CrossSiam: k-Fold Cross Representation Learning

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Abstract: One of the most important tasks for multi-agents such as drones is to automatically make decisions based on images captured by on-board cameras. These agents must be highly accurate and reliable. For this purpose, we applied k-fold cross validation to the task of classifying images using deep learning, which is a method that compares and evaluates models appropriately model of a given problem; this technique is easy to understand and easy to implement, and it produces results in lower bias estimates. However, k-fold cross validation reduces the amount of data per neural network, which reduces the accuracy. In order to address this problem, we propose CrossSiam. CrossSiam is a one of the representation learning methods to train feature encoders to mimic the embedding space of the validation data of each neural network. We show that the proposed method has a higher classification accuracy than the ParaSiam (baseline). This approach can be very important in the field where reliability is required, such as automated vehicles and drones in disaster situations.

1 INTRODUCTION

In recent years, multi-agent system comprising vehicles, such as robots and drones, have been attracting attention in many domains, including disaster relief. These artificial agents should be able to make their own decisions with high accuracy and reliability. Deep learning is currently the focus of considerable research attention as an accurate decision-making method based on images and videos; it is the state of the art in several tasks, for which multi-agents are expected to perform (Suzuki et al., 2021). In particular, for image classification tasks where a large dataset is available, AlexNet (Krizhevsky et al., 2012), VGG (Simonyan and Zisserman, 2014), ResNet (He et al., 2016), and EfficientNet (Tan and Le, 2019) have achieved excellent accuracy outperforming other conventional models. The reliability is a major issue of deep learning. Because it mostly performs black-box decision making; moreover, it is difficult to correct mistakes by post-processing due to the complexity. Therefore, more reliable method than those deep learning methods is required in many tasks.

k-Fold cross validation is a common and simple method to improve the reliability of machine learning. It extracts sub-datasets consisting of k train/validation data by splitting the training dataset into k groups. This method does not use the test data while training, but allows the model to evaluate the training results through validation. Improving robust decisions with multiple models and multi-agents is effective for both accuracy and computational cost. Because it is possible to have multiple models on different agents. However, k-fold cross validation is rarely applied to deep learning for the following two reasons.

- It increases the computational cost in proportion to the number of number of divisions of the training dataset.
- It decreases the number of training data per model, thus, decreasing the accuracy.

In particular, the decrease in accuracy resulting from the decrease in number of training data can be fatal when the dataset is small.

In this study, we propose a learning method called CrossSiam. We show that this method can mitigate the accuracy degradation caused by the application of k-fold cross validation to deep learning.

2 RELATED WORK

2.1 Representation Learning

Representation learning is a method for obtaining valuable representations for classification and other purposes through self-supervised learning.

The major representation learning methods, such as SimCLR (Chen et al., 2020) and BYOL (Grill et al.,

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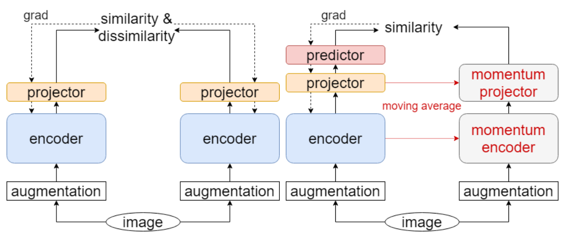

(a) SimCLR (b) BYOL

Figure 1: Major Siamese representation learning architectures.

2020), share a common approach. First, x_1, x_2 are obtained by applying two data augmentations to a sample x. Second, z_1, z_2, which are feature representations corresponding to x_1, x_2, are obtained from the neural network. Finally, the neural network learns to make the two obtained feature representations z_1, z_2 consistent. To achieve this policy, each method adopts a different technique for obtaining the network and loss functions (Figure 1).

SimCLR (Figure 1a) is one of the earliest of these methods and is trained via the following algorithm.

$$\begin{aligned}
x_1, x_2 &= \mathrm{aug}(x), \mathrm{aug}(x) \\
z_1, z_2 &= g_\theta(f_\theta(x_1)), g_\theta(f_\theta(x_2)) \\
loss &= L_{simclr}(z_1, z_2) + L_{simclr}(z_2, z_1)
\end{aligned}$$

where $L_{simclr}(z_1, z_2)$ is defined in Equation 1.

$$-\sum_{i=1}^{N} \log \frac{\exp(\mathrm{sim}(z_{i1}, z_{i2}))}{\sum_{j\neq i}^{N} \sum_{k\in[1,2]} \exp(\mathrm{sim}(z_{i1}, z_{jk}))}. \quad (1)$$

Here, aug denotes random data augmentation, and sim denotes the cosine similarity. In addition, f_θ is a neural network such as ResNet (He et al., 2016) without the classification layer, and g_θ is a neural network consisting of one to three layers.

BYOL (Figure 1b) is an advanced version of SimCLR and MoCo (He et al., 2020). There are two significant differences between BYOL and SimCLR. The first is that ξ, which is the model parameter updated by a moving average of θ, as proposed by MoCo. This implies that instead of predicting each z directly, prediction of z' output is learned using the model parameter ξ. The second modification is the addition of a network h_θ to predict z and train the output p to predict z'. The algorithm is as follows:

$$\begin{aligned}
x_1, x_2 &= \mathrm{aug}(x), \mathrm{aug}(x) \\
z_1, z_2 &= g_\theta(f_\theta(x_1)), g_\theta(f_\theta(x_2)) \\
z'_1, z'_2 &= g_\xi(f_\xi(x_1)), g_\xi(f_\xi(x_2)) \\
p_1, p_2 &= h_\theta(z_1), h_\theta(z_2) \\
loss &= \mathrm{sim}(p_1, \mathrm{sg}(z'_2)) + \mathrm{sim}(p_2, \mathrm{sg}(z'_1)),
\end{aligned}$$

Here, sg denotes the stop gradient.

2.2 k-Fold Cross Validation

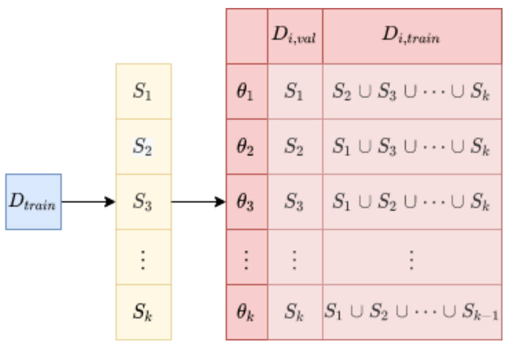
D_{train}
S_1
S_2
S_3
$\vdots$
S_k
$D_{i,val}$
$D_{i,train}$
θ_1 S_1 $S_2 \cup S_3 \cup \cdots \cup S_k$
θ_2 S_2 $S_1 \cup S_3 \cup \cdots \cup S_k$
θ_3 S_3 $S_1 \cup S_2 \cup \cdots \cup S_k$
$\vdots$ $\vdots$ $\vdots$
θ_k S_k $S_1 \cup S_2 \cup \cdots \cup S_{k-1}$

Figure 2: k-Fold Cross Validation.

k-Fold cross validation is a common evaluation method in machine learning. The following steps are used for training and evaluation (Figure 2):

1. Divide the training data D_{train} into k groups $S_1, S_2, \ldots, S_k$.
2. Let S_i be training data and the rest be validation data.
3. Train and evaluate the model θ_i based on train/validation data
4. Apply Steps 2–3 for all i.

This method improves the reliability of machine learning. For example, in hyperparameter search, when optimizing on a fixed set of train/validation data, there is a possibility of overfitting on that combination. k-Fold cross validation prevents overfitting by optimizing on k types of train/validation data. Cross validation can prevent overfitting by optimizing on k types of train/validation data.

2.3 Semi-supervised Semantic Segmentation with Cross Pseudo Supervision

This method is proposed in (Chen et al., 2021) for semi-supervised semantic segmentation. It utilizes unlabeled dataset for training in addition to supervised semantic segmentation. In this method, the unlabeled data is split into two parts and two corresponding neural networks are prepared, each of which is used as training data. The output of the neural network that is not included in the training data is transformed and used as the pseudo-label for the unlabeled data. This method enables more robust learning than existing methods.

In our study, we extend this method to self-supervised learning, i.e., we consider the classification task for the case where the labeled dataset is zero.

Furthermore, we train not only 2-fold but also 5-fold, because a larger number of partitions increases the amount of training data per model and the expected accuracy, while increasing the computational complexity.

3 METHOD

In applying k-fold cross validation to representation learning, we denote the kth neural net as θ_k, the training dataset as $D_{k,train}$, and the validation dataset as $D_{k,val}$.

3.1 Baseline

ParaSiam, the baseline method of representation learning with k-fold cross validation, has a loss function similar to BYOL (Grill et al., 2020).

$$\begin{aligned}
x &\in D_{k,train} \\
x_1, x_2 &= \text{aug}(x), \text{aug}(x) \\
z_1, z_2 &= g_{\theta_k}(f_{\theta_k}(x_1)), g_{\theta_k}(f_{\theta_k}(x_2)) \\
z'_1, z'_2 &= g_{\xi_k}(f_{\xi_k}(x_1)), g_{\xi_k}(f_{\xi_k}(x_2)) \\
p_1, p_2 &= h_{\theta_k}(z_1), h_{\theta_k}(z_2) \\
loss &= \sum_{i=1,2} \sum_{j=1,2} \text{sim}(p_i, \text{sg}(z'_j))
\end{aligned}$$

where k indicates the ID of the network and corresponding training data of subset, θ_k and ξ_k are the kth model parameters.

3.2 CrossSiam

CrossSiam is the proposed method to improve representation learning with k-fold cross validation. Although the loss function is similar to BYOL and ParaSiam, the target of prediction is other network validation data like (Chen et al., 2021).

$$\begin{aligned}
x &\in D_{k,train} \cap D_{l,val} (k \neq) \\
x_1, x_2 &= \text{aug}(x), \text{aug}(x) \\
z_1, z_2 &= g_{\theta_k}(f_{\theta_k}(x_1)), g_{\theta_k}(f_{\theta_k}(x_2)) \\
z'_1, z'_2 &= g_{\xi_l}(f_{\xi_l}(x_1)), g_{\xi_l}(f_{\xi_l}(x_2)) \\
p_1, p_2 &= h_{\theta_k}(z_1), h_{\theta_k}(z_2) \\
loss &= \sum_{i=1,2} \sum_{j=1,2} \text{sim}(p_i, \text{sg}(z'_j))
\end{aligned}$$

where l is one of IDs of the other networks. This function indicates that z', the target of kth network prediction, is the output of the lth network, with the constraint that the input x is the kth training data and the validation data of the lth network.

4 EXPERIMENTS

In this study, we trained models to learn representation with ParaSiam and CrossSiam(the proposed method). To evaluate these models, first, after the representation learning, we calculate the accuracy of classification when only the final layer is trained with the fixed embedding space. Second, we calculate the difference between embedding space of $D_{i,train}$, $D_{i,val}$, and D_{test} in CrossSiam and ParaSiam, respectively, and consider whether there is any unfair leakage from validation data to the model, in other words learning from validation data. The details of the training configurations are shown in APPENDIX.

4.1 Linear Evaluation

Linear evaluation is a common evaluation method for representation learning, such as BYOL (Grill et al., 2020). It measures the classification accuracy of a full connection layer added to a fixed embedding space to determine whether the embedding space learns meaningful features. In other words, we evaluate whether the linear separability of the embedding space can learn without labels.

While applying k-fold cross validation, the same segmented training data in representation learning is used for learning linear evaluation. The network and learning details are the same. The detailed configuration is shown in APPENDIX.

4.2 Compared Distribution

One of the roles of validation data is to monitor the training data for overfitting. Conversely, in cases where validation data cannot monitor overfitting, the following two conditions may occur:

- Training data and validation data are too close
- Validation data and the test data are too far apart

CrossSiam learns to predict the embedding space of validation data for one network as it is predicted by another network. Although this method improves accuracy, it has the risk of leaking validation data through network predictions.

To evaluate the possibility of unfair leaks, we compare embedding space of $D_{i,train}$,$D_{i,val}$, $D_{i,train}$,D_{test}, $D_{i,val}$,D_{test}.

In this study, we use Fréchet distance (FD) (Dowson and Landau, 1982) as a method to compare two different embedding distributions:

$$\begin{aligned}
\text{FD}(X, Y) &= ||\mu_X - \mu_Y||_2^2 \\
&+ Tr(\Sigma_X + \Sigma_Y + 2(\Sigma_X \Sigma_Y)^{\frac{1}{2}}) \quad (2)
\end{aligned}$$

where X, Y are embedding spaces from two different datasets, μ_X, μ_Y are the mean features of X, Y, Σ_X, Σ_Y are the covariance matrices of X, Y.

4.3 Splitting Dataset for k-Fold Cross Validation

In k-fold cross validation, the dataset is divided into k subsets. Then, if the labels in each subset are not equal, the learning is adversely affected.

In this study, when the dataset is divided by k-fold cross validation, each subset is constrained to have equal number of included classes. This allows us to separate the class inequality problem from the evaluation of the proposed method.

4.4 Dataset and Model Specifications

We employed CIFAR10 as the dataset. It contains 50,000 training data and 10,000 test data for 10 classes of images with a size 32×32. We chose ResNet-18 (He et al., 2016) as the base CNN model. We trained the model from scratch with a minibatch size of 512 for $800 \times \frac{k}{k-1}$ epochs. We include more details in the Appendix. We set 2 and 5 as the number of folds.

5 RESULTS AND DISCUSSION

5.1 Linear Evaluation

Table 1: Linear Evaluation.

network	folds	linear evaluation
ParaSiam	2	$87.99 \pm 0.12\%$
CrossSiam	2	$91.22 \pm 0.19\%$
ParaSiam	5	$91.41 \pm 0.18\%$
CrossSiam	5	$91.60 \pm 0.12\%$

We show the results of linear evaluation in Table 1. Each item shows the training model, the number of folds, and the mean and variance of the classification accuracy for k models, respectively.

We compare ParaSiam and CrossSiam. When the number of folds is two, the classification accuracy of CrossSiam is higher than that of ParaSiam. This result shows the usefulness of CrossSiam. Conversely, when the number of folds is five, CrossSiam has a slightly smaller improvement in classification accuracy than ParaSiam.

The reason why the improvement is greater in 2-fold than in 5-fold validations can be explained by the following reasons.

1. CrossSiam is especially effective when the amount of data is small
2. CrossSiam is affected by the batch size when calculating validation data

In the future, we plan to conduct experiments to prove these hypotheses.

5.2 FD

We show the results of the FD in Table 2. Each item shows the learning model, the number of folds, FD between D_{train} and D_{test}, FD between D_{train} and D_{val}, and FD between D_{val} and D_{test}, and we show the results of The ratio of FD(D_{train}, D_{val}) and FD(D_{val}, D_{test}) to FD(D_{val}, D_{test}) in Table 3.

To investigate whether validation data has lost its ability to monitor overfitting or not, we focused on the following points:

- Whether training data and validation data are too close or not, and
- Whether validation data and the test data are too far apart or not.

The first item is indicated by FD$(D_{k,train}, D_{k,val})$. The second item is indicated by FD$(D_{k,val}, D_{k,test})$.

In experiments (Table 2), FD$(D_{k,train}, D_{k,val})$ of CrossSiam is smaller than the one of ParaSiam at 2-fold validation, and FD$(D_{k,train}, D_{k,val})$ of CrossSiam is larger than the one of ParaSiam at 5-fold validation. From this, it is difficult to show the relationship between the distances of $D_{k,train}$ and $D_{k,val})$ in ParaSiam and CrossSiam at any fold.

Conversely, FD$(D_{k,val}, D_{k,test})$ of CrossSiam is larger compared to that of ParaSiam at both 2-fold and 5-fold validation. This indicates that there is a possibility of a leak from validation to network training in CrossSiam.

We should evaluate the method with FD$(D_{k,train}, D_{k,val})$ and FD$(D_{k,val}, D_{k,test})$ ratio for FD(D_{train}, D_{test}), because accuracy of classification is generally proportional to affinity between D_{train} and $D_{test})$ (Deng and Zheng, 2021). Table 3 shows that FD$(D_{k,train}, D_{k,val})$ ratio of CrossSiam is smaller compared to that of ParaSiam and FD$(D_{k,val}, D_{k,test})$ ratio of CrossSiam is larger compared to the one of ParaSiam at both 2-fold and 5-fold validation.

These results do not rule out the possibility of overfitting. Conversely, it is unclear whether the validation data can be used as a monitoring indicator when overfitting actually occurs. Decreasing FD$(D_{k,train}, D_{k,val})$ and increasing FD$(D_{k,val}, D_{k,test})$ are the requirement for overfitting. In the future, we will investigate whether $D_{k,val}$ follows $D_{k,train}$ or $D_{k,test}$ when overfitting actually occurs.

Table 2: FD(·) between each datasets.

network	folds	D_{train}, D_{test}	D_{train}, D_{val}	D_{val}, D_{test}
ParaSiam	2	0.00529	0.00497	0.00035
CrossSiam	2	0.00110	0.00032	0.00071
ParaSiam	5	0.00196	0.00186	0.00064
CrossSiam	5	0.00078	0.00044	0.00079

Table 3: FD(·) ratio for FD(D_{train}, D_{test}) between each datasets.

network	folds	D_{train}, D_{val}	D_{val}, D_{test}
ParaSiam	2	0.939	0.066
CrossSiam	2	0.289	0.642
ParaSiam	5	0.948	0.323
CrossSiam	5	0.564	1.008

6 FUTURE WORK

6.1 Training Method Adapted to k-Fold Cross Validation

In this study, k-fold cross validation is used for both CrossSiam and ParaSiam, and they are trained similarly to the method without validation data. Conversely, there are many learning methods that use validation data. For example, early stopping terminates learning when the loss or accuracy of the validation data and training data are far apart.

In CrossSiam(the proposed method), the embedding spaces of the validation data are targeted, and the in-distribution and out-of-distribution of them is available. This method cannot be used in ParaSiam (baseline), because the target data is also the training data and is likely to be judged as in-distribution. We will conduct experiments to take advantage of this feature of CrossSiam, and show greater accuracy improvement and robustness to out-of-distribution.

6.2 Multi-agents Intelligence with Different Decision Criteria

In the case of a multi-agent system such as unmanned robots and drones, it is necessary for the agents themselves to decide the behavior of swarms from camera images. If this decision is made in CrossSiam, there are two methods to improve reliability when each drone makes a decision based on a model learned by k-fold cross validation.

- Prediction of a single drone assembly by k different models.
- Prediction of k kinds of drones through each model.

The first aforementioned method improves the recognition accuracy of the model. However, all agents behave similarly; hence, if one drone misses a decision, it is highly likely that other drones will also miss the decision. The computational cost is also k times higher.

The second method does not improve the recognition accuracy of the model by itself. However, even if one drone misses a decision due to fluctuations in learning, other drones may not miss the decision. In other words, an ensemble of multiple drones becomes possible. This method can be more robust than that of an ensemble with multiple drones, which make the same decision in the same situation.

However, the system will be unreliable if it is unable to completely control the movement of the network. It is desirable to learn the ensemble so that the output of each model is as consistent as possible. The proposed method can realize an ensemble system and reduce the output of each network to a common criterion.

7 CONCLUSIONS

In this study, we propose a method to improve the reliability of multi-agents such as unmanned robots and drones by making autonomous decisions based on camera information. First, we apply k-fold cross validation to representation learning as a baseline. This method splits the dataset into k parts and performs training and evaluation based on a combination of k sub-datasets. Conversely, dividing the dataset reduces the amount of training data, which reduces the accuracy of the network. To improve the accuracy, we proposed CrossSiam. By mimicking the embedding space of each other's validation data, this method is able to train robustly and accurately.

To show the usefulness of CrossSiam, we compared it with ParaSiam, a network that simply applied k-fold cross validation to representation learning. We conducted two experiments for evaluation. The first involved linear evaluation, which measures the classification accuracy when embedding space is fixed and only 1 fully connected layer is used for supervised learning. The experimental results showed that the proposed method achieved higher accuracy than the baseline for 2-fold and 5-fold cross validation. In particular, the accuracy of 2-fold CrossSiam was much higher than that of 2-fold ParaSiam. The second involved Fréchet distance (FD), the distribution difference between each dataset like training, validation and test. The experimental results show that distance between the embeddings of training data and validation data is smaller and distance between the embeddings of validation data and test data is larger for CrossSiam than for ParaSiam. This means that, undesirably, CrossSiam has the requirement of leaking verification data to the network compared to ParaSiam. However, it is unclear whether leakage actually occurs. In the future, we will conduct experiments to see if each validation data can be used to suppress overfitting. We also show that CrossSiam can be trained on datasets with a high percentage of out-of-distribution. We will experiment to show the suitability of this approach for autonomous control of multiple drones.

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APPENDIX

Architecture

In this study, we use f_θ as ResNet-18 Encoder, ResNet-18 without the last full connection layer (Table 4), projector g_θ constructed as in Table 6, and predictor h_θ constructed as in Table 5 like in BYOL (Grill et al., 2020).

Training Details for Representation Learning

We used the SGD optimizer (Shamir and Zhang, 2013) to train model parameters θ in representation

Table 4: ResNet-18 Encoder.

Group name	Output size	Block type
conv1	32×32	$[7 \times 7, 64, \text{stride}2]$
conv2	32×32	$\begin{bmatrix} 3 \times 3, 64 \\ 3 \times 3, 64 \end{bmatrix} \times 2$
conv3	16×16	$\begin{bmatrix} 3 \times 3, 128 \\ 3 \times 3, 128 \end{bmatrix} \times 2$
conv4	8×8	$\begin{bmatrix} 3 \times 3, 256 \\ 3 \times 3, 256 \end{bmatrix} \times 2$
conv5	4×4	$\begin{bmatrix} 3 \times 3, 512 \\ 3 \times 3, 512 \end{bmatrix} \times 2$
	1×1	average pool

Table 5: Projector.

Layer name	Input size	Output size
Linear	512	2048
BN	2048	2048
ReLU	2048	2048
Linear	2048	2048
BN	2048	2048

Table 6: Predictor.

Layer name	Input size	Output size
Linear	2048	512
BN	512	512
ReLU	512	512
Linear	512	2048

learning. The base hyperparameters are listed in Table 7 with the cosine learning rate decay schedule (Loshchilov and Hutter, 2017).

Table 7: Optimizer Hyperparameters for Representation Learning.

Parameter name	Value
base learning rate	0.06
final learning rate	0.00
weight decay	0.0005
base epochs	800
batch size	512

The number of training epochs is inversely proportional to the amount of each training data of subset. In other words, the number of epochs at k-Fold is $800 \times \frac{k}{k-1}$.

Training Details for Linear Evaluation

We fixed ResNet-18 encoders with representation learning, and added full connection layers for predicting the 10 classes of CIFAR-10.

We used the SGD optimizer (Shamir and Zhang, 2013) for linear evaluation training. The base hyperparameters are listed in Table 8 with cosine learning rate decay schedule (Loshchilov and Hutter, 2017).

Table 8: Optimizer Hyperparameters for Linear Evaluation.

Parameter name	Value
base learning rate	30.0
final learning rate	0.0
weight decay	0.0
epochs	100
batch size	256