into a fused control signal

$$\hat{\mathbf{T}}_{nhw:}^{(L)} = \begin{cases} \mathbf{A}_{nhw:}^{(L)} & \text{if inlier at } h, w \\ \mathbf{T}_{nhw:}^{(L)} & \text{if outlier at } h, w \end{cases} \quad (9)$$

where outliers are determined as described in Sec. II-B2. Thus, control signals fill in the activities that seem corrupted.

6) *Variant Generation*: Variant generation is a special case of sampling, where a template image is supplied and the DCGMM generates similar ones. This requires forward-propagating the template image in estimation mode through the DCGMM, and subsequently sampling a control signal from the top-level GMM layer O according to the obtained top-level activities $\mathbf{A}_{hw:}^{(O)}$. For all layers $L < O$ sampling is performed as detailed in Sec. II-B3. An interesting option is to control the similarity to the template image. This can be done either by selecting a suitable S for top- S -sampling, or by limiting top-down signals to activities in higher DCGMM layers:

$$\mathbf{T}^{(L)} \equiv \mathbf{A}^{(L-1)} \text{ for } L \geq \hat{L}, \quad (10)$$

where \hat{L} is a free parameter. The closest match between template image and generated image is to be expected for $\hat{L} = 0$, whereas $\hat{L} > O$ should result in very diverse results.

III. EXPERIMENTS

We define various DCGMM instances (with 2 or 3 GMM layers) for evaluation, see Tab. I, plus a single-layer DCGMM baseline which is nothing but a vanilla GMM. A DCGMM instance is defined by the parameters of its layers: **Folding**($f_Y, f_X, \Delta_Y, \Delta_X$), **(Max-)Pooling**($k_Y, k_X, \Delta_Y, \Delta_X$) and **GMM**(K). Unless stated otherwise, training is always conducted for 25 epochs, using the recommended parameters from [7]. Sharpening is always performed for $G = 1\,000$ iterations with a step size of 0.1.

A. Datasets

For the evaluation we use the following image datasets:

MNIST [19] is the common benchmark for computer vision

systems and classification problems. It consists of 60 000 28×28 gray scale images of handwritten digits (0-9).

FashionMNIST [33] consists of images of clothes in 10 categories and is structured like the MNIST dataset.

Although these datasets are not particularly challenging for classification, their dimensionality of 784 is at least one magnitude higher than datasets in the literature, which are used for validating other hierarchical GMM approaches in the literature.

B. Sampling, Sparsity and Interpretability

We show that trained DCGMM parameters are sparse and have an intuitive interpretation in terms of sampling. To this effect, we train DCGMM instance $2L-a$ (see Tab. I). After training (see Sec. II-B1), we plot and interpret the centroids of the GMM layers 2 (G2) and 4 (G4). The centroids of layer 2 (left of Fig. 2) are easily interpretable and reflect the patterns that can occur in any of the 2×2 input patches to layer G2 of size 20×20 . The $36 = 6 \times 6$ centroids of G4 (right of Fig. 2) express typical responsibility patterns computed from each of the 2×2 input patches to G2. They are, very sparsely populated. Another interpretation of G4 centroids can be found in terms of sampling (see Sec. II-B3), which would first select a random G4 component to generate a sample of dimensions $H, W, C = 1, 1, 2 \times 2 \times 5 \times 5$, and pass it on as a control signal to G2. Traversing Folding layer 3 only reshapes the control signal to dimension $H, W, C = 2, 2, 5 \times 5$, depicted in the middle of Fig. 2. This signal controls component selection in each of the 2×2 positions in G2. Due to their sparsity, we can directly read off the components likely to be selected for sampling at each position. Thus, G2 generates a control signal whose 2×2 positions of dimensions $H, W, C = 20, 20, 1$ overlap in the input plane (this is resolved by sharpening in Folding layer 1). In this case, it is easy to see that sampling produces a particular representation of the digit zero.

C. Outlier Detection

For outlier detection, we compare DCGMM architectures from Tab. I, using the log-likelihood of the highest layer as a criterion as detailed in Sec. II-B2. We first train a DCGMM instance on classes 0-4, and subsequently use the trained classes for inlier- and class 5-9 for outlier-detection. We vary c in the range $[-2, 2]$, resulting in different outlier and

TABLE I: Configurations of different DCGMM architectures.

layer \ ID	1L	2L-a	2L-b	2L-c	2L-d	2L-e	3L-a	3L-b
1	F(28,28,1,1)	F(20,20,8,8)	F(7,7,7,7)	F(8,8,2,2)	F(28,28,1,1)	F(4,4,2,2)	F(3,3,1,1)	F(28,28,1,1)
2	G(25)	G(25)	G(25)	G(25)	G(25)	G(25)	G(25)	G(25)
3		F(2,2,1,1)	F(4,4,1,1)	F(11,11,1,1)	F(1,1,1,1)	F(13,13,1,1)	P(2,2)	F(1,1,1,1)
4		G(36)	G(36)	G(36)	G(36)	G(36)	F(4,4,1,1)	G(25)
5							G(25)	F(1,1,1,1)
6							P(2,2)	G(25)
7							F(6,6,1,1)	
8							G(49)	
comment	vanilla GMM	1 conv. layer	1 conv. layer	1 conv. layer	no convolutions	1 conv. layer	2 conv. layers	no convolutions

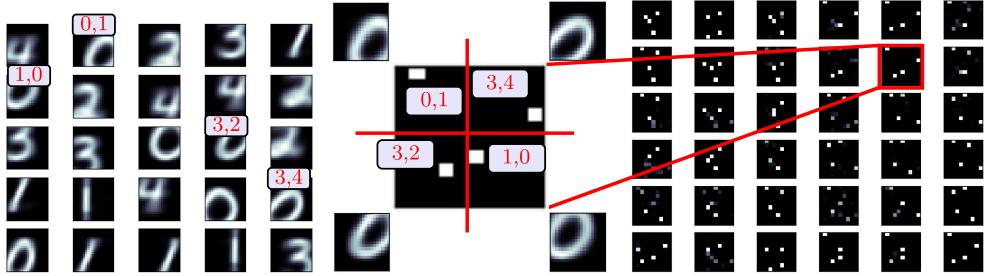


Fig. 2: Sampling from DCGMM instance 2L-a, see Tab. I. Learned GMM centroids (left: G2, right: G4) are presented along with an illustration of sampling, having initially selected the layer 4 component highlighted in red. In the middle, the selected G4 centroid is shown.

inlier percentages. Fig. 3 shows the ROC-like curves which clearly indicate that the deep convolutional DCGMM instances perform best. However, deep but non-convolutional instances like 2L-d and 3L-b consistently perform badly.

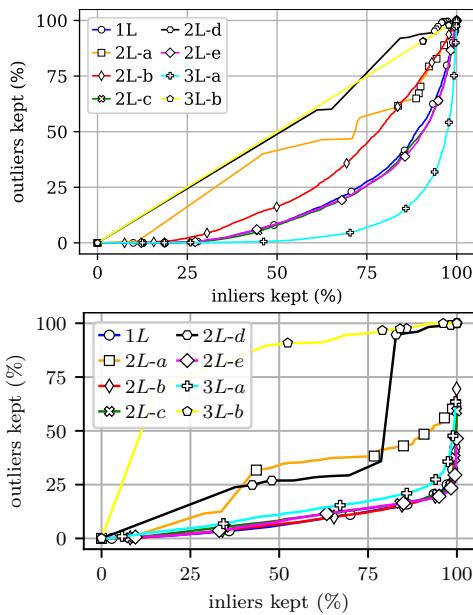


Fig. 3: Visualization of outlier detection capabilities (different DCGMMs) for MNIST (above) and FashionMNIST (below).

D. Clustering

We compare DCGMMs to vanilla GMMs using established clustering metrics, namely the Dunn index [5] and the Davies-Bouldin score [3]. The DCGMM instances from Tab. I are tested on both image datasets. We observe (see Tab. II and Fig. 3) that mainly the deep but non-convolutional DCGMM instances perform well in clustering, whereas convolutional instances, even if they are deep, are compromised. These metrics do not measure the classification accuracy obtained by clustering but intrinsic clustering-related properties.

E. Sampling and Sharpening

The results presented here were obtained by training on classes 0-4 of both datasets, and have to be confirmed by visual

TABLE II: Dunn index (higher is better) and Davies-Bouldin (DB) score (smaller is better), evaluated for all tested DCGMM architectures on MNIST and FashionMNIST. Best are marked bold for 10 repetitions (worst case).

Dataset	DCGMM Metric								
		1L	2L-a	2L-b	2L-c	2L-d	2L-e	3L-a	3L-b
MNIST	Dunn index	0.14	0.14	0.13	0.12	0.19	0.15	0.15	
	DB score	2.59	2.73	3.06	2.62	2.57	2.65	2.53	
Fashion-MNIST	Dunn index	0.14	0.15	0.16	0.15	0.11	0.11	0.096	0.13
	DB score	2.37	2.77	2.62	2.7	2.40	2.92	3.2	2.35

inspection of generated samples. The restriction to classes 0-4 is purely for visualization purposes.

a) *Effects of Convolutional Architectures:* An important property of DCGMM is the ability to analyze *local* input patches. In this experiment, we evaluate sampling for various two-layer architectures with different local patch sizes (i.e., convolution filter): global (2L-d), large (2L-a), semi-local (2L-c) and local (2L-e) and observe effects when performing top-1-sampling. The results of Fig. 4 indicate that as filter sizes decrease, the diversity but also the sharpness of generated samples increases at essentially no additional computational cost. Analogous FashionMNIST results are given in Fig. 5.

b) *Controlling Diversity by Top-S-Sampling:* Using instance 2L-c, Fig. 5 demonstrates how sample diversity is related to S . A higher value yields more diverse samples (see Fig. 6), but increases the risk of generating corrupted samples or outliers. As the FashionMNIST results show, a good value of S is clearly problem-dependent.

c) *Generating Sharp Images:* Fig. 7 shows the effect of sharpening for DCGMM instance 2L-c using top-1-sampling. We can observe that the overall shape of a sample is not changed but that the outlines are sharper, an effect visible especially for FashionMNIST. Thus, sharpening does no harm and rather improves the visual quality of generated samples.

IV. PROBABILISTIC INTERPRETATION OF DCGMMs

A probabilistic interpretation of the DCGMM model is possible despite its complex structure. The simple reason is that DCGMM instances produce outputs which are inherently normalizable, meaning that the integral over an infinite domain (e.g., data space) remains finite. Thus, DCGMM outputs can

2 4 4 3 0 3 2 0	3 0 0 0 3 0 3 1
0 3 4 0 2 4 3 1	2 4 1 3 3 4 3 0
0 3 4 0 0 2 0 3	1 3 1 1 3 3 0 2
4 0 0 3 3 1 3 2	0 3 3 2 3 0 1 3
3 0 2 3 3 2 2 3	3 1 0 2 3 2 3 0
3 2 4 1 c a / 0 3 4	4 1 1 0 3 0 3 3
2 3 1 0 4 0 4 0	1 1 1 0 0 0 1 3
3 4 0 0 3 0 3 3	0 3 0 1 1 3 4 2
3 3 3 0 0 2 2 3	2 0 0 0 0 1 4 0
0 0 0 2 1 3 0 0	0 0 2 4 4 2 2 3
3 / 1 1 4 4 4 1	4 4 3 2 3 3 3 1
1 1 2 4 4 4 3 2	1 3 3 3 1 1 4 2
2 4 0 2 3 3 3 0	0 2 1 1 2 0 0 0
0 2 2 3 0 0 0 2	0 1 4 0 0 0 2 4
1 3 0 0 3 1 1 1	4 2 2 3 4 1 3 2
4 4 4 1 1 1 2 4	3 3 8 1 1 3 3 3

Fig. 4: Convolutional architecture is helpful for sampling: top-1 sampling shown on MNIST for DCGMM architectures 1L (vanilla GMM, upper left), 2L-d (non-convolutional 2-layer, upper right), 2L-c (convolutional 2-layer, lower left) and 2L-e (convolutional 2-layer, lower right). Please observe duplicated samples in the non-convolutional architectures, marked by identical red letters. This figure is larger so duplicated samples can be better observed.

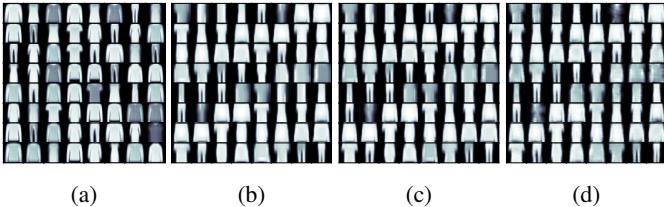


Fig. 5: Convolutional architecture is helpful for sampling: top-1 sampling shown on FashionMNIST, for DCGMM architectures 1L (vanilla GMM, a), 2L-d (non-convolutional 2-layer, b), 2L-c and 2L-e (both convolutional 2-layer, c and d).

be interpreted as a probability, which is not the case for DNN/CNNs due to the use of scalar products.

Here, we prove that GMMs are normalizable in the sense that the integral of the log-probability $\mathcal{L}(\mathbf{x}) = \log \sum_k \pi_k p_k(\mathbf{x})$ is finite. This holds for any GMM layer in a hierarchy regardless of its input, provided that the input is finite (which is assured as Pooling and Folding layers cannot introduce infinities). For simplicity, we integrate over the whole d -dimensional space \mathbb{R}^d . Since the component probabilities are Gaussian and strictly positive, and therefore the mixing weights are normalized and ≥ 0 , the sum is strictly positive. Thus, it is sufficient to show that the integral over the inner sum

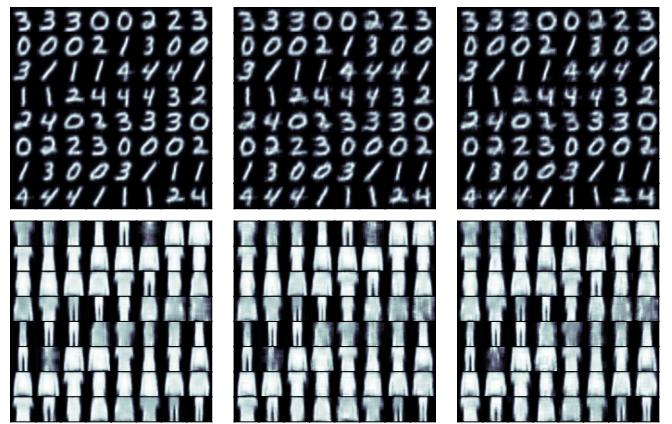


Fig. 6: Impact of higher values of S in top-S sampling, shown for DCGMM instance 2L-c for MNIST and FashionMNIST. From left to right: $S=2,5,10$.

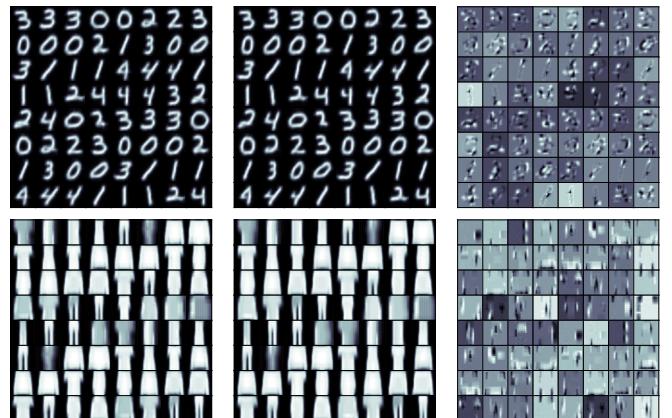


Fig. 7: Impact of sharpening on top-S-sampling with $S=1$, see Sec. II-B3, shown for DCGMM instance 2L-c. Shown are unsharpened samples (left), sharpened samples (middle) and differences (right). Samples at the same position were generated by the same top-level prototype.

(argument of the logarithm) is finite. We thus have

$$\begin{aligned} \int_{\mathbb{R}^d} \sum_k \pi_k p_k(\mathbf{x}) d\mathbf{x} &= \sum_k \pi_k \int_{\mathbb{R}^d} p_k(\mathbf{x}) \\ &= \sum_k \pi_k \sqrt{\det(2\pi\Sigma)} \end{aligned} \quad (11)$$

which is trivially finite because Gaussians are normalized.

V. CONCEPTUAL AND PRACTICAL DIFFERENCES TO OTHER HIERARCHICAL GMM MODELS

In this work, we outline the main conceptual differences to what we consider the closest related work, namely the hierarchical GMM models presented in [30]–[32]. Besides some differences, they share the notion that a GMM performs sampling by transforming what is termed a random *latent variable*. This process usually follows a simple distribution like $\mathcal{N}(0, \mathbf{I})$.

To clarify a purely semantic point: In this work, and close to the original derivation of the EM algorithm for GMMs [4], we consider the latent variable z of a GMM to be the one that enters into the complete-data log-likelihood of the corresponding latent-variable model. Another point where we differ in terminology is our perception of lower layers being closer to the input in density estimation mode. The lowest layer has index 1, counting upwards.

On the conceptual side, the cited models all share the notion that the proposed deep GMMs have a one-to-one correspondence to a flat model, which is actually the one whose log-likelihood is optimized. Consequently, layers are not optimized independently of each other, but are intrinsically linked. This is most easily visible from the fact that the component weights in each layer are not normalized. Only the aggregated weights of all sampling paths through the deep model have this property.

In contrast, our model does not assume (or require) a one-to-one correspondence to a flat GMM. The layers in our model are GMMs in their own right, having, e.g., their own, normalized weights and losses, and compute the posterior probabilities $\gamma_{nj} = p(z_j = 1 | \mathbf{x}_n)$ of their *own* latent variables. The dependency between layers is realized simply by the fact that posterior probabilities of one GMM layer are inputs to the subsequent GMM layer (potentially after being transformed by convolution and pooling layers).

The first practical consequence of this independent layers type of formulation is that layers can be optimized independently of each other. In particular, it is not necessary to enumerate all possible paths through the deep GMM as in [31] for training, which can only be approximated. Normal GMM optimization is rather performed for each layer, given the outputs of previous layers. This leads to a huge gain in scalability and allows deep GMMs with many layers to be trained on high-dimensional data, such as images, in a matter of minutes.

Another consequence concerns the introduction of pooling and convolution operations: since the layers of our model are not constrained by a joint flat GMM assumption, we are free to apply arbitrary transformations to their outputs before passing these on to subsequent GMM layers. The probabilistic interpretation of our model comes from the fact that each GMM in the model is independent and has the probabilistic interpretation that all GMMs share.

A last consequence concerns sampling. In our formulation of deep GMMs, a single GMM layer is trained on (estimated) latent variables from a preceding layer. When sampling, it can generate a valid instance z of these latent variables. Therefore, it is reasonable to use the generated z for *selecting* the GMM component to sample from in layer X , instead of the $\pi^{(X)}$. Of course, a suitable merging of both quantities is possible. Sampling, as described here, is a non-linear instead of an affine transformation, which is similar to the modeling related works. Nevertheless, we retain the notion of paths through the DCGMM instance, given by the components selected for sampling in each layer. Due to the fact that the number

of paths grows exponentially with the number of layers, deeper DCGMM instances can describe much richer sample distributions.

VI. SUMMARY, DISCUSSION AND CONCLUSION

The **Objective of the article** was to establish the conceptual foundations of deep GMM hierarchies (see also Sec. IV) that leverage important mechanisms from the CNN domain. Conceptual differences and shared properties w.r.t. principal related works are discussed in V. Convolution and pooling layers make it possible to apply the model to high-dimensional image data with off-the-shelf hardware (typical training runs take approximately 2 minutes on a GeForce GTX 1080).

Results show the illustration of important functionalities such as outlier detection, clustering and sampling, which no other work on hierarchical GMMs can present for such high-dimensional image datasets. We also propose a method to generate sharp images with GMMs, which has been a problem in the past [28]. An interesting facet of our experimental results is that non-convolutional DCGMMs seem to perform better at clustering, whereas convolutional ones are better at outlier detection and sampling.

A **Key point** is the compositionality in natural images. This property is at the root of DCGMM's ability to produce realistic samples with relatively few parameters. When considering top-S-sampling in a layer L with $H^{(L)}W^{(L)} = P^{(L)}$ positions, the number of distinct control signals generated layer L is $S^{P^{(L)}}$. A DCGMM instance with multiple GMM layers $\{L_i\}$ can thus sample $\prod_L S^{P^{(L)}}$ different patterns, which grows with the depth of the hierarchy *and* the number of distinct positions in a layer, making a strong argument in favor of deep convolutional hierarchies such as DCGMM. This is an argument similar to the one about different paths through a hierarchical MFA model in [31], [32]. However, the number of paths grow more strongly for DCGMMs because sampling is performed independently for each GMM position.

Practical advantages over other hierarchical models such as [30]–[32] are most notably the introduction of convolution and pooling layers. Our experimental validation can be performed on high-dimensional data, such as images, with moderate computational cost. This contradicts low-dimensional problems such as the artificial Smiley task or the *Ecoli* and related problems. Our experimental validation does not exclusively focus on clustering performance (problematic with images), but on demonstrating the capacity for realistic sampling and outlier detection. Lastly, training DCGMMs by SGD facilitates efficient parallelizable implementations, as demonstrated by the TF2 implementation provided.

Next steps consist of exploring more DCGMM architectures, mainly sampling, for generating natural images.

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