Simultaneous Feature and Expert Selection within Mixture of Experts

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Abstract

A useful strategy to deal with complex classification scenarios is the “divide and conquer” approach. The mixture of experts (MOE) technique makes use of this strategy by jointly training a set of classifiers, or experts, that are specialized in different regions of the input space. A global model, or gate function, complements the experts by learning a function that weights their relevance in different parts of the input space. Local feature selection appears as an attractive alternative to improve the specialization of experts and gate function, particularly, for the case of high dimensional data. Our main intuition is that particular subsets of dimensions, or subspaces, are usually more appropriate to classify instances located in different regions of the input space. Accordingly, this work contributes with a regularized variant of MoE that incorporates an embedded process for local feature selection using $L_1$ regularization, with a simultaneous expert selection. The experiments are still pending.

Keywords: Mixture of experts, local feature selection, embedded feature selection, regularization.

1. Mixture of Experts with embedded variable selection

Our main idea is to incorporate a local feature selection scheme inside each expert and gate function of a MoE formulation. Our main intuition is that, in the context of classification, different partitions of the input data can be best represented by specific
subsets of features. This is particularly relevant in the case of high dimensional spaces, where the common presence of noisy or irrelevant features might obscure the detection of particular class patterns. Specifically, our approach takes advantage of the linear nature of each local expert and gate function in the classical MoE formulation [17], meaning that $L_1$ regularization can be directly applied. Below, we first briefly describe the classical MoE formulation for classification. Afterwards, we discuss the proposed modification to the MoE model that provides embedded feature selection.

1.1. Mixture of Experts

In the context of supervised classification, there is available a set of $N$ training examples, or instance-label pairs $(x_n,y_n)$, representative of the domain data $(x,y)$, where $x_n \in \mathbb{R}^D$ and $y_n \in C$. Here $C$ is a discrete set of $Q$ class labels $\{c_1,\ldots,c_Q\}$. The goal is to use training data to find a function $f$ that minimizes a loss function which scores the quality of $f$ to predict the true underlying relation between $x$ and $y$. From a probabilistic point of view [4], a useful approach to find $f$ is using a conditional formulation:

$$ f(x) = \arg \max_{c_i \in C} p(y = c_i | x). $$

In the general case of complex relations between $x$ and $y$, a useful strategy consists of approximating $f$ through a mixture of local functions. This is similar to the case of modeling a mixture distribution [34] and it leads to the MoE model.

We decompose the conditional likelihood $p(y|x)$ as:

$$ p(y|x) = \sum_{i=1}^{K} p(y, m_i | x) = \sum_{i=1}^{K} p(y|m_i, x) p(m_i | x), \quad (1) $$

where Equation (1) represents a MoE model with $K$ experts $m_i$. Figure [I] shows a schematic diagram of the MoE approach. The main idea is to obtain local models in such a way that they are specialized in a particular region of the data. In Figure [I], $x$ corresponds to the input instance, $p(y|m_i, x)$ is the expert function, $p(m_i | x)$ is the
gating function, and \( p(y|x) \) is the weighted sum of the experts. Note that the output of each expert model is weighted by the gating function. This weight can be interpreted as the relevance of expert \( m_i \) for the classification of input instance \( x \). Also note that the gate function has \( K \) outputs, one for each expert. There are \( K \) expert functions that have \( Q \) components, one for each class.

![Diagram of Mixture of Experts](image)

**Figure 1: Mixture of experts scheme.**

The traditional MoE technique uses multinomial logit models, also known as softmax functions [4], to represent the gate and expert functions. An important characteristic of this model is that it forces competition among its components. In MoE, such components are expert functions for the gates and class-conditional functions for the experts. The competition in softmax functions enforces the specialization of experts in different areas of the input space [41].

Using multinomial logit models, a gate function is defined as:

\[
p(m_i|x) = \frac{\exp(\nu_i^T x)}{\sum_{j=1}^{K} \exp(\nu_j^T x)}
\]

where \( i \in \{1, \ldots, K\} \) refers to the set of experts and \( \nu_i \in \mathbb{R}^D \) is a vector of model parameters. Component \( \nu_{ij} \) of vector \( \nu_i \) models the relation between the gate and dimension \( j \) of input instance \( x \).

Similarly, an expert function is defined as:
\[ p(y = c_i | x, m_i) = \frac{\exp(\omega_{li}^T x)}{\sum_{j=1}^{M} \exp(\omega_{ji}^T x)} \]  

(3)

where \( \omega_{li} \) depends on class label \( c_i \) and expert \( i \). In this way, there are a total of \( Q \times K \) vectors \( \omega_{li} \). Component \( \omega_{ij} \) of vector \( \omega_{li} \) models the relation between expert function \( i \) and dimension \( j \) of input instance \( x \).

There are several methods to find the value of the hidden parameters \( \nu_{ij} \) and \( \omega_{lij} \) \cite{26}. An attractive alternative is to use the EM algorithm. In the case of MoE, the EM formulation augments the model by introducing a set of latent variables, or \textit{responsibilities}, indicating the expert that generates each instance. Accordingly, the EM iterations consider an expectation step that estimates expected values for \textit{responsibilities}, and a maximization step that updates the values of parameters \( \nu_{ij} \) and \( \omega_{lij} \). Specifically, the posterior probability of the \textit{responsibility} \( R_{in} \) assigned by the gate function to expert \( m_i \) for an instance \( x_n \) is given by \cite{26}:

\[ R_{in} = p(m_i | x_n, y_n) = \frac{p(y_n | x_n, m_i) \ p(m_i | x_n)}{\sum_{j=1}^{K} p(y_n | x_n, m_j) \ p(m_j | x_n)} \]  

(4)

Considering these responsibilities and Equation (1), the expected complete log-likelihood \( \langle L_c \rangle \) used in the EM iterations is \cite{26}:

\[ \langle L_c \rangle = \sum_{n=1}^{N} \sum_{i=1}^{K} R_{in} \ [\log p(y_n | x_n, m_i) + \log p(m_i | x_n)] \]  

(5)

1.2. Regularized Mixture of Experts (RMoE)

To embed a feature selection process in the MoE approach, we use the fact that in Equations (2) and (3) the multinomial logit models for gate and experts functions contain linear relations for the relevant parameters. This linearity can be straightforwardly used in feature selection by considering that a parameter component \( \nu_{ij} \) or \( \omega_{lij} \)
with zero value implies that dimension \( j \) is irrelevant for gate function \( p(m_i|x) \) or expert model \( p(y|m_i,x) \), respectively. Consequently, we propose to penalize complex models using \( L_1 \) regularization. Similar consideration is used in the work of [29] but in the context of unsupervised learning. The idea is to maximize the likelihood of data while simultaneously minimizing the number of parameter components \( \nu_{ij} \) and \( \omega_{lij} \) different from zero. Considering that there are \( Q \) classes, \( K \) experts, and \( D \) dimensions, the expected \( L_1 \) regularized log-likelihood \( \langle L_c^R \rangle \) is given by:

\[
\langle L_c^R \rangle = \langle L_c \rangle - \lambda \nu \sum_{i=1}^{K} \sum_{j=1}^{D} |\nu_{ij}| - \lambda \omega \sum_{l=1}^{Q} \sum_{i=1}^{K} \sum_{j=1}^{D} |\omega_{lij}|.
\] (6)

To maximize Equation (6) with respect to model parameters, we use first the standard fact that the likelihood function in Equation (5) can be decomposed in terms of independent expressions for gate and expert models [26]. In this way, the maximization step of the EM based solution can be performed independently with respect to gate and expert parameters [26]. In our problem, each of these optimizations has an extra term given by the respective regularization term in Equation (6). To handle this case, we observe that each of these optimizations is equivalent to the expression to solve a regularized logistic regression [20]. As shown in [20], this problem can be solved by using a coordinate ascent optimization strategy [37] given by a sequential two-step approach that first models the problem as an unregularized logistic regression and afterwards incorporates the regularization constraints.

In summary, we handle Equation (6) by using a EM based strategy that at each step solves the maximization with respect to model parameters by decomposing this problem in terms of gate and expert parameters. Each of these problems is in turn solved using the strategy proposed in [20]. Next, we provide details of this procedure.

**Optimization of the unregularized log-likelihood**

In this case, we solve the unconstrained log-likelihood given by Equation (5). First, we optimize the log-likelihood with respect to vector \( \omega_{li} \). The maximization of the expected log-likelihood \( \langle L_c \rangle \) implies deriving Equation (5) with respect to \( \omega_{li} \):
\[
\frac{\partial}{\partial \omega_{li}} \sum_{n=1}^{N} \sum_{i=1}^{K} R_{in} \left[ \log p(y_n | x_n, m_i) \right] = 0, \quad (7)
\]

and applying the derivative, we have:

\[
- \sum_{n=1}^{N} R_{in} (p(y_n | x_n, m_i) - y_n) x_n = 0. \quad (8)
\]

In this case, the classical technique of least-squares cannot be directly applied because of the soft-max function in \( p(y_n | x_n, m_i) \). Fortunately, as described in [18] and later in [26], Equation (8) can be approximated by using a transformation that implies inverting the soft-max function. Using this transformation, Equation (8) is equivalent to an optimization problem that can be solved using a weighted least squares technique [4]:

\[
\min_{\omega_{li}} \sum_{n=1}^{N} R_{in} \left( \omega_{li}^T x_n - \log y_n \right)^2 \quad (9)
\]

A similar derivation can be performed with respect to vectors \( \nu_i \). Again deriving Equation (5), in this case with respect to parameters \( \nu_{ij} \) and applying the transformation suggested in [18], we obtain:

\[
\min_{\nu_{ij}} \sum_{n=1}^{N} \left( \nu_{ij}^T x_n - \log R_{in} \right)^2 \quad (10)
\]

Optimization of the regularized likelihood

Following the procedure of [20], we add the regularization term to the optimization problem given by Equation (9), obtaining an expression that can be solved using quadratic programming [35]:

\[
\min_{\omega_{li}} \sum_{n=1}^{N} R_{in} \left( \log y_n - \omega_{li}^T x_n \right)^2 \\
\text{subject to:} \quad ||\omega_{li}||_1 \leq \lambda \omega \quad (12)
\]
Similarly, we can also obtain a standard quadratic optimization problem to find parameters $\nu_{ij}$:

$$\min_{\nu_i} \sum_{n=1}^{N} (\log R_{in} - \nu_i^T x_n)^2$$

subject: to $||\nu_i||_1 \leq \lambda$  \hspace{1cm} (13)

A practical advantage of using quadratic programming is that most available optimization packages can be utilized to solve it [6]. Specifically, in the case of $T$ iterations, there are a total of $T \times K \times (Q + 1)$ convex quadratic problems related to the maximization step of the EM algorithm. To further reduce this computational load, we slightly modify this maximization by applying the following two-steps scheme:

- Step-1: Solve $K$ quadratic problems to find gate parameters $\nu_{ij}$ assuming that each expert uses all the available dimensions. In this case, there are $T - 1$ iterations.

- Step-2: Solve $K \times (Q + 1)$ quadratic problems to find expert parameters $\omega_{lij}$ applying the feature selection process. In this case, there is a single iteration.

Using the previous scheme we reduce from $T \times K \times (Q + 1)$ to $K \times (T + 1) + K \times (Q + 1)$ the number of quadratic problems that we need to solve in the maximization step of the EM algorithm. In our experiments, we do not notice a drop in performance by using this simplification, but we are able to increase processing speed in one order of magnitude.

In summary, starting by assigning random values to the relevant parameters $\nu_{ij}$ and $\omega_{lij}$, our EM implementation consists of iterating the following two steps:

- Expectation: estimating responsibilities for each expert using Equation (4), and then estimating the outputs of gate and experts using Equations (2) and (3).

- Maximization: updating the values of parameters $\nu_{ij}$ and $\omega_{lij}$ in Equations (12) and (13) by solving $K \times (T + 1) + K \times (Q + 1)$ quadratic problems according to the approximation described above in Step-1 and Step-2.
2. Expert Selection

The MoE or RMoE assumes that all the gate functions affects to every data. But for example in object detection, we can assume that there are some group of objects i.e. group of vehicles, animals, kitchen stuff, where each group is assigned to a gate function. We think that considering all groups of objects can confuse the classifiers. Therefore we propose to select a subset of gates function according to each data. We denominate this idea as a “expert selection”.

Recalling that the likelihood in regular mixture of experts is:

\[
L = \prod_{n=1}^{N} \prod_{i=1}^{K} p(y_n|x_n, m_i) p(m_i|x_n) 
\] (14)

Now, in order to select a gate, we change the multinomial logit representation of the gate function (Equation 2) in this way:

\[
p(m_i|x_n) = \frac{\exp \mu_{in} (\nu_i^T x)}{\sum_{j=1}^{K} \exp \mu_{jn} (\nu_j^T x)}
\] (15)

where all the components of Equation 2 remain the same, except \( \mu \). The variable \( \mu_{in} \in \{0,1\}^K \) is the vector of model parameters of the expert selector. It depends on data \( x_n \) and expert \( i \), where \( i \in \{1,\ldots,K\} \) for the set of expert gates. When \( \mu_{in} = 1/0 \), it indicates that the gate \( i \) is relevant/irrelevant for data \( n \). In the case of \( \mu_{in} = 0 \), the value is constant and we can say that the data \( n \) is ignorant about expert \( i \) and assign a constant value. In this way, it is done the expert selection.

In order to use EM algorithm, we show the expected log-likelihood by considering the responsabilities, i.e. the posteriori probability of experts and the respective regularization terms with the addition of the term corresponding to the expert selector:

\[
\langle L_c \rangle = \sum_{n=1}^{N} \sum_{i=1}^{K} R_{in} \left[ \log p(y_n|x_n, m_i) + \log p(m_i|x_n) \right]
\]

\[-\lambda_{\mu} \sum_{i=1}^{K} \sum_{j=1}^{D} |\nu_{ij}| - \lambda_{\omega} \sum_{l=1}^{Q} \sum_{i=1}^{K} \sum_{j=1}^{D} |\omega_{lij}| - P(\mu) \] (16)

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The penalization $P$ depends on the regularization norm, mainly 0-norm or 1-norm. Now, we define the posteriori probability of the gates $m_i$ as:

$$ R_{in} = \frac{p(y_n|x_n, m_i)p(m_i|x_n)}{\sum_{j=1}^{K} p(y_n|x_n, m_j) p(m_j|x_n)} \quad (17) $$

Next, we repeat the strategy of Lee et al. by first optimizing the unregularized expected log-likelihood and then, adding the restriction. In order to facilitate the calculations, we define some auxiliary variables. As the derivative is linear in the sum, we calculate the contribution of a single data and call it as $E'$:

$$ E' = -\log \sum_{k=1}^{K} p(y_n|x_n, m_k) p(m_k|x_n) \quad (18) $$

We solve this process using an EM algorithm, where in the E-step, we calculate the responsabilities in this case by using the equation $17$. In the M-step, we assume the responsabilities as known and we find the optimal parameters $\nu$, $\omega$ and $\mu$.

Since the use of the responsability values, the term $p(y_n|x_n, m_k)$ can be evaluated separately and then the parameter $\omega$ can be optimized using the equation used in RMoE. In the case of $p(m_k|x_n)$, by fixing the parameter $\mu$, we can optimize the parameter $\nu$.

We use some notations in order to facilitate the calculus: the term $p(y_n|x_n, m_k)$ as $g_k^n$, $p(m_k|x_n)$ as $h_{kn}$ and $\exp(\mu_i \nu_i x_n)$ as $z_i$, we derive the equation respect to $\nu_{in}$ for having:

$$ \frac{\partial E'}{\partial \nu_i} = \frac{\partial E'}{\partial z_i} \frac{\partial z_i}{\partial \nu_i} \quad (19) $$

Now we have three terms and we evaluate the derivative over each one:
\[ \frac{\partial E'}{\partial h_k} = \partial - \log \sum_{j=1}^{K} g_j h_j \]
\[ \frac{\partial E'}{\partial h_k} = -\frac{g_k}{\sum_{j=1}^{K} g_j h_j} \]
\[ \frac{\partial E'}{\partial h_k} = -\frac{R_{kn}}{h_k} \]  
\[ (20) \]

\[ \frac{\partial h_k}{\partial z_i} = \frac{\partial \frac{\exp(h_k)}{\sum_{j=1}^{K} \exp(h_j)}}{\partial z_i} \]
\[ \frac{\partial h_k}{\partial z_i} = \delta_{ki} h_i - h_i h_k \]  
\[ (21) \]

We integrate these elements for obtain:

\[ \frac{\partial E'}{\partial v_i} = \left( \sum_{k=1}^{K} \frac{R_{kn}}{h_k} (\delta_{ki} h_i - h_i h_k) \right) \mu_i x \]
\[ \frac{\partial E'}{\partial v_i} = (R_{in} - h_i) \mu_i x \]  
\[ (22) \]

By considering all the data, the regularization term and applying the trick of Bishop by taking the logarithms of the outputs and equaling to zero, we have:

\[ \min_{\nu_i} \sum_{n=1}^{N} \left( \log(R_{in}) - \nu_i^T \mu_{in} x_n \right)^2 \]
subject: to \[ ||\nu_i||_1 \leq \lambda \nu \]  
\[ (23) \]

In this case it is a modified version of equation [13] and we can apply a QP package to solve it. Finally, we fix the parameters \( \nu \) and \( \omega \) for optimizing the parameter \( \mu \). The
regularization over the parameter of expert selector has originally norm 0; on the other hand, it can be relaxed by considering norm 1. We state both approaches:

A. Optimization of $\mu$ considering norm 0

As the parameter $\mu$ depends on data $x_n$, we need to solve the optimization problem:

$$
\min_{\mu_{in}} \ -\log \sum_{k=1}^{K} p(y_n|x_n, m_k) p(m_k|x_n) \\
\text{subject: to} \quad ||\mu_{in}||_0 \leq \lambda_{\mu}
$$

The minimization of equation 24 requires an exploration of $C^K_{\lambda_{\mu}}$ combinations, however, by assuming a low number of gates $K < 50$ and a lower number of active experts $\lambda_{\mu} < 10$, this numerical optimization is feasible in practice.

B. Optimization of $\mu$ considering norm 1

A more applicable approach is relaxing the constraint of 0-norm by replacing by the use of a 1-norm, also known as LASSO regularization. Given that $\mu$ is in the same component of $\nu$, its solution has many equal steps. In particular, we find almost the same equations. Using the same notations of Equation 19, we have for the individual log-likelihood:

$$
\frac{\partial E'}{\partial \mu_{in}} = \frac{\partial E'}{\partial z_i} \frac{\partial z_i}{\partial \mu_{in}} \\
\frac{\partial E'}{\partial \mu_{in}} = \left[ \sum_{k=1}^{K} \frac{\partial E'}{\partial h_k} \frac{\partial h_k}{\partial z_i} \right] \frac{\partial z_i}{\partial \mu_{in}}
$$

We get the same Equations 20 and 21. In the case of the last component we have:

$$
\frac{\partial z_{li}}{\partial \mu_{in}} = \frac{\partial \mu_{in} \nu_i x}{\partial \mu_{in}} \\
\frac{\partial z_{li}}{\partial \mu_{in}} = \nu_i x
$$
We ensemble all components equations to have:

$$\frac{\partial E'}{\partial \mu_{in}} = \left( \sum_{k=1}^{K} \frac{R_{kn}}{h_k} (\delta_{ki} h_i - h_i h_k) \right) \nu_i x$$

$$\frac{\partial E'}{\partial \mu_{in}} = (R_{in} - h_i) \nu_i x$$

In order to find the optimum parameter $\mu_{in}$, we fix $n$ and consider from $i = 1$ to $K$. By equaling each equation to zero, we have:

$$(R_{in} - h_i) \nu_i x = 0 \quad (27)$$

Next, we approximate the previous equation using the logarithms over the outputs (Bishop):

$$(\log(R_{in}) - \mu_{in} \nu_i x_n) \nu_i x = 0 \quad (28)$$

Now, we fix $n$ in order to find jointly the parameters of $\mu$ for a fixed data $n$. Therefore when we add the $K$ equations, we have an equation system:

$$\left( \sum_{i=1}^{K} (\log(R_{in}) - \mu_{in} \nu_i x_n) \nu_i x_n \right) = 0 \quad (29)$$

This equation can be represented as a minimization problem considering the sum of squares residuals between $\log(R_{in})$ and $\mu_{in} \nu_i x_n$; where we add restriction of norm 1 over $\mu_{sn}$ that represents all selected experts for data $n$. In this case, we have:

$$\min_{\mu} \frac{||\log(R_{n}) - \mu_{sn} \nu x_n||_2^2}{2}$$

subject: to $||\mu_{sn}||_1 \leq \lambda_{\mu} \quad (30)$
This equation can be solved with a quadratic program optimization package where the variable is $\mu_{sn}$. In the training phase, we require to solve this optimization $N$ times. And in the test phase, it is necessary to solve this optimization problem for each test data.

By using norm 0 or 1, we can find the parameters of the expert selector. All the process is summarized as an EM algorithm where in the M-step, first, we freeze $\nu$ and $\omega$ and find $\mu$; then we freeze $\mu$ and iterate for finding the local optimum $\nu$ and $\omega$; then in the E-step, we find the responsabilities $R_{in}$ using the new parameters $\nu$, $\omega$ and $\mu$. In the beginning, we initialize all parameters randomly. In the following section, we will detail the results of our experiments.

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