EXPLOITING MODEL CAPACITY BY CONSTRAINING WITHIN-BATCH FEATURES TO BE ORTHOGONAL

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ABSTRACT

Deeper networks with large model capacity perform better in general due to the various techniques in deep learning. But at the same time features of the large capacity network have the potential to be redundant. In this work, we propose a new regularization method to exploit given network capacity effectively. By minimizing the redundancy among in-layer filters and the correlation between in-batch features at the same time, we achieve the better performance with the same network architecture. Experiments with CIFAR-10/100 show that constraining both the in-layer filters to be orthonormal and the in-batch features to be orthogonal simultaneously is beneficial in utilizing the model capacity.

1 INTRODUCTION

Recent trend of deep learning shows deeper model performs better in general (Krizhevsky et al., 2012; Simonyan & Zisserman, 2015; He et al., 2016). This is due to the efforts to resolve vanishing/exploding gradients problem in deep models such as normalizing outputs of layers to be identical distributions (Ioffe & Szegedy, 2015), connecting layers with shortcuts to make direct paths for gradient flow (He et al., 2016), and initializing weights appropriately to prevent vanishing (or exploding) of gradients (Saxe et al., 2014; Mishkin & Matas, 2016). Although those works enabled learning of deep models, learned filters of deeper networks with large capacity are more likely to be redundant compared to shallow ones. If we use the given model capacity effectively, we can achieve better generalization with the same models.

(Xie et al., 2017) proposed a method to regularize in-layer filters to be orthonormal during training to solve the gradient vanishing/exploding problem in plain (i.e. without shortcuts) deep networks. The orthonormality among filters in layer-k makes the output features from the layer-k have small correlation with each other and enhance the diversity among the filters. However, the minimum correlation between *features* cannot be guaranteed by regularizing the in-layer *filters* to be orthonormal.

In this work, we present a method to exploit given model capacity effectively by constraining *in-batch features* to be orthogonal and *in-layer filters* to be orthonormal. Since the output features of the layer-k is generated from the input data via all of the preceding layers, it helps to regularize all the relevant filters globally. The proposed method keeps the in-batch features from the layers in a set $S_{feature}$ to be orthogonal and the filters of the layers in a set S_{filter} to be orthonormal at the same time. Experimental results show that the proposed method gives further performance benefit from the original orthonormal filter regularizer.

2 METHODOLOGY

Objective function to guarantee the orthonormality between filters in each layer can be described as,

$$L_{filter} = \frac{1}{N_l} \sum_{l \in S_{filter}} \frac{1}{n_{out}^2} ||W_l W_l^T - \mathbf{I}||_2^2, \qquad W_l \in \mathbb{R}^{n_{out} \times n_{in}}, \tag{1}$$

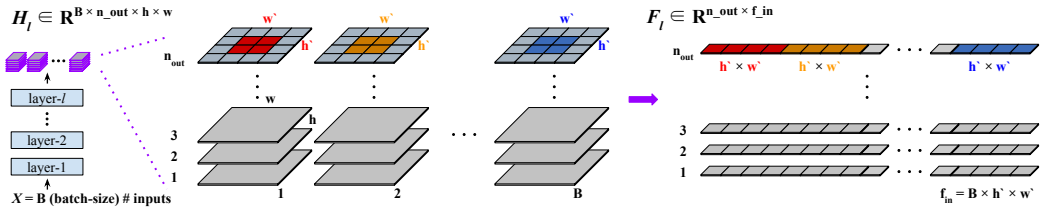

Figure 1: Transformation from the 4-dimensional feature map H_l of layer-l (left) to the 2-dimensional feature matrix F_l (right). Concatenation of center-cropped features across batch-axis defines per-filter representative features.

where S_{filter} is a set of target layers to be optimized via orthonormal filter regularizer, and N_l is the number of layers in the set. W_l, n_{in}, and n_{out} are a learnable filter bank of $l-th$ layer, the number of parameters in each filter, and the number of filters in W_l. For example, 3×3 convolutional kernel with 64 filters for the 32-channel input feature map; n_{in} and n_{out} are 288 ($= 3 \times 3 \times 32$) and 64 respectively. $\mathbf{I} \in \mathbb{R}^{n_{out} \times n_{out}}$ in Eq. (1) is an identity matrix. During training, correlation between n_{out} number of n_{in} dimensional filters is minimized by the loss function L_{filter}.

In order to define the features to be orthogonalized during training, 4-dimensional output feature map $H_l \in \mathbb{R}^{B \times n_{out} \times h \times w}$ of the target layer-l is transformed to the 2-dimensional feature matrix $F_l \in \mathbb{R}^{n_{out} \times f_{in}}$ as shown in Figure 1. B is the batch-size and f_{in} is the dimension of each transformed feature vector (i.e. each row of F_l). Since each transformed feature vector should be representative of each corresponding filter, we define the per-filter feature as a concatenation of the features of all the input examples in a batch. Each per-example feature is center-cropped as shown in Figure 1. Target loss for the orthogonality among features is as follows,

$$L_{feature} = \frac{1}{N_l} \sum_{l \in S_{feature}} \frac{1}{n_{out}^2} ||\hat{F}_l \hat{F}_l^T - \mathbf{I}||_2^2, \qquad \hat{F}_l \in \mathbb{R}^{n_{out} \times f_{in}}, \tag{2}$$

where $S_{feature}$ and N_l are a set of target layers for the in-batch feature orthogonalization and the number of layers in the set, respectively. F_l is the target in-batch feature transformed from the output feature H_l, and $\hat{F}_l$ is the unit-vectorized version of F_l (i.e. each row of $\hat{F}_l$ is a unit vector converted from corresponding row of F_l). $\hat{F}_l \hat{F}_l^T$ is a matrix with ones on a diagonal, thus the orthogonality between features of F_l is guaranteed by this loss.

Incorporating both L_{filter} and $L_{feature}$ with a task solving loss L_{task} (e.g., negative-log-likelihood for classification), total loss is described as,

$$L = (1 - \lambda_1 - \lambda_2) L_{task} + \lambda_1 L_{filter} + \lambda_2 L_{feature}, \tag{3}$$

where the loss weighting constants λ_1, λ_2, and their sum $\lambda_1 + \lambda_2$ should be in the range of [0,1).

3 Experiments

We conducted experiments on the CIFAR-10/100 datasets that have 10/100 classes with 50k/10k training/test images (Krizhevsky & Hinton, 2009). First, we experimentally confirmed that the orthonormal filter regularization is effective not only in the plain deep models but also in deep models with residual connection.[1] Based on our experiments, ResNet with both L2 and orthonormal filter regularizers is better than the model only with the orthonormal filter regularizer. For example, error rate with mean (std) of 4 trials in cifar-10; ResNet-32 with orthonormal filter regularizer only:

[1](Xie et al., 2017) also showed the effectiveness of the orthonormal filter regularization in deep networks with shorcuts; e.g., ResNet-110 with the orthonormal filter regularizer (error rate: 10.0%) is better than original ResNet-110 with L2 regularizer (13.5%), but the error rate reported in the original paper (He et al., 2016) was much smaller (6.61%).

Table 1: Classification error rates (%) of 4 trials with mean (std) on CIFAR-10/100; *Baseline* refers to the original ResNet (He et al., 2016), *Filter* refers to the orthonormal filter regularizer (only) (Xie et al., 2017), *Feature* refers to the orthogonal feature regularizer (only), and *Both* refers to both of the regularizers.

	cifar-10				cifar-100			
	ResNet-32	ResNet-56	ResNet-110	ResNet-152	ResNet-32	ResNet-56	ResNet-110	ResNet-152
Baseline	7.57 (0.207)	6.98 (0.306)	6.60 (0.340)	6.44 (0.349)	31.43 (0.211)	28.15 (0.412)	26.82 (0.531)	26.71 (0.683)
Filter	7.64 (0.128)	6.64 (0.158)	6.00 (0.097)	5.85 (0.220)	31.12 (0.519)	**27.46 (0.272)**	26.08 (0.433)	25.50 (0.166)
Feature	7.85 (0.128)	6.69 (0.129)	6.20 (0.135)	6.41 (0.265)	31.46 (0.224)	27.85 (0.127)	26.16 (0.161)	25.76 (0.157)
Both	**7.44 (0.131)**	**6.34 (0.132)**	**5.78 (0.173)**	**5.84 (0.048)**	**31.00 (0.365)**	27.61 (0.240)	**25.63 (0.181)**	**25.13 (0.270)**

8.20% (0.246), ResNet-32 with both orthonormal filter and L2 regularizers: 7.64% (0.103), so we use both regularizers for reproducing (Xie et al., 2017) in our experiments.

There are two types of residual blocks (He et al., 2016); basic block (consists of 2 consecutive convolutions), bottleneck block (consists of 3 consecutive convolutions with bottleneck structure). Bottleneck-type ResNet performs similar to the basic-type with much smaller parameters in ResNet-56, 110, 152, and the basic-type performs better in ResNet-32; e.g., bottleneck-type ResNet-56 (# params: 0.59M, error rate: 6.98%), basic-type ResNet-56 (# params: 0.86M, error rate: 6.99%). For our baseline architecture, bottleneck-type is used for ResNet-56, 110, 152 and basic-type is used for ResNet-32. Details of the architecture comparison are summarized in Appendix (Table 2 and 3).

Augmentation follows the original paper (He et al., 2016); images are zero-padded with 4 pixels on each side, randomly cropped to produce 32×32 images, flipped horizontally with probability 0.5, and normalized by subtracting channel means and dividing by channel standard deviations.

S_{filter} includes all the convolution layers and $S_{feature}$ includes all the convolution layers except for the first convolution layer, and w' and h' in Figure 1 are 2. Learning rate 0.1 is decayed by $\frac{1}{10}$ at $80-th$ and $120-th$ epoch during training until $160-th$ epoch. Weight decay constant is 0.0001 and stochastic gradient descent with momentum 0.9 is used. Based on 50k training images, performance on the 10k test images at the last ($160-th$) epoch was reported. All the experiments are conducted with PyTorch.[2]

Error rates of 4 trials with mean (std) are summarized in Table 1 (details of each model is described in the caption). $\lambda_{1,2}$ in Eq. (3) of *Baseline*, *Filter*, *Feature*, and *Both* are (0.0, 0.0), (0.25, 0.0), (0.0, 0.25), and (0.25, 0.25), respectively. *Feature* is beneficial, but worse than *Filter* in general. And *Both* performs the best. Result of *Both* implicitly shows that the source of the performance benefit in *Feature* is different from that of *Filter*. We investigated the average correlation between features with respect to each model (details are in Appendix; Table 4). In summary, orthonormality among filters helps to reduce the correlation between features but the gap between *Baseline* and *Filter* is small. The average correlation of *Both* is the lowest among the models, which is slightly lower than *Feature*; i.e. both *Filter* and *Feature* contribute complementarilly to achieve the best performance.

4 Conclusion and Future Works

We showed that constraining the in-batch features to be orthogonal and the in-layer filters to be orthonormal can help to exploit given model capacity effectively. Directly handling the output features to be orthogonal is beneficial, and it performs the best when it is equipped with the orthonormal filter regualizer. Although the proposed method is shown to be effective with the small datasets, further experimental validation with large-scale datasets is needed. Our future work includes more experimental analysis with different configurations (e.g., using convolution layers in the last residual block for $S_{feature}$ shows better performance in ResNet-152; 5.72 (0.178)) and datasets (e.g., ImageNet).

[2]https://github.com/pytorch/vision/tree/master/torchvision/models

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5 APPENDIX

Table 2 compares two residual blocks in ResNet (He et al., 2016), and the performance with the model capacity of the two types are in Table 3. Table 4 shows average correlation between features.

Table 2: ResNet architecture for CIFAR-10/100; basic block vs bottleneck block. Downsampling with stride 2 is performed by res-block2 and res-block3.

layer name	output size	basic block	bottleneck block	# blocks
init conv	32×32	3×3, 16 (stride=2)		
res-block 1	32×32	$\begin{bmatrix} 3 \times 3, 16 \\ 3 \times 3, 16 \end{bmatrix}$	$\begin{bmatrix} 1 \times 1, 16 \\ 3 \times 3, 16 \\ 1 \times 1, 64 \end{bmatrix}$	$\times n_1$
res-block 2	16×16	$\begin{bmatrix} 3 \times 3, 32 \\ 3 \times 3, 32 \end{bmatrix}$	$\begin{bmatrix} 1 \times 1, 32 \\ 3 \times 3, 32 \\ 1 \times 1, 128 \end{bmatrix}$	$\times n_2$
res-block 3	8×8	$\begin{bmatrix} 3 \times 3, 64 \\ 3 \times 3, 64 \end{bmatrix}$	$\begin{bmatrix} 1 \times 1, 64 \\ 3 \times 3, 64 \\ 1 \times 1, 256 \end{bmatrix}$	$\times n_3$
final block	1×1	avgpool, cls#-dim fc, softmax		

Table 3: Comparison of the two types; # of blocks, # of paramerters, and error rate (%) with mean (std) of 4 trials. Bottleneck-type ResNet performs similar to the basic-type ResNet with much smaller parameters.

		ResNet-32	ResNet-56	ResNet-110	ResNet-152
basic block	(n_1, n_2, n_3)	(5, 5, 5)	(9, 9, 9)	(18, 18, 18)	(25, 25, 25)
	# params	0.47M	0.86M	1.73M	2.41M
	error rate (%)	7.57 (0.207)	6.99 (0.100)	6.54 (0.203)	6.40 (0.113)
bottleneck block	(n_1, n_2, n_3)	(3, 3, 4)	(6, 6, 6)	(12, 12, 12)	(16, 16, 18)
	# params	0.38M	0.59M	1.15M	1.66M
	error rate (%)	7.80 (0.287)	6.98 (0.306)	6.60 (0.340)	6.44 (0.349)

Table 4: Average correlation between features; mean of $L_{feature}$ at the last epoch (4 trials). Orthonormality between filters in *Filter* helps to reduce the average correlation of features from *Baseline*, but the gap is small. *Both* shows the lowest correlation which is slightly lower than *Feature*.

	cifar-10				cifar-100			
	ResNet-32	ResNet-56	ResNet-110	ResNet-152	ResNet-32	ResNet-56	ResNet-110	ResNet-152
Baseline	0.121	0.103	0.143	0.147	0.101	0.089	0.113	0.136
Filter	0.114	0.096	0.110	0.118	0.091	0.084	0.099	0.111
Feature	0.034	0.039	0.040	0.041	0.026	0.040	0.042	0.045
Both	0.021	0.032	0.033	0.034	0.021	0.034	0.035	0.037