A DISCRIMINATIVE GAUSSIAN MIXTURE MODEL WITH SPARSITY

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ABSTRACT

In probabilistic classification, a discriminative model based on the softmax function has a potential limitation in that it assumes unimodality for each class in the feature space. The mixture model can address this issue, although it leads to an increase in the number of parameters. We propose a sparse classifier based on a discriminative GMM, referred to as a sparse discriminative Gaussian mixture (SDGM). In the SDGM, a GMM-based discriminative model is trained via sparse Bayesian learning. Using this sparse learning framework, we can simultaneously remove redundant Gaussian components and reduce the number of parameters used in the remaining components during learning; this learning method reduces the model complexity, thereby improving the generalization capability. Furthermore, the SDGM can be embedded into neural networks (NNs), such as convolutional NNs, and can be trained in an end-to-end manner. Experimental results demonstrated that the proposed method outperformed the existing softmax-based discriminative models.

1 INTRODUCTION

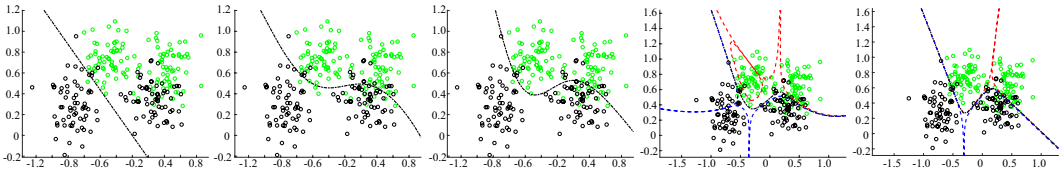
In probabilistic classification, a discriminative model is an approach that assigns a class label c to an input sample $\boldsymbol{x}$ by estimating the posterior probability $P(c \mid \boldsymbol{x})$. The posterior probability $P(c \mid \boldsymbol{x})$ should correctly be modeled because it is not only related to classification accuracy, but also to the confidence of decision making in real-world applications such as medical diagnosis support. In general, the model calculates the class posterior probability after nonlinear feature extraction using the softmax function. Classically, a combination of the kernel method and the softmax function has been used. The recent mainstream method is to use a deep neural network for representation learning and softmax for the calculation of the posterior probability.

Such a general procedure for developing a discriminative model potentially contains a limitation due to unimodality. The softmax-based model, such as a fully connected layer with a softmax function that is often used in deep neural networks, assumes a unimodal Gaussian distribution for each class (details are shown in Appendix A). Therefore, even if the feature space is transformed into discriminative space via the feature extraction part, $P(c \mid \boldsymbol{x})$ cannot correctly be modeled if the multimodality remains, which leads to a decrease in accuracy.

Mixture models can address this issue. Mixture models are widely used for generative models, with a Gaussian mixture model (GMM) as a typical example. Mixture models are also effective in discriminative models; for example, discriminative GMMs have been applied successfully in various fields, e.g., speech recognition (Tüske et al. 2015; Wang 2007). However, the number of parameters increases if the number of mixture components increases, which may lead to over-fitting; this is useful if we can reduce the number of redundant parameters while maintaining multimodality.

In this paper, we propose a discriminative model with two important properties; multimodality and sparsity. The proposed model is referred to as the sparse discriminative Gaussian mixture (SDGM). In the SDGM, a GMM-based discriminative model is formulated and trained via sparse Bayesian learning. This learning algorithm improves the generalization capability by obtaining sparse weights while maintaining multimodality of the mixture model.

The technical highlight of this study is twofold: One is that the SDGM finds the multimodal structure in the feature space and the other is that redundant Gaussian components are removed owing to sparse learning. Figure 1 shows a comparison of the decision boundaries with other discrimina-



(a) FC + softmax (b) Gaussian process (c) RVM (d) Discriminative GMM (e) SDGM (ours)

Figure 1: Comparison of decision boundaries. The black and green circles represent training samples from classes 1 and 2, respectively. The dashed black line indicates the decision boundary between classes 1 and 2 and thus satisfies $P(c = 1 \mid \boldsymbol{x}) = (c = 2 \mid \boldsymbol{x}) = 0.5$. The dashed blue and red lines represent the boundaries between the posterior probabilities of the mixture components.

tive models. The two-class data are from Ripley's synthetic data (Ripley 2006), where two Gaussian components are used to generate data for each class. The fully connected (FC) layer with the softmax function, which is often used in the last layer of deep neural networks (NNs), assumes a unimodal Gaussian for each class, resulting in an inappropriate decision boundary. Kernel Bayesian methods, such as the Gaussian process (GP) classifier (Wenzel et al. 2019) and relevance vector machine (RVM) (Tipping 2001), estimate nonlinear decision boundaries using nonlinear kernels, whereas these methods cannot find multimodal structures. Although the discriminative GMM finds multimodal structure, this model retains redundant Gaussian components. However, the proposed SDGM finds a multimodal structure of data while removing redundant components, which leads to an accurate decision boundary.

Furthermore, the SDGM can be embedded into NNs, such as convolutional NNs (CNNs), and trained in an end-to-end manner with an NN. The proposed SDGM is also considered as a mixture, nonlinear, and sparse expansion of the logistic regression and thus the SDGM can be used as the last layer of an NN for classification by replacing it with the fully connected (FC) layer with a softmax activation function.

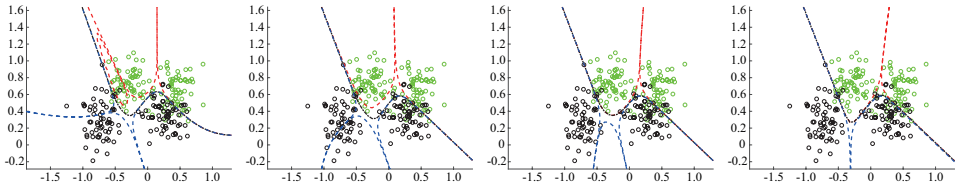
The contributions of this study are as follows:

- We propose a novel sparse classifier based on a discriminative GMM. The proposed SDGM has both multimodality and sparsity, thereby flexibly estimating the posterior distribution of classes while removing redundant parameters. Moreover, the SDGM automatically determines the number of components by simultaneously removing the redundant components during learning.
- From the perspective of the Bayesian kernel methods, the SDGM is considered as the expansion of the GP and RVM. The SDGM can estimate the posterior probabilities more flexibly than the GP and RVM owing to multimodality. The experimental comparison using benchmark data demonstrated superior performance to the existing Bayesian kernel methods.
- This study connects both fields of probabilistic models and NNs. From the equivalence of a discriminative model based on a Gaussian distribution to an FC layer, we demonstrate that the SDGM can be used as a module of a deep NN. We also demonstrate that the SDGM exhibits superior performance to the FC layer with a softmax function via end-to-end learning with an NN on the image recognition task.

2 Related Work and Position of This Study

The position of the proposed SDGM among the related methods are summarized in Figure 2. Interestingly, by summarizing the relationships, we can confirm that the three separately developed fields, generative models, discriminative models, and kernel Bayesian methods, are related to each other. Starting from the Gaussian distribution, all the models shown in Figure 2 are connected via four kinds of arrows. There is an undeveloped area in the upper right part, and the development of the area is the contribution of this study.

A (unimodal) Gaussian distribution is used as the most naive generative model in machine learning and is the foundation of this relationship diagram. A GMM is the mixture expansion of the Gaussian distributions. Since the GMM can express an (almost) arbitrary continuous distributions using



(a) 1 epoch (b) 100 epochs (c) 200 epochs (d) 250 epochs

Figure 3: Snapshots of the training process of SDGM. The meanings of lines and circles are same as Figure 1. There are three components for each class in the initial stage of learning. As the training progresses, one of the components for each class becomes small gradually and is finally removed.

multiple Gaussian components, it has been utilized for a long time. Since Gaussian fitting requires numerous parameters, the sparsified versions of Gaussian (Hsieh et al. 2011) and GMM (Gaiffas & Michel 2014) have been proposed.

The discriminative models and the generative models are mutually related (Lasserre et al. 2006; Minka 2005). According to Lasserre et al. (2006), the only difference between these models is their statistical parameter constraints. Therefore, given a generative model, we can derive a corresponding discriminative model. For example, discriminative models corresponding to the Gaussian mixture model have been proposed (Axelrod et al. 2006; Bahl et al. 1996; Klautau et al. 2003; Tsai & Chang 2002; Tsuji et al. 1999; Tüske et al. 2015; Wang 2007). They indicate more flexible fitting capability for classification problems than the generative GMM because the discriminative models have a lower statistical bias than the generative models. Furthermore, as shown by Tüske et al. (2015); Variani et al. (2015), these models can be used as the last layer of the NN because these models output the class posterior probability.

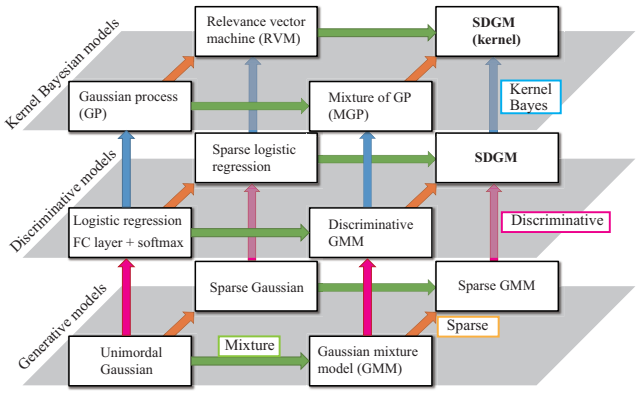


Figure 2: Position of the SDGM among the related methods.

From the perspective of the kernel Bayesian methods, the GP classifier (Wenzel et al. 2019) is the Bayesian kernelized version of the logistic regression. The RVM (Tipping 2001) is the sparse version of the GP classifier and is the most important related study. The learning algorithm of the SDGM is based on that of the RVM; however, it is extended for the mixture model.

If we use kernelization, the SDGM becomes one of the kernel Bayesian methods, and is considered as the mixture expansion of the RVM or sparse expansion of the mixture of GP (MGP). Therefore, the classification capability and sparsity are compared with kernel Bayesian methods in Section 4.1. Otherwise, the SDGM is considered as one of the discriminative models, and can be embedded in an NN. The comparison with other discriminative models is conducted in Section 4.2 via image classification by combining a CNN.

3 Sparse Discriminative Gaussian Mixture (SDGM)

The SDGM takes a continuous variable as its input and outputs the posterior probability of each class, acquiring a sparse structure by removing redundant components via sparse Bayesian learning. Figure 3 shows how the SDGM is trained by removing unnecessary components while maintaining discriminability. In this training, we set the initial number of components to three for each class. As the training progresses, one of the components for each class gradually becomes small and is removed.

3.1 NOTATION

Let $\boldsymbol{x} \in \mathbb{R}^D$ be a continuous input variable and t_c ($c \in \{1, \dots, C\}$, C is the number of classes) be a discrete target variable that is coded in a one-of-C form, where $t_c = 1$ if $\boldsymbol{x}$ belongs to class c, $t_c = 0$ otherwise. Also, let z_{cm} be a discrete latent variable, and $z_{cm} = 1$ when $\boldsymbol{x}$ from class c belongs to the m-th component ($m \in \{1, \dots, M_c\}$, M_c is the number of components for class c), $z_{cm} = 0$ otherwise. For simplicity, in this paper, the probabilities for classes and components are described using only c and m; e.g., we use $P(c, m \mid \boldsymbol{x})$ instead of $P(t_c = 1, z_{cm} = 1 \mid \boldsymbol{x})$.

3.2 MODEL FORMULATION

The posterior probabilities of each class c given $\boldsymbol{x}$ are calculated as follows:

$$P(c \mid \boldsymbol{x}) = \sum_{m=1}^{M_c} P(c, m \mid \boldsymbol{x}), \quad P(c, m \mid \boldsymbol{x}) = \frac{\pi_{cm} \exp[\boldsymbol{w}_{cm}^{\mathrm{T}} \boldsymbol{\phi}]}{\sum_{c'=1}^{C} \sum_{m'=1}^{M_{c'}} \pi_{c'm'} \exp[\boldsymbol{w}_{c'm'}^{\mathrm{T}} \boldsymbol{\phi}]}, \tag{1}$$

$$\boldsymbol{\phi} = \Big[1, \boldsymbol{x}^{\mathrm{T}}, x_1^2, x_1 x_2, \dots, x_1 x_D, x_2^2, x_2 x_3, \dots, x_D^2\Big]^{\mathrm{T}}, \tag{2}$$

where π_{cm} is the mixture weight that is equivalent to the prior of each component $P(c, m)$. It should be noted that we use $\boldsymbol{w}_{cm} \in \mathbb{R}^H$, which is the weight vector representing the m-th Gaussian component of class c. The dimension of $\boldsymbol{w}_{cm}$, i.e., H, is the same as that of $\boldsymbol{\phi}$; namely, $H = 1 + D(D+3)/2$.

Derivation. Utilizing Gaussian distribution as a conditional distribution of $\boldsymbol{x}$ given c and m, $P(\boldsymbol{x} \mid c, m)$, the posterior probability of c given $\boldsymbol{x}$, $P(c \mid \boldsymbol{x})$, is calculated as follows:

$$P(c \mid \boldsymbol{x}) = \sum_{m=1}^{M_c} \frac{P(c, m) P(\boldsymbol{x} \mid c, m)}{\sum_{c=1}^{C} \sum_{m=1}^{M_c} P(c, m) P(\boldsymbol{x} \mid c, m)}, \tag{3}$$

$$P(\boldsymbol{x} \mid c, m) = \frac{1}{(2\pi)^{\frac{D}{2}} |\boldsymbol{\Sigma}_{cm}|^{\frac{1}{2}}} \exp\left[-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_{cm})^{\mathrm{T}} \boldsymbol{\Sigma}_{cm}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_{cm})\right], \tag{4}$$

where $\boldsymbol{\mu}_{cm} \in \mathbb{R}^D$ and $\boldsymbol{\Sigma}_{cm} \in \mathbb{R}^{D \times D}$ are the mean vector and the covariance matrix for component m in class c. Since the calculation inside an exponential function in (4) is quadratic form, the conditional distributions can be transformed as follows:

$$P(\boldsymbol{x} \mid c, m) = \exp[\boldsymbol{w}_{cm}^{\mathrm{T}} \boldsymbol{\phi}], \tag{5}$$

where

$$\boldsymbol{w}_{cm} = \Big[-\frac{D}{2} \ln 2\pi - \frac{1}{2} \ln |\boldsymbol{\Sigma}_{cm}| - \frac{1}{2} \sum_{i=1}^{D} \sum_{j=1}^{D} s_{cmij} \mu_{cmi} \mu_{cmj}, \sum_{i=1}^{D} s_{cmi1} \mu_{cmi}, \dots, \sum_{i=1}^{D} s_{cmiD} \mu_{cmi}, -\frac{1}{2} s_{cm11}, -s_{cm12}, \dots, -s_{cm1D}, -\frac{1}{2} s_{cm22}, \dots, -\frac{1}{2} s_{cmDD} \Big]^{\mathrm{T}}. \tag{6}$$

Here, s_{cmij} is the (i, j)-th element of $\boldsymbol{\Sigma}_{cm}^{-1}$.

3.3 DUAL FORM VIA KERNELIZATION

Since $\boldsymbol{\phi}$ is a second-order polynomial form, we can derive the dual form of the SDGM using polynomial kernels. By kernelization, we can treat the SDGM as the kernel Bayesian method as described in Section 2.

Let $\boldsymbol{\psi}_{cm} \in \mathbb{R}^N$ be a novel weight vector for the c, m-th component. Using $\boldsymbol{\psi}_{cm}$ and the training dataset $\{\boldsymbol{x}_n\}_{n=1}^N$, the weight of the original form $\boldsymbol{w}_{cm}$ is represented as

$$\boldsymbol{w}_{cm} = [\boldsymbol{\phi}(\boldsymbol{x}_1), \cdots, \boldsymbol{\phi}(\boldsymbol{x}_N)] \boldsymbol{\psi}_{cm}, \tag{7}$$

where $\boldsymbol{\phi}(\boldsymbol{x}_n)$ is the transformation $\boldsymbol{x}_n$ of using (2). Then, (5) is reformulated as follows:

$$\begin{aligned} P(\boldsymbol{x} \mid c, m) &= \exp[\boldsymbol{w}_{cm}^{\mathrm{T}} \boldsymbol{\phi}] \\ &= \exp[\boldsymbol{\psi}_{cm}^{\mathrm{T}} [\boldsymbol{\phi}(\boldsymbol{x}_1)^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}), \cdots, \boldsymbol{\phi}(\boldsymbol{x}_N)^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x})]^{\mathrm{T}}] \\ &= \exp[\boldsymbol{\psi}_{cm}^{\mathrm{T}} K(\mathbf{X}, \boldsymbol{x})], \end{aligned} \tag{8}$$

where $K(\mathbf{X}, \boldsymbol{x})$ is a N-dimensional vector that contains kernel functions defined as $k(\boldsymbol{x}_n, \boldsymbol{x}) = \boldsymbol{\phi}(\boldsymbol{x}_n)^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}) = (\boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{x} + 1)^2$ for its elements and $\mathbf{X}$ is a data matrix that has $\boldsymbol{x}_n^{\mathrm{T}}$ in the n-th row. Whereas the computational complexity of the original form in Section 3.2 increases in the order of the square of the input dimension D, the dimensionality of this dual form is proportional to N. When we use this dual form, we use N and $k(\boldsymbol{x}_n, \cdot)$ instead of H and $\boldsymbol{\phi}(\cdot)$, respectively.

3.4 LEARNING ALGORITHM

Algorithm 1: Learning algorithm of the SDGM

Input: Training data set $\mathbf{X}$ and teacher vector $\mathbf{T}$.
Output: Trained weight $\boldsymbol{w}$ obtained by maximizing (11).
Initialize the weights $\boldsymbol{w}$, hyperparameters $\boldsymbol{\alpha}$, mixture coefficients $\boldsymbol{\pi}$, and posterior probabilities $\boldsymbol{r}$;
while $\boldsymbol{\alpha}$ *have not converged* **do**
  Calculate J using (10);
  while $\boldsymbol{r}$ *have not converged* **do**
    while $\boldsymbol{w}$ *have not converged* **do**
      Calculate gradients using (12);
      Calculate Hessian (13);
      Maximize (11) w.r.t. $\boldsymbol{w}$;
      Calculate $P(c, m \mid \boldsymbol{x}_n)$ and $P(c \mid \boldsymbol{x}_n)$;
    end
    $r_{ncm} = P(c, m \mid \boldsymbol{x}_n)/P(c \mid \boldsymbol{x}_n)$;
  end
  Calculate Λ using (16);
  Update $\boldsymbol{\alpha}$ using (17);
  Update $\boldsymbol{\pi}$ using (18);
end

Algorithm 1 shows the training of the SDGM. In this algorithm, the optimal weight is obtained as maximum a posterior solution. We can obtain a sparse solution by optimizing the prior distribution set to each weight simultaneously with weight optimization.

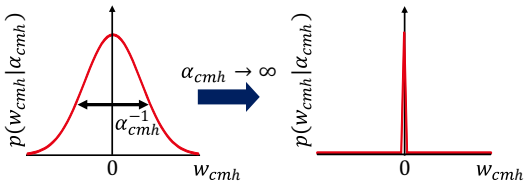


Figure 4: Prior for each weight w_{cmh}. By maximizing the evidence term of the posterior of $\boldsymbol{w}$, the precision of the prior α_{cmh} achieves infinity if the corresponding weight w_{cmh} is redundant.

A set of training data and target value $\{\boldsymbol{x}_n, t_{nc}\}$ $(n = 1, \cdots, N)$ is given. We also define $\boldsymbol{\pi}$ and $\boldsymbol{z}$ as vectors that comprise π_{cm} and z_{ncm} as their elements, respectively. As the prior distribution of the weight w_{cmh}, we employ a Gaussian distribution with a mean of zero. Using a different precision parameter (inverse of the variance) α_{cmh} for each weight w_{cmh}, the joint probability of all the weights is represented as follows:

$$P(\boldsymbol{w} \mid \boldsymbol{\alpha}) = \prod_{c=1}^{C} \prod_{m=1}^{M_c} \prod_{h=1}^{H} \sqrt{\frac{\alpha_{cmh}}{2\pi}} \exp\left[-\frac{1}{2} {w_{cmh}}^2 \alpha_{cmh}\right], \tag{9}$$

where $\boldsymbol{w}$ and $\boldsymbol{\alpha}$ are vectors with w_{cmh} and α_{cmh} as their elements, respectively. During learning, we update not only $\boldsymbol{w}$ but also $\boldsymbol{\alpha}$. If $\alpha_{cmh} \to \infty$, the prior (9) is 0; hence a sparse solution is obtained by optimizing $\boldsymbol{\alpha}$ as shown in Figure 4.

Using these variables, the expectation of the log-likelihood function over $\boldsymbol{z}$, J, is defined as follows:

$$J = \mathbb{E}_{\boldsymbol{z}} \left[\ln P(\mathbf{T}, \boldsymbol{z} \mid \mathbf{X}, \boldsymbol{w}, \boldsymbol{\pi}, \boldsymbol{\alpha})\right] = \sum_{n=1}^{N} \sum_{c=1}^{C} r_{ncm} t_{nc} \ln P(c, m \mid \boldsymbol{x}_n),$$

where $\mathbf{T}$ is a matrix with t_{nc} as its element. The variable r_{ncm} in the right-hand side corresponds to $P(m \mid c, \boldsymbol{x}_n)$ and can be calculated as $r_{ncm} = P(c, m \mid \boldsymbol{x}_n)/P(c \mid \boldsymbol{x}_n)$.

The posterior probability of the weight vector $\boldsymbol{w}$ is described as follows:

$$P(\boldsymbol{w} \mid \mathbf{T}, \boldsymbol{z}, \mathbf{X}, \boldsymbol{\pi}, \boldsymbol{\alpha}) = \frac{P(\mathbf{T}, \boldsymbol{z} \mid \mathbf{X}, \boldsymbol{w}, \boldsymbol{\pi}, \boldsymbol{\alpha}) P(\boldsymbol{w} \mid \boldsymbol{\alpha})}{P(\mathbf{T}, \boldsymbol{z} \mid \mathbf{X}, \boldsymbol{\alpha})} \tag{10}$$

An optimal $\boldsymbol{w}$ is obtained as the point where (10) is maximized. The denominator of the right-hand side in (10) is called the evidence term, and we maximize it with respect to $\boldsymbol{\alpha}$. However, this maximization problem cannot be solved analytically; therefore we introduce the Laplace approximation described as the following procedure.

With $\boldsymbol{\alpha}$ fixed, we obtain the mode of the posterior distribution of $\boldsymbol{w}$. The solution is given by the point where the following equation is maximized:

$$\mathbb{E}_{\boldsymbol{z}} \left[\ln P(\boldsymbol{w} \mid \mathbf{T}, \boldsymbol{z}, \mathbf{X}, \boldsymbol{\pi}, \boldsymbol{\alpha})\right] = \mathbb{E}_{\boldsymbol{z}} \left[\ln P(\mathbf{T}, \boldsymbol{z} \mid \mathbf{X}, \boldsymbol{w}, \boldsymbol{\pi}, \boldsymbol{\alpha})\right] + \ln P(\boldsymbol{w} \mid \boldsymbol{\alpha}) + \text{const.}$$

$$= J - \boldsymbol{w}^{\mathrm{T}}\mathbf{A}\boldsymbol{w} + \text{const.}, \tag{11}$$

where $\mathbf{A} = \operatorname{diag} \alpha_{cmh}$. We obtain the mode of (11) via Newton's method. The gradient and Hessian required for this estimation can be calculated as follows:

$$\nabla \mathbb{E}_{\boldsymbol{z}} \left[\ln P(\boldsymbol{w} \mid \mathbf{T}, \boldsymbol{z}, \mathbf{X}, \boldsymbol{\pi}, \boldsymbol{\alpha})\right] = \nabla J - \mathbf{A}\boldsymbol{w}, \tag{12}$$

$$\nabla\nabla \mathbb{E}_{\boldsymbol{z}} \left[\ln P(\boldsymbol{w} \mid \mathbf{T}, \boldsymbol{z}, \mathbf{X}, \boldsymbol{\pi}, \boldsymbol{\alpha})\right] = \nabla\nabla J - \mathbf{A}. \tag{13}$$

Each element of ∇J and $\nabla\nabla J$ is calculated as follows:

$$\frac{\partial J}{\partial w_{cmh}} = (r_{ncm} t_{nc} - P(c, m \mid \boldsymbol{x}_n))\phi_h, \tag{14}$$

$$\frac{\partial^2 J}{\partial w_{cmh} \partial w_{c'm'h'}} = P(c', m' \mid \boldsymbol{x}_n)(P(c, m \mid \boldsymbol{x}_n) - \delta_{cc'mm'})\phi_h \phi_{h'}, \tag{15}$$

where $\delta_{cc'mm'}$ is a variable that takes 1 if both $c = c'$ and $m = m'$, 0 otherwise. Hence, the posterior distribution of $\boldsymbol{w}$ can be approximated by a Gaussian distribution with a mean of $\hat{\boldsymbol{w}}$ and a covariance matrix of Λ, where

$$\Lambda = -(\nabla\nabla \mathbb{E}_{\boldsymbol{z}} \left[\ln P(\hat{\boldsymbol{w}} \mid \mathbf{T}, \boldsymbol{z}, \mathbf{X}, \boldsymbol{\pi}, \boldsymbol{\alpha})\right])^{-1}. \tag{16}$$

Since the evidence term can be represented using the normalization term of this Gaussian distribution, we obtain the following updating rule by calculating its derivative with respect to α_{cmh}.

$$\alpha_{cmh} \leftarrow \frac{1 - \alpha_{cmh}\lambda_{cmh}}{\hat{w}_{cmh}^2}, \tag{17}$$

where λ_{cmh} is the diagonal component of Λ. The mixture weight π_{cm} can be estimated using r_{ncm} as follows:

$$\pi_{cm} = \frac{1}{N_c} \sum_{n=1}^{N_c} r_{ncm}, \tag{18}$$

where N_c is the number of training samples belonging to class c. As described above, we obtain a sparse solution by alternately repeating the update of hyper-parameters, as described in (17) and (18) and the posterior distribution estimation of $\boldsymbol{w}$ using the Laplace approximation. As a result of the optimization, some of α_{cmh} approach to infinite values, and w_{cmh} corresponding to α_{cmh} have prior distributions with mean and variance both zero as shown in (4); hence such w_{cmh} are removed because their posterior distributions are also with mean and variance both zero. During the procedure, the $\{c, m\}$-th component is eliminated if π_{cm} becomes 0 or all the weights w_{cmh} corresponding to the component become 0.

4 EXPERIMENTS

4.1 COMPARATIVE STUDY USING BENCHMARK DATA

To evaluate the capability of the SDGM quantitatively, we conducted a classification experiment using benchmark datasets. The datasets used in this experiment were Ripley's synthetic data (Ripley 2006) (Ripley hereinafter) and four datasets cited from (Rätsch et al. 2001); Banana, Waveform, Titanic, and Breast Cancer. Ripley is a synthetic dataset that is generated from a two-dimensional ($D = 2$) Gaussian mixture model, and 250 and 1,000 samples are provided for training and test, respectively. The number of classes is two ($C = 2$), and each class comprises two components. The remaining four datasets are all two-class ($C = 2$) datasets, which comprise different data size and dimensionality. Since they contain 100 training/test splits, we repeated experiments for 100 times and then calculated average statistics.

For comparison, we used three kernel Bayesian methods: a Gaussian process classifier, a mixture of Gaussian process classifier (Tresp 2001; Luo & Sun 2017), and a relevance vector machine (RVM) (Tipping 2001). In the evaluation, we compared the recognition error rates for discriminability and the number of nonzero weights for sparsity on the test data. The results of RVM were cited from (Tipping 2001). By way of summary, the statistics were normalized by those of the SDGM and the overall mean was shown.

Table 1 shows the recognition error rates and the number of nonzero weights for each method. The results in Table 1 demonstrated that the SDGM achieved abetter accuracy on average compared to the other kernel Bayesian methods. The SDGM is developed based on a Gaussian mixture model and

Table 1: Recognition error rate (%) and number of nonzero weights

	Accuracy (error rate (%))				Sparsity (number of nonzero weights)			
		Baselines				Baselines		
Dataset	SDGM	GP	MGP	RVM	SDGM	GP	MGP	RVM
Ripley	**9.1**	**9.1**	9.3	9.3	6	250	1250	**4**
Waveform	10.1	10.4	**9.6**	10.9	**11.0**	400	2000	14.6
Banana	10.6	**10.5**	10.7	10.8	**11.1**	400	2000	11.4
Titanic	**22.6**	**22.6**	22.8	23.0	74.5	150	750	**65.3**
Breast Cancer	**29.4**	30.4	30.7	29.9	15.73	200	1000	**6.3**
Normalized mean	**1.00**	1.01	1.01	1.03	1.00	25.76	128.79	**0.86**

is particularly effective for data where a Gaussian distribution can be assumed, such as the Ripley dataset. In terms of sparsity, the SDGM achieved a relatively small number of nonzero weights thanks to its sparse Bayesian learning. The results above indicated that the SDGM demonstrated generalization capability and a sparsity simultaneously.

4.2 Image classification

In this experiment, the SDGM is embedded into a deep neural network. Since the SDGM is differentiable with respect to the weights, SDGM can be embedded into a deep NN as a module and is trained in an end-to-end manner. In particular, the SDGM plays the same role as the softmax function since the SDGM calculates the posterior probability of each class given an input vector. We can show that a fully connected layer with the softmax is equivalent to the discriminative model based on a single Gaussian distribution for each class by applying a simple transformation (see Appendix A), whereas the SDGM is based on the Gaussian mixture model.

To verify the difference between them, we conducted image classification experiments. Using a CNN with a softmax function as a baseline, we evaluated the capability of SDGM by replacing softmax with the SDGM. We also used a CNN with a softmax function trained with L_1 regularization and a CNN with the discriminative GMM as other baselines.

In this experiment, we used the original form of the SDGM. To achieve sparse optimization during end-to-end training, we employed an approximated sparse Bayesian learning based on Gaussian dropout proposed by Molchanov et al. (2017). This is because it is difficult to execute the learning algorithm in Section 3.4 with backpropagation due to computational costs.

4.2.1 Datasets and experimental setups

We used the following datasets and experimental settings in this experiment.

MNIST: This dataset includes 10 classes of handwritten binary digit images of size 28×28 (LeCun et al. 1998). We used 60,000 images as training data and 10,000 images as testing data. As a feature extractor, we used a simple CNN that consists of five convolutional layers with four max pooling layers between them and a fully connected layer. To visualize the learned CNN features, we first set the output dimension of the fully connected layer of the baseline CNN as two ($D = 2$). Furthermore, we tested by increasing the output dimension of the fully connected layer from two to ten ($D = 10$).

Fashion-MNIST: Fashion-MNIST (Xiao et al. 2017) includes 10 classes of binary fashion images with a size of 28×28. It includes 60,000 images for training data and 10,000 images for testing data. We used the same CNN as in MNIST with 10 as the output dimension.

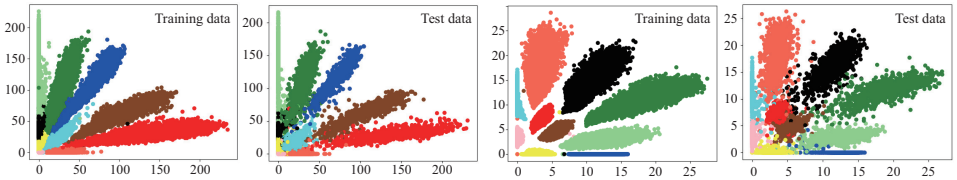
CIFAR-10: This dataset consists of 60,000 32×32 color images in 10 classes, with 6,000 images per class (Krizhevsky & Hinton 2009). There are 50,000 training images and 10,000 test images. For CIFAR-10, we trained DenseNet (Huang et al. 2017) with a depth of 40 and a growth rate of 12.

For each dataset, the network was trained with a batch size of 64 for 100 epochs with a learning rate of 0.01 We used a weight decay of 1.0×10^{-5} and the Nesterov optimization algorithm (Sutskever et al. 2013) with a momentum of 0.9. The network weights were initialized using the Glorot uniform (Glorot & Bengio 2010).

It should be noted that we did not employ additional techniques to increase classification accuracy such as data augmentation, hyperparameter tuning, and pre-trained models; therefore, the accuracy of the baseline model did not reach the state-of-the-art. This is because we considered that it is not essential to confirm the effectiveness of the proposed method.

Table 2: Recognition error rates (%) on image classification

	MNIST ($D = 2$)	MNIST ($D = 10$)	Fashion-MNIST	CIFAR-10
CNN + Softmax	3.19	1.01	8.78	11.07
CNN + Softmax + L_1 regularization	3.70	1.58	9.20	10.30
CNN + Discriminative GMM	2.43	**0.72**	8.30	**10.05**
CNN + SDGM	**1.81**	0.86	**8.05**	10.46



(a) Softmax (b) Ours

Figure 5: Visualization of CNN features on MNIST ($D = 2$) after end-to-end learning. In this visualization, five convolutional layers with four max pooling layers between them and a fully connected layer with a two-dimensional output are used. (a) results when a fully connected layer with the softmax function is used as the last layer. (b) when SDGM is used as the last layer instead. The colors red, blue, yellow, pink, green, tomato, saddlebrown, lightgreen, cyan, and black represent classes from 0 to 9, respectively. Note that the ranges of the axis are different between (a) and (b).

4.2.2 Results

Figure 5 shows the two-dimensional feature embeddings on the MNIST dataset. Different feature embeddings were acquired for each method. When softmax was used, the features spread in a fan shape and some parts of the distribution overlapped around the origin. However, when the SDGM was used, the distribution for each class exhibited an ellipse shape and margins appeared between the class distributions. This is because the SDGM is based on a Gaussian mixture model and functions to push the samples into a Gaussian shape.

Table 2 shows the recognition error rates on each dataset. SDGM achieved better performance than softmax. Although sparse learning was ineffective in two out of four comparisons, replacing softmax with SDGM was effective in all the comparisons. As shown in Figure 5, SDGM can create margins between classes by pushing the features into a Gaussian shape. This phenomenon positively affected classification capability.

5 Conclusion

In this paper, we proposed a sparse classifier based on a Gaussian mixture model (GMM), which is named sparse discriminative Gaussian mixture (SDGM). In the SDGM, a GMM-based discriminative model was trained by sparse Bayesian learning. This learning algorithm improved the generalization capability by obtaining a sparse solution and automatically determined the number of components by removing redundant components. The SDGM can be embedded into neural networks (NNs) such as convolutional NNs and could be trained in an end-to-end manner.

In the experiments, we demonstrated that the SDGM could reduce the number of weights via sparse Bayesian learning, thereby improving its generalization capability. The comparison using benchmark datasets suggested that SDGM outperforms the conventional kernel Bayesian classifiers. We also demonstrated that SDGM outperformed the fully connected layer with the softmax function when it was used as the last layer of a deep NN.

One of the limitations of this study is that the proposed sparse learning reduces redundant Gaussian components but cannot obtain the optimal number of components, which should be improved in future work. We will also develop a sparse learning algorithm for a whole deep NN structure including the feature extraction part. This will improve the ability of the CNN for larger data classification. Further applications using probabilistic property of the proposed model such as semi-supervised learning, uncertainty estimation, and confidence calibration will be considered.

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