Feature Selection Using Batch-Wise Attenuation and Feature Mask Normalization

Yiwen Liao∗  Raphaël Latty†  Bin Yang∗

Abstract

Feature selection is generally used as one of the most important pre-processing techniques in machine learning, as it helps to reduce the dimensionality of data and assists researchers and practitioners in understanding data. Thereby, better performance and reduced computational consumption, memory complexity and even data amount can be expected by utilizing feature selection. However, only few studies leverage the power of deep neural networks to solve the problem of feature selection. In this paper, we propose a feature mask module (FM-module) for feature selection based on a novel batch-wise attenuation and feature mask normalization. The proposed method is almost free from hyperparameters and can be easily integrated into common neural networks as an embedded feature selection method. Experiments on popular image, text and speech datasets have been shown that our approach is easy to use and has superior performance in comparison with other state-of-the-art deep learning based feature selection methods.

1 Introduction

Feature selection is an important research field in the machine learning community. Typically, given a dataset consisting of samples with \(D\) features, feature selection aims to select \(K\) from the \(D\) features with \(K < D\). Subsequently, samples consisting of the selected features are used as a new dataset to solve some given learning tasks, such as classification or regression [1]. In this paper, the learning tasks performed with the selected features are called downstream tasks. Thereby, feature selection helps to reduce data dimensions for a more robust classification or regression in downstream learning tasks. Furthermore, it can be used by researchers and practitioners to understand which features are critical for a given task. Specifically, in some fields, feature selection techniques are utilized to analyze measurements and to find out the salient quantities, such as in the field of gene analysis [2].

∗University of Stuttgart, Institute of Signal Processing and System Theory.
†Advantest Europe GmbH, Applied Research and Venture Team.
Due to its importance, feature selection is already well established in the literature, especially in the field of conventional machine learning \[1,3\]. Early feature selection methods (e.g. correlation analysis \[3\] and information theory \[4,5\]) typically rely on statistical properties of data. However, they usually focus on the relations between one single feature and the target label, or focus on the features themselves, failing to take advantage from the possibly available label information. Moreover, complex relations might be overlooked in conventional feature selection methods, because they typically presume simple linear relations among different features and labels.

Recently, deep learning has achieved dramatic success in many machine learning fields \[6\]. Naturally, designing feature selection methods using deep learning concepts or in combination with neural networks has become a new research area. Many deep learning related techniques are leveraged to provide new ideas for feature selection, such as the attention mechanism \[7,8\] and autoencoder structures \[9,10\]. Moreover, due to the nature of the non-linearity of deep neural networks, more efficient and robust embedded feature selection methods can be expected if neural networks are used as backbone algorithms. For example, several popular deep learning based embedded feature selection approaches integrate the sparsity penalty from the conventional feature selection approaches into neural networks, such as \[11,12,2\]. Nonetheless, existing deep learning based feature selection methods still face multiple challenges. First, many of them often necessitate new loss terms in addition to the original downstream learning objective. Thereby, the search for an optimal loss term and a good combination of hyperparameters becomes a new bottleneck for these methods. Second, the integration of additional network modules (e.g. attention modules) may result in redundantly large network architectures. This is usually infeasible for high-dimensional data, which are, however, the most common data type in feature selection tasks. Last but not least, many previous deep learning based feature selection methods often neglect the relations between features, i.e., features are considered more or less independently. This might lead to suboptimum feature selection performance.

In order to address the issues mentioned above and provide new insights of deep learning based feature selection, we propose a feature mask module (FM-module) for feature selection in neural networks based on a novel batch-wise attenuation and feature mask normalization. The FM-module can be jointly trained with common neural networks, such as multiple layer perceptrons (MLP) or convolutional neural networks (CNN). Once the entire network is trained, the FM-layer can directly output a feature mask vector, of which each element represents the importance score of the corresponding feature of the input data. Therefore, we can use the importance scores to select the most representative and informative feature subset. Randomly selected exemplary results on the MNIST dataset are shown in Figure 1 to present the surprising performance of the proposed method. In a nutshell, the major contributions of this work can be summarized as follows:
A novel feature mask module (FM-module) is proposed, which can be jointly trained with an arbitrary neural network. The trained FM-module can directly generate importance scores (feature mask) for input features to perform feature selection.

The relation between the original features is taken into account by applying the proposed feature mask normalization. Moreover, the batch-wise attenuation forces the same feature mask for all samples within a training batch during each iteration. This targets better to feature selection than the conventional sample-wise attention mechanism.

The proposed method does not introduce additional hyperparameters to original learning objectives in comparison with other existing deep learning based approaches, and it is thus easy to use.

The features selected by the proposed method are reliable and result in similar downstream performance with different learning algorithms.

2 Related Work

According to the literature [1, 3], feature selection methods can be roughly categorized into three groups: wrapper methods, filter methods and embedded methods. In this paper, we only focus on embedded methods, since most deep learning based feature selection methods can be considered as embedded methods. It should be noted that, in our context, “deep learning based” means that a feature selection method either uses deep neural networks as a part of it, or takes advantage from the techniques developed within the deep learning community. Furthermore, according to [3], feature selection is sometimes called variable selection. In order not to confuse with the random variable in probability theory, we only use the term “feature selection” in this paper.

Early deep learning based feature selection methods were frequently inspired by conventional embedded methods, i.e. based on penalizing a sparsity term in learning objectives or based on the
analysis of the weights in hidden layers. Representative studies include [2] and [13]. In [2], the authors proposed the Deep Feature Selection (DFS) by utilizing $\ell_1$- and $\ell_2$-regularization simultaneously. Unlike previous methods [14], the first layer of DFS is innovatively designed as a sparse one-to-one linear layer, i.e. each input feature only connects to one specific neuron in the first hidden layer. This novel design has become a paradigm for many successors such as [11, 12]. In [13], the first hidden layer of a trained network is directly used to obtain the importance scores of each individual input feature by calculating individual contributions of each input feature using the activation potentials. This method does not introduce new architectures or loss terms to the network for the original learning task, but requires additional efforts to compute the feature importance vector after the training, and its performance thus significantly depends on the architecture of the neural networks.

Another modern research direction is to use attention mechanism to select features automatically. In [7], the so-called attention based feature selection (AFS) was proposed by constructing attention subnetworks to generate a selection probability matrix. Each attention subnetwork outputs one probability whether one input feature should be selected. In addition to the attention mechanism, $\ell_2$-regularization terms have been used in AFS as well.

Moreover, to design special layers or modules for feature selection is a new trend in research such as [12, 11, 9]. For example, in the concrete autoencoder [9], the authors propose a concrete selection layer by sampling random variables from concrete distributions. By using a temperature annealing schedule, the concrete random variables can smoothly approximate one-hot coding vectors and can thus be used to select features. Analogously, the binary stochastic filtering (BSF) [12] samples random variables from a Bernoulli distribution to stochastically select features.

### 3 Problem Formulation

This section introduces the feature selection problem in the context of embedded selection methods. Given a dataset $X_{\text{all}} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N]^\top \in \mathbb{R}^{N \times D}$ with $\mathbf{x}_i = [x_{i,1}, x_{i,2}, \ldots, x_{i,D}]^\top \in \mathbb{R}^D$, the corresponding ground truth set for $X_{\text{all}}$ is denoted as $y = [y_1, y_2, \ldots, y_N]^\top$ if the downstream problem is a supervised learning task. Feature selection aims to select a subset $S \subseteq \{1, 2, \cdots, D\}$ of the original $D$ features with $|S| = K$ and $K < D$. Let $\tilde{\mathbf{x}}_i$ be the feature vector after feature selection, then each entry of $\tilde{\mathbf{x}}_i$ can be denoted as $x_{i,j}$ with $j \in S$. Thereby, $f(\cdot)$ is used to denote the mapping from the original feature space to the selected feature space: $f(\cdot) : \mathbb{R}^D \mapsto \mathbb{R}^K$. Consequently, under the embedded feature selection setup, the subset $S$ is obtained in such a way that the loss function of the downstream learning task is minimized over the data distribution $p_{\text{data}}$.

Formally, the objective is defined as

$$
\arg\min_{f, g} \mathbb{E}_{(\mathbf{x}, y) \sim p_{\text{data}}} \left[ \mathcal{L}(g(f(\mathbf{x})), y) \right]
$$

(1)
where $\mathcal{L}(\cdot, \cdot)$ is the loss function for the downstream learning task, and $g(\cdot)$ is the function for the downstream learning task to be learned during training. However, in most cases, the real data distribution $p_{\text{data}}$ is unknown and we instead minimize the loss defined in Eq. 1 over the empirical distribution defined on the available dataset under the assumption that all samples are independent and identically distributed (i.i.d.).

In most cases, we do not directly search the optimal $f(\cdot)$ because the selection procedure is not differentiable and consequently difficult to optimize. Instead we search $f(x; m) = m \odot x$ such as in [12, 11, 7]. Correspondingly, the elements of the resulting feature mask vector $m \in \mathbb{R}^{D}_{\geq 0}$ can be interpreted as importance scores for each individual feature for a given downstream learning task. By sorting the importance scores in a descending order, the top-$K$ features can then be selected. Note that the mask $m$ can be a function of the input $x$ as in [7], while it can also be independent as in [11].

### 4 Method

The core idea of the proposed method is the batch-wise attenuation within a minibatch during each training iteration and the feature mask normalization. Once the feature importance mask is obtained by an arbitrary neural network trained on the given dataset, it is easy to select the top $K$ features by comparing the importance scores of each individual input feature. Thereby, in this paper, we propose a novel Feature Mask Module (FM-module) to enable feature selection jointly trained with deep neural networks as shown in Figure 2.

![Figure 2: The proposed FM-module. In each iteration, a minibatch $X$ is first mapped to $Z$ under a non-linear transformation. Then, a primitive feature mask $\bar{z}$ is obtained by averaging $Z$ over this minibatch. Finally, a fixed mask vector $m$ at the this iteration is calculated by applying a novel feature mask normalization.](image-url)
4.1 Feature Mask Module

Let the given training dataset with \( N \) samples be denoted as a matrix \( X_{\text{all}} \in \mathbb{R}^{N \times D} \), then each row vector \( x_i^\top \in \mathbb{R}^{1 \times D} \) with \( i \in \{1, 2, \ldots, N\} \) represents a single sample vector. The feature mask module (FM-module) \( f_{\text{FM}}(\cdot) \) aims to generate one fixed feature mask \( m \in \mathbb{R}^D \) from the entire dataset as: \( m = f_{\text{FM}}(X_{\text{all}}) \).

The FM-module is a generic subnetwork that can be integrated into common neural networks. In general, as shown in Figure 2, the FM-module consists of three sub-modules: i) non-linear transformation (orange); ii) batch-wise attenuation (blue); iii) feature mask normalization (green).

**Non-linear Transformation**  Let a minibatch with size of \( B \) be denoted as \( X \in \mathbb{R}^{B \times D} \). The minibatch \( X \) is mapped to \( Z = [z_1, z_2, \ldots, z_B]^\top \in \mathbb{R}^{B \times D} \) under a non-linear transformation. By using this module, the complex (non-linear) relations between different input features can be captured during the training procedure, i.e. the corresponding feature selection result takes the relation of all input features into consideration and a reliable feature selection can be expected. This idea is similar to [7], which compresses the input samples into lower dimensional representations and maps back to a matrix having the same size as the input feature matrix. In this paper, as an example, we stack two dense layers to realize this non-linear transformation:

\[
z_i = W_2 \cdot \tanh(W_1 \cdot x_i + b_1) + b_2
\]

where \( W_1 \in \mathbb{R}^{E \times D}, W_2 \in \mathbb{R}^{D \times E}, b_1 \in \mathbb{R}^E \) and \( b_2 \in \mathbb{R}^D \) with \( E < D \). It should be noted that the non-linear transformation module is generic and thus not restricted to the example mentioned above. Stacking more layers or using other layer types (e.g., convolutional layers) is also permitted within this non-linear transformation module.

**Batch-wise Attenuation**  A row vector of the resulting \( Z \) from the non-linear transformation module is dependent of its corresponding input vector. This means that each sample \( x_i \) in the original minibatch has its own map \( z_i \) in \( Z \). However, this is not desirable for feature selection since it is generally assumed that all samples in the given data should have the same significant features. Therefore, by explicitly averaging \( Z \) over the minibatch, a fixed vector for all samples within a minibatch can be obtained at each training iteration. Specifically, for each minibatch, we calculate

\[
\bar{z} = \frac{1}{B} \sum_{i=1}^{B} z_i
\]

**Feature Mask Normalization**  This module is proposed to normalize the resulting \( \bar{z} \), i.e. all elements of the feature mask are normalized. That is to say, the relative importance of different input features are considered by the normalization during training. Consequently, the resulting feature importance scores (the entries of the final feature mask vector \( m \)) are more reliable. In this
work, inspired by [15], we use \( \text{softmax}(\cdot) \) to realize this module:

\[
\mathbf{m} = \text{softmax}(\mathbf{z}), \quad \text{with} \quad m_i = \frac{e^{z_i}}{\sum_{j=1}^{D} e^{z_j}}
\]  

(4)

Thereby, the FM-module can be integrated with an arbitrary neural network targeting a given downstream learning task by element-wise multiplying \( \mathbf{m} \) with each input sample. Accordingly, the downstream learning network is trained on \( \mathbf{m} \odot \mathbf{x}_i \) rather than the original \( \mathbf{x}_i \) with \( i \in \{1, 2, \ldots, B\} \) at each iteration. In this way, the FM-module is trained jointly with the downstream task. Once the FM-module is trained, the final feature mask \( \mathbf{m} \) can be separately calculated over the entire training dataset, i.e. by applying the trained FM-module to the whole dataset \( X_{\text{all}} \) in Eq. 2 to Eq. 4. Accordingly, each individual entry \( m_i \) of \( \mathbf{m} \) indicates the importance of the corresponding feature \( x_i \). Consequently, we can select the top \( K \) features based on the resulting feature importance scores. In contrast to conventional attention mechanism, the calculated feature mask \( \mathbf{m} \) remains fixed while solving the downstream learning task with the selected input features.

4.2 Network and Objective Function

![Figure 3: The network with an FM-module for feature selection. The FM-module (orange) can generate a fixed feature mask \( \mathbf{m} \) from the data \( X \). The learning network \( g(\cdot) \) (green) can be an arbitrary network parameterized by \( \Theta \) according to a specific learning task.](image)

In this section, we briefly introduce how to use the proposed FM-module in common neural networks. Specifically, let \( g(\cdot; \Theta) \) be an arbitrary neural network for the given downstream learning task parameterized by \( \Theta \) such as classification or regression, and \( \mathcal{L}(\cdot, \cdot) \) denote the corresponding loss function. The given dataset is denoted as \( \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\} \). A common learning task without feature selection can be defined as

\[
\arg\min_{\Theta} \mathbb{E}_{(x,y) \sim p_{\text{data}}} \left[ \mathcal{L}(g(x; \Theta), y) \right]
\]

(5)

In order to learn the feature mask vector \( \mathbf{m} \), the FM-module can be added before the downstream network \( g(\cdot; \Theta) \) as shown in Figure 3. Thereby, each input for \( g(\cdot; \Theta) \) becomes \( f_{\text{FM}}(\mathbf{x}) = \mathbf{m} \odot \mathbf{x}_i \). Consequently, the overall learning objective becomes

\[
\arg\min_{\Theta, \Theta_{\text{FM}}} \mathbb{E}_{(x,y) \sim p_{\text{data}}} \left[ \mathcal{L}(g(f_{\text{FM}}(\mathbf{x}; \Theta_{\text{FM}}); \Theta), y) \right]
\]

(6)

\[ ^{\text{In our running example, } \Theta_{\text{FM}} = \{W_1, W_2, b_1, b_2\} \text{ defined in Subsection 4.1}} \]
What makes the proposed FM-Module appealing is that no additional regularization terms or carefully designed loss terms need to be added to the original downstream learning objective. This means that the entire network shown in Figure 3 can be directly trained to minimize exactly the same loss function $L(\cdot, \cdot)$ for $g(\cdot; \Theta)$. For example, if the downstream task is classification, a canonical objective function could be the cross entropy loss.

5 Experiments

To evaluate the proposed FM-module, we carried out experiments on multiple datasets from different domains. Additionally, six other state-of-the-art deep learning based feature selection methods were considered for comparison to show the superiority of the FM-module.

5.1 Setups

The proposed FM-module with other six reference methods were trained on five datasets in both supervised and unsupervised manners. All methods shared the same architecture of the learning network $g(\cdot)$ for a fair comparison, since they were all embedded feature selection approaches. In particular, the learning network $g(\cdot)$ used in all experiments had two dense layers, with 128 and 64 neurons, respectively. After each dense layer, a LeakyReLU layer [16] with the rate of 0.2 was used as the activation function. Before the output layer, a Dropout layer [17] with the dropout rate of 0.3 was used to reduce overfitting. It should be noted that each individual experiment was repeated five times with different random seeds to eliminate the occasionality of the training procedure in neural networks. In the following, we only report the averaged results with their standard deviations. Furthermore, in all conducted experiments, the accuracy on the test set was used to measure the performance of a feature selection method to be consistent with previous studies.

5.1.1 Reference Methods

In this work, we selected the following state-of-the-art approaches from the literature as reference methods for comparison: i) Attention based Feature Selection (AFS) [7]; ii) Concrete Autoencoder (ConAE) [9]; iii) CancelOut [11]; iv) Binary Stochastic Filtering (BSF) [12]; v) Deep Feature Selection (DFS) [2]; vi) Feature Selection using Deep Neural Networks (FSDNN) [13]. The key hyperparameters of all reference methods were individually optimized by us for the considered datasets by grid search on a hold-out validation subset (10% of the training samples). Furthermore, we used all raw features (RawF) as the performance upper bound, while used randomly selected features (RSF) as a lower bound. It should be noted that the usage of raw features indicates that we did not do any additional feature extraction for a given dataset, although the dataset itself may consist of data based on extracted features.
5.1.2 Datasets

Five well-known datasets, which frequently benchmark feature selection algorithms, were used in conducted experiments, including three image datasets, MNIST [18], Fashion-MNIST (fMNIST) [19] and COIL20 [20], one speech dataset Isolet [21] and one text dataset PCMAC [1]. It should be noted that the latter three datasets consist of only limited number of samples. This is a challenge for deep learning based approaches requiring a large amount of data. Moreover, the Isolet and PCMAC datasets consist of extracted features, meaning that all features have physical meaning. A detailed information of the datasets is listed in Table 1.

| # Features | # Train | # Test | Classes | Type |
|------------|---------|--------|---------|------|
| MNIST      | 784     | 60000  | 10000   | 10   | Image |
| fMNIST     | 784     | 60000  | 10000   | 10   | Image |
| COIL20     | 1024    | 1152   | 288     | 20   | Image |
| Isolet     | 617     | 1248   | 312     | 26   | Speech |
| PCMAC      | 3289    | 1555   | 388     | 2    | Text  |

5.1.3 Classifiers

In order to verify whether the selected features are robust to different classifiers for the downstream learning tasks, the selected features from our method and reference approaches should be evaluated on different classifiers. Therefore, five well-known classifiers were trained on the selected features: i) Random Forest (RF); ii) Linear Support Vector Machine (SVM); iii) k-Nearest Neighbor (kNN); iv) Logistic Regression (LR); v) Neural Network (NN). The five classifiers above were implemented using scikit-learn [22] and TensorFlow [23]. The hyperparameters of the classifiers were set based on the performance on the raw features. In general, the five classifiers showed similar results on all experiments. Therefore, due to the length limitation, we only report the results based on random forest, which is more frequently used in previous studies [7]. Results of other classifiers are additionally attached in Appendix.

5.2 Basic Experiments

The basic experiments aim to show whether the proposed FM-module can generally outperform other considered state-of-the-art feature selection methods. Table 2 shows the resulting classification accuracy using the top-50 features selected by the reference methods and the proposed method on the random forest classifier. In total, the proposed FM-module can select the most informative and representative features in comparison with all other six state-of-the-art methods on the five datasets in respect of the downstream classification accuracy. In particular, although DFS achieved
moderately similar performance as our method in the conducted experiments, the FM-module does not possess that many hyperparameters as DFS: DFS uses $\ell_1$- and $\ell_2$-regularization in both feature selection part and learning subnetwork. Consequently, four critical hyperparameters for the regularization terms have to be carefully fine-tuned in DFS. In contrast, our method does not introduce new loss terms and is thus easier to use.

Table 2: Downstream classification accuracy based on top-50 selected features in a supervised learning setup (random forest as the classifier).

| Method   | MNIST   | fMNIST  | COIL20 | Isolet  | PCMAC  |
|----------|---------|---------|--------|---------|--------|
| RSF      | 0.842 (± 0.038) | 0.828 (± 0.008) | 0.991 (± 0.007) | 0.835 (± 0.027) | 0.584 (± 0.038) |
| RawF     | 0.969 (± 0.000) | 0.876 (± 0.000) | 1.000 (± 0.000) | 0.931 (± 0.000) | 0.930 (± 0.000) |
| AFS      | 0.905 (± 0.022) | 0.833 (± 0.001) | 0.984 (± 0.009) | 0.825 (± 0.002) | 0.759 (± 0.061) |
| CancelOut| 0.743 (± 0.033) | 0.611 (± 0.024) | 0.970 (± 0.005) | 0.846 (± 0.013) | 0.878 (± 0.001) |
| BSF      | 0.912 (± 0.018) | 0.833 (± 0.012) | 0.988 (± 0.010) | 0.890 (± 0.019) | 0.788 (± 0.025) |
| DFS      | 0.936 (± 0.005) | 0.852 (± 0.001) | 0.998 (± 0.002) | 0.900 (± 0.006) | 0.621 (± 0.036) |
| FSDNN    | 0.877 (± 0.011) | 0.811 (± 0.011) | 0.998 (± 0.002) | 0.837 (± 0.054) | 0.749 (± 0.014) |
| ConAE    | 0.908 (± 0.022) | 0.806 (± 0.017) | 0.983 (± 0.007) | 0.771 (± 0.011) | 0.613 (± 0.000) |
| FM (ours)| **0.954 (± 0.003)** | **0.854 (± 0.003)** | **0.999 (± 0.002)** | **0.901 (± 0.013)** | **0.889 (± 0.010)** |

As mentioned before, in our experiment, RawF and RSF were used as the upper and lower bounds for the evaluation of a feature selection method, respectively. We argue that a carefully designed algorithm should have better performance than randomly selected features (RSF). Although previous works often overlook the experiments with random features, we surprisingly found that randomly selected features led to better results than some carefully designed methods in some cases. For example, the method CancelOut has poorer performance than RSF on the three image datasets. Moreover, FSDNN had moderately poorer performance than RSF on the fMNIST datasets. Fortunately, the FM-module outperforms the RFS with a significant gap on all considered datasets.

In addition to the random forest as the downstream classifier, the results in Appendix show the classification results on other four considered classifiers to justify whether the proposed method can select features which are consistent for different types of classifiers. In general, the features selected by the proposed FM-module lead to the best classification performance in the most considered experiments. This means that the selected features are more informative and reliable.

Furthermore, the FM-module and other considered methods have only small standard deviation in respect of different network initialization seeds. This is feasible and shows that all methods have consistent performance regarding different initialization.
5.3 Performance over Different Numbers of Features

To identify whether the FM-module can select different numbers of features with reliable downstream classification performance, different feature subsets were selected and compared in this subsection. Figure 4 shows an exemplary experimental result on the dataset MNIST using the random forest as the classifier. Six different numbers of features were investigated: 10, 25, 50, 100, 250 and 500. They correspond to 1.3%, 3.2%, 6.4%, 12.8%, 31.9% and 63.8% of all raw features (pixels) of the original dataset.

The overall results show that the proposed FM-module can select informative features in comparison with other six state-of-the-art approaches with a certain number of features. We can notice that, in MNIST, FM-module can result in an accuracy more than 90% with about only 3.2% of all pixels of the original image data. Furthermore, by using FM-module, 100 selected features (only about 12.8% of all features) can already lead to similar performance with that of all features. This is valuable for studying the salient features of a given dataset and reducing the data dimension more effectively and efficiently.

It should be also mentioned that ConAE has to be individually trained for each different number of features to be selected, because ConAE requires a predefined number of features as a training parameter. In contrast, other methods, including our FM-module, do not require the number of target features as a parameter for training the algorithm. Instead, the methods except for ConAE all output a feature importance vector. Different numbers of features can thus be selected by choosing the features corresponding to the highest importance scores. This is more practical and efficient, because we often do not have idea how many features should be selected in advance.

![Figure 4: Downstream classification over different numbers of selected features on MNIST (random forest as the classifier).](image-url)
5.4 Unsupervised Settings

The proposed FM-module is designed to be easily integrated into different networks. Therefore, FM-module can be applied to unsupervised learning tasks as well. In this case, the learning objective becomes minimizing the reconstruction loss between the input data and the reconstructed data. Thereby, the minimization of the mean squared error loss is a common learning objective. To build up the unsupervised learning environment, $g(\cdot)$ in Figure 3 becomes an autoencoder with three hidden dense layers with LeakyReLU as activation functions, having 128, 64 and 128 neurons, respectively. The mean squared error (MSE) was used as the learning objective. All hyperparameters of all methods were set to be same as those in supervised learning in the previous subsections.

|        | MNIST   | fMNIST  | COIL20  | Isolet  | PCMAC  |
|--------|---------|---------|---------|---------|--------|
| RSF    | 0.842\(\pm 0.038\) | 0.828\(\pm 0.008\) | 0.991\(\pm 0.007\) | 0.835\(\pm 0.027\) | 0.584\(\pm 0.038\) |
| RawF   | 0.969\(\pm 0.000\) | 0.876\(\pm 0.000\) | 1.000\(\pm 0.000\) | 0.931\(\pm 0.000\) | 0.930\(\pm 0.000\) |
| AFS    | 0.883\(\pm 0.010\) | 0.808\(\pm 0.023\) | 0.970\(\pm 0.029\) | 0.759\(\pm 0.025\) | 0.548\(\pm 0.003\) |
| CancelOut | 0.875\(\pm 0.018\) | 0.805\(\pm 0.020\) | 0.977\(\pm 0.019\) | 0.782\(\pm 0.037\) | 0.583\(\pm 0.021\) |
| BSF    | 0.868\(\pm 0.022\) | 0.803\(\pm 0.007\) | 0.950\(\pm 0.020\) | 0.833\(\pm 0.006\) | 0.556\(\pm 0.023\) |
| DFS    | 0.817\(\pm 0.123\) | 0.815\(\pm 0.019\) | 0.918\(\pm 0.099\) | 0.818\(\pm 0.046\) | 0.643\(\pm 0.105\) |
| FSDNN  | 0.935\(\pm 0.002\) | 0.815\(\pm 0.002\) | 0.943\(\pm 0.046\) | 0.825\(\pm 0.023\) | 0.667\(\pm 0.038\) |
| ConAE  | 0.868\(\pm 0.027\) | 0.808\(\pm 0.024\) | 0.976\(\pm 0.010\) | 0.790\(\pm 0.030\) | 0.575\(\pm 0.011\) |
| FM (ours) | **0.936\(\pm 0.009\)** | **0.842\(\pm 0.003\)** | **0.998\(\pm 0.002\)** | **0.865\(\pm 0.005\)** | **0.692\(\pm 0.033\)** |

Table 3: Downstream classification accuracy based on top-50 selected features in an unsupervised learning setup (random forest as the classifier).

In particular, the feature selection methods were trained in an unsupervised manner and the resulting selected features were evaluated by classifiers targeting classification tasks. Table 3 shows the classification accuracy on random forest classifier trained on the unsupervised learned selected features. The FM-module achieved the best performance in the downstream classification on all five datasets. This shows that the proposed method is flexible to be applied to different learning environments, e.g., in both supervised and unsupervised learning. Moreover, it can be noticed that the selected features did not show significant performance difference or deterioration on MNIST, fMNIST and COIL20 from the supervised learning to unsupervised learning. One plausible reason might be that the MSE loss function can also guide the feature selection algorithms to select similar informative features as the categorical cross entropy loss on image datasets. However, when it comes to the speech or text datasets (Isolet and PCMAC), where the input features are sometimes sparse (containing many zeros), the mean squared error as the learning objective is difficult to min-
imize. Hence, the performance on selected features is poorer than that in a supervised learning setup.

5.5 Insight of FM-module

In comparison with other considered state-of-the-art approaches, the proposed FM-module enjoys a key property that it is free from special hyperparameters such as additional decays for the $\ell_1$- or $\ell_2$-terms. Nonetheless, this subsection investigates the advantages and limitations of the proposed FM-module to provide a deep insight of this method.

5.5.1 A Visual Understanding of FM-module

In order to obtain a more intuitive understanding of the superiority of the proposed FM method, we visualize the learned feature importance vector of all considered reference methods as shown in Figure 5. To make the comparison more clearly, we re-scaled the resulting feature importance vector into the range between 0 and 1. Moreover, the feature vector was reshaped into $28 \times 28$ for the MNIST dataset. Apparently, the proposed FM method can select the most informative features, i.e. the pixels distributed in the center of the image. Although DFS and FSDNN can also select the centered pixels, they often assign similar importance scores to nearing pixels. In this case, redundant pixels might be selected and have no further information contribution to the subsequent learning tasks. On the contrary, other methods, such as CancelOut, assign high importance scores to the pixels at the edges of the image. However, the pixels around the edges have values of zero and do not provide any information for classification. Thereby, non-related features are mistakenly selected by these methods. In Figure 6, we highlight the top-50 features based on the scores in Figure 5. The visualization of the top-50 features further matches the observation above. Interestingly, the number of selected features of ConAE does not equal to 50, because ConAE might repeatedly select the same feature during the training.

![Figure 5: The visualization of the learned feature importance vectors for the reference methods and the proposed FM-module. The resulting vectors are reshaped to $28 \times 28$ for better visualization.](image)

5.5.2 Ablation Study of FM-module

This subsection studies the necessity of the batch-wise attenuation (BA) and the feature mask normalization (FMN) within the FM-module. Table 4 presents the overview results of the ablation
study. Generally, the usage of both submodules contributes to the final performance (e.g. classification accuracy on a random forest classifier). For example, the batch-wise attenuation has significant contribution when not using feature mask normalization (w/o FMN), while BA leads to limited performance improvement if using FMN. We argue that the utilization of FMN has two advantages: one is the introduction of the non-negativity of the resulting feature mask due to $\text{softmax}(\cdot)$, the other is the consideration of the relative importance among individual features due to the denominator of $\text{softmax}(\cdot)$. The latter property of FMN lacks of attention in previous studies. On the other hand, the batch-wise attenuation forces that the feature mask vector to be same for all input samples, differentiating the proposed method from conventional attention mechanism. Using the same feature mask vector for all samples is more intuitive and reasonable for feature selection and shows better results in conducted experiments.

Table 4: Ablation study of the FM-module (exemplary classification accuracy on MNIST using a random forest classifier).

|       | w/o FMN          | w/ FMN          |
|-------|------------------|------------------|
| w/o BA | 0.720 ($\pm$ 0.005) | 0.932 ($\pm$ 0.005) |
| w/ BA  | 0.898 ($\pm$ 0.008) | 0.954 ($\pm$ 0.003) |

5.5.3 Time Complexity

This subsection investigates the time complexity of considered state-of-the-art methods and the proposed FM-module. We let the batch size be denoted as $B$, number of raw features be denoted as $D$, number of selected features be $K$. Furthermore, without loss of generality, the learning network is a dense network with $g(\cdot)$ has $DN_1 + N_{\text{others}}$ parameters, $N_1$ represents the number of neurons in the first hidden layer, and $N_{\text{others}}$ represents the number of all other parameters within this network. Moreover, the AFS and FM methods require the input data first to be transformed into a lower dimensional representation, and the corresponding dimension is denoted as $E$. In the following, we omit the bias term in all layers for simplicity.

Table 5 shows the resulting complexity, where we omit the complexity of the learning network $g(\cdot)$. In other words, we only compared the time complexity of the special network or layer pro-
posed to perform feature selection of each method. Generally, CancelOut, BSF and DFS has the lowest time complexity $\mathcal{O}(BD)$ during training, because the initialized feature importance vector is directly multiplied to the input data element-wisely. On the contrary, AFS, ConAE and the proposed method has a higher time complexity due to the matrix multiplication. Furthermore, in AFS [7], the authors state that their method can be generalized to a version with deeper attention modules. In this case, the time complexity of AFS becomes $\mathcal{O}(DN_A)$, where $N_A$ is the complexity of each individual attention module, which is significantly larger than $BDE$. Moreover, in FSDNN, only an ordinary network is trained and the feature selection is achieved by a post-processing, while all other methods can directly output the feature importance vector once after training. Although the proposed method does not have the smallest time complexity, in practice, this gap can be omitted because the learning part $g(\cdot)$ typically has notably greater time complexity. In order to show this, the last column of Table 5 shows the actual time consumption for the seven methods trained on MNIST with 100 epochs as an example. Apparently, only little time consumption difference can be observed among different methods, and this difference can be expected to be even smaller when we turn to a deeper learning network $g(\cdot)$.

Table 5: Time complexity of reference methods and the proposed method.

| Method    | Time Complexity                  | Actual Time Consumption (in second) |
|-----------|----------------------------------|-------------------------------------|
| AFS       | $\mathcal{O}(BD^2E)$ or $\mathcal{O}(DN_A)$ | 119.2                               |
| CancelOut | $\mathcal{O}(BD)$               | 106.9                               |
| BSF       | $\mathcal{O}(BD)$               | 99.5                                |
| DFS       | $\mathcal{O}(BD)$               | 103.1                               |
| FSDNN     | $\mathcal{O}(BDN_1)$            | 163.0                               |
| ConAE     | $\mathcal{O}(BD^2K)$            | 104.8                               |
| FM (ours) | $\mathcal{O}(BD^2E)$            | 105.8                               |

5.5.4 Deeper FM-module

As discussed before, stacking multiple layers can lead to a deeper version of the FM-module, i.e. $z_i = f_1 \circ f_2 \circ \cdots \circ f_\ell(x_i)$, where $f_i(\cdot)$ is one non-linear transformation layer, such as a dense layer with a $\tanh(\cdot)$ function. According to our experiment, this extension of FM-module is not necessary. Specifically, we evaluated the performance of the FM-module with different hidden layers, ranging from one hidden layer (the proposed version) and six hidden layers. The resulting downstream classification accuracy for the MNIST dataset was between 0.950 to 0.959. This

---

4The implementation of FSDNN for generating feature importance vector was not based on GPU, so the actual time consumption is significantly larger than others.
empirically shows that current FM-module with one hidden layer only, i.e., the structure defined in Subsection 4.1 can guarantee a reliable performance and select the most important features. The reason might be that the current FM-module already has enough capacity to generate the feature mask from the data.

5.5.5 Sensitivity to Initialization

The initialization is an important issue in deep learning based feature selection approaches. For example, the AFS and CancelOut are sensitive to the initialization [7, 11]. To eliminate this concern, we justified our method on the following different initialization methods: i) weights initialized from a uniform distribution; ii) weights initialized from a normal distribution; iii) weights initialized with constants (ones); iv) weights initialized by using Xavier methods [24]. The standard deviation of final classification accuracy of different initialization methods was within 0.4%. This shows that our method is empirically non-sensitive to different initialization methods.

6 Conclusion

This paper has proposed a novel feature mask module (FM-module) for feature selection in combination with neural networks leveraging a novel batch-wise attenuation and feature mask normalization. In comparison to existing deep learning based approaches, our method does not include additional loss terms in the overall learning objective, and the module can therefore be easily trained with common networks in a joint fashion. Experiments show that the FM-module can be used for both supervised and unsupervised feature selection tasks. Comprehensive experiments on several datasets from different domains demonstrate the effectiveness and superiority of our approach in comparison with other state-of-the-art methods. Further research might explore the possibility to leverage the FM-module to perform network pruning and reduction. Moreover, the authors plan to apply the FM-module to other scientific domains, such as gene analysis or semiconductor test data analysis.

Acknowledgment This research was supported by Advantest as part of the Graduate School “Intelligent Methods for Test and Reliability” (GS-IMTR) at the University of Stuttgart.
References

[1] Jundong Li, Kewei Cheng, Suhang Wang, Fred Morstatter, Robert P Trevino, Jiliang Tang, and Huan Liu. Feature selection: A data perspective. *ACM Computing Surveys (CSUR)*, 50(6):1–45, 2017.

[2] Yifeng Li, Chih-Yu Chen, and Wyeth W Wasserman. Deep feature selection: theory and application to identify enhancers and promoters. *Journal of Computational Biology*, 23(5):322–336, 2016.

[3] Isabelle Guyon and André Elisseeff. An introduction to variable and feature selection. *Journal of machine learning research*, 3(Mar):1157–1182, 2003.

[4] Gavin Brown, Adam Pocock, Ming-Jie Zhao, and Mikel Luján. Conditional likelihood maximisation: a unifying framework for information theoretic feature selection. *The journal of machine learning research*, 13(1):27–66, 2012.

[5] Hanchuan Peng, Fuhui Long, and Chris Ding. Feature selection based on mutual information criteria of max-dependency, max-relevance, and min-redundancy. *IEEE Transactions on pattern analysis and machine intelligence*, 27(8):1226–1238, 2005.

[6] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep learning*, volume 1. 2016.

[7] Ning Gui, Danni Ge, and Ziyin Hu. Afs: An attention-based mechanism for supervised feature selection. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 3705–3713, 2019.

[8] Qian Wang, Jiaxing Zhang, Sen Song, and Zheng Zhang. Attentional neural network: Feature selection using cognitive feedback. In *Advances in neural information processing systems*, pages 2033–2041, 2014.

[9] Abubakar Abid, Muhammed Fatih Balin, and James Zou. Concrete autoencoders for differentiable feature selection and reconstruction. In *Proceedings of the 36th International Conference on Machine Learning, PMLR*, 2019.

[10] Kai Han, Yunhe Wang, Chao Zhang, Chao Li, and Chao Xu. Autoencoder inspired unsupervised feature selection. In *2018 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 2941–2945. IEEE, 2018.

[11] Vadim Borisov, Johannes Haug, and Gjergji Kasneci. Cancelout: A layer for feature selection in deep neural networks. In *International Conference on Artificial Neural Networks*, pages 72–83. Springer, 2019.

[12] Andrii Trelín and Aleš Procházka. Binary stochastic filtering: feature selection and beyond, 2020.
[13] Debaditya Roy, K Sri Rama Murty, and C Krishna Mohan. Feature selection using deep neural networks. In *2015 International Joint Conference on Neural Networks (IJCNN)*, pages 1–6. IEEE, 2015.

[14] Hui Zou and Trevor Hastie. Regularization and variable selection via the elastic net. *Journal of the royal statistical society: series B (statistical methodology)*, 67(2):301–320, 2005.

[15] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Advances in neural information processing systems*, pages 5998–6008, 2017.

[16] Andrew L Maas, Awni Y Hannun, and Andrew Y Ng. Rectifier nonlinearities improve neural network acoustic models. In *Proceedings of the 30th International Conference on Machine Learning (ICML)*, 2010.

[17] Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: a simple way to prevent neural networks from overfitting. *The journal of machine learning research*, 15(1):1929–1958, 2014.

[18] Yann LeCun, Léon Bottou, Yoshua Bengio, and Patrick Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.

[19] Han Xiao, Kashif Rasul, and Roland Vollgraf. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms. *arXiv preprint arXiv:1708.07747*, 2017.

[20] Sameer A Nene, Shree K Nayar, Hiroshi Murase, et al. Columbia object image library (coil-100). 1996.

[21] Mark Fanty and Ronald Cole. Spoken letter recognition. In *Advances in Neural Information Processing Systems*, pages 220–226, 1991.

[22] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.

[23] Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, et al. Tensorflow: A system for large-scale machine learning. In *12th {USENIX} symposium on operating systems design and implementation ({OSDI} 16)*, pages 265–283, 2016.

[24] Xavier Glorot and Yoshua Bengio. Understanding the difficulty of training deep feedforward neural networks. In *Proceedings of the thirteenth international conference on artificial intelligence and statistics*, pages 249–256, 2010.