# Supplementary Material

#### 

## 459 Appendix

#### **Table of Contents**

462	A Summary of Notations					
463	В	Robust Loss Optimization in DRO	13			
64		B.1 Robust Loss Optimization	13			
65		B.2 Hyperparameter settings	14			
66	С	Theoretical Proof	14			
67		C.1 Proof of Lemma 1	14			
68		C.2 Proof of Theorem 2	15			
69	D	Experimental Details and Additional Results	16			
70		D.1 Detailed Dataset Description	16			
71		D.2 Hardware Details for Experimentation	17			
72		D.3 Single-view and Multi-view Examples	17			
73		D.4 Additional Result on Cifar10 and Cifar100	17			
74		D.5 Additional Baseline Results on TinyImageNet	17			
75		D.6 Performance from Ensemble Members	18			
76		D.7 Comparison with Common Calibration Techniques	18			
77		D.8 Ablation Study	19			
78		D.9 Parameter Size and Inference Speed	20			
79		D.10 Diversity on Sparse Sub-networks	20			
80		D.11 Qualitative Analysis	20			
1	Е	Broader Impact, Limitations, and Future Work	21			
32		E.1 Broader Impact	21			
33		E.2 Limitations and Future Works	22			
34	F	Source Code	22			
35	G	References	22			
86 87 88						

## **489** Organization of Appendix

In this appendix, we first present a table summarizing the major notations used by the main paper. Next, we provide detailed information about the training process and hyperaprameters setting. We provide the detailed proof of Lemma 1 and Theorem 2 in Section C. After that, we provide additional experimental details and results. Finally, we discuss the broader impacts, limitations, and future work of our DRE technique. The link to the source code can be found in the end of the Appendix.

## **495 A** Summary of Notations

Table 4 below shows the major notations used in the main paper. We further assign each notation into one of four major categories: dataset, DRO formulation, sparse training, and theoretical results.

Symbol Group	Notation	Description
	X	Set of training images
	Y	Set of training class labels
Detect	C	Total classes
Dataset	$\hat{y}$	Predicted class label
	N	Total number of training samples
		Dimensionality of each data sample
	$D_f$	<i>f</i> -divergence
DRO	$\eta$	Parameter controlling size of uncertainty set in DRO framework
	$ z_n $	Weight associated with $n^{th}$ data sample
	M	Number of sparse sub-networks
	<i>K</i>	Density of the given network
Sparse Training	$  \Theta  $	Parameter associated with given neural network
	$\hat{p}$	Confidence associated with predicted class
	$l(\mathbf{x}_n, \Theta)$	Loss associated with $n^{th}$ data sample
	β	Learning rate of the given network
	P	Total number of patches in each data sample
	d	Dimensionality of each patch
	$\mathbf{v}_{c,l}$	Major $l^{th}$ feature associated with class c
		Total number of features in each class class
Theoretical Results	$D_N^S$	Collection of single-view data samples
Theoretical Results	$D_N^M$	Collection of multi-view data samples
	Û Û	Collection of features
	H	Number of convolution layers
	$F_c(\mathbf{x})$	Logistic output for the $c^{th}$ class for the data sample x
	$\mathcal{P}_{\mathbf{v}_{c,l}}$	Collection of patches containing feature $\mathbf{v}_{c,l}$ in sample $\mathbf{x}_j$
	SOFT <sub>c</sub>	Softmax output for class c

Table 4: Symbols with Descriptions.

## **498 B Robust Loss Optimization in DRO**

<sup>499</sup> In this section, we first provide a detailed description on how we optimize the robust loss function in <sup>500</sup> (1). We then explain how to set the uncertainty set by choosing a proper hyperparameter.

## 501 B.1 Robust Loss Optimization

The optimization problem specified in (1) involves an inequality constraint so directly solving it may incur a higher computational overhead. Therefore, we consider a regularized version of the robust loss to train each base learner by using the following loss:

$$\mathcal{L}^{Robust} = \max_{\mathbf{z} \ge \mathbf{0}, \mathbf{z}^{\top} \mathbb{1} = 1} \sum_{n=1}^{N} z_n l_n(\Theta) - \lambda D_f\left(\mathbf{z} || \frac{\mathbb{1}}{N}\right)$$
(9)

where  $l_n(\Theta) = l(\mathbf{x}_n, \Theta)$ . Solving the above maximization problem leads to a closed-form solution for  $\mathbf{z}^*$  as shown by the following lemma: <sup>507</sup> **Lemma 3.** Assuming that  $D_f$  is the KL divergence, then solving (9) leads to the following solution

$$\mathcal{L}^{Robust} = \sum_{n=1}^{N} z_n^* l_n(\Theta) \tag{10}$$

508 where  $z_n^*$  is given by

$$z_n^* = \frac{\exp\left(\frac{l_n(\Theta)}{\lambda}\right)}{\sum_{j=1}^N \exp\left(\frac{l_j(\Theta)}{\lambda}\right)}$$
(11)

509

It can be verified that there is a one-to-one correspondence between  $\eta$  in (2) and  $\lambda$  in (9). Given their roles in the corresponding equations, a large  $\eta$  implies a small  $\lambda$  and a small  $\eta$  implies a large  $\lambda$ .

#### 512 B.2 Hyperparameter settings

The hyperparameter in the regularization term is chosen based on the difficulty of a dataset. Specifi-513 cally, for DRE, we always consider the  $\lambda \to \infty$  for the first sparse sub-network which is equivalent 514 to Expected Risk Minimization (ERM). For the second and third sub-networks, we choose this 515 hyperparameter based on the difficulty of data samples. It should be noted that we need to set higher 516 517  $\lambda$  values for more difficult datasets as difficult samples are more common on those datasets. Using 518 this notion, for Cifar10, we choose small  $\lambda$  values so that the model can focus on the difficult samples that are few. For this, we choose  $\lambda = 10$  for the second sparse sub-network and  $\lambda = 500$  for the 519 third sparse sub-network. Considering Cifar100 is more difficult, we would have more difficult 520 samples and therefore higher  $\lambda$  value is preferred. For this, we choose  $\lambda = 50$  for the second sparse 521 sub-network and  $\lambda = 500$  for the third one. In the case of TinyImageNet, we have many difficult 522 samples and therefore we choose relatively large  $\lambda$  values. Specifically, we choose  $\lambda = 100$  for the 523 second sparse sub-network and  $\lambda = 1,000,000$  for the third sparse sub-network. 524

#### 525 C Theoretical Proof

<sup>526</sup> In this section, we provide detailed proofs of the theoretical results presented in the main paper.

#### 527 C.1 Proof of Lemma 1

528 *Proof.* For  $y_n = c$ , with respect to data sample  $\{\mathbf{x}_n, y_n\}$ , the gradient can be evaluated as

$$-\nabla_{\Theta_{c,h}} l(\Theta; \mathbf{x}_n, y_n) = [1 - \text{SOFT}_c(F(\mathbf{x}_n))] \sum_{p \in [P]} \text{ReLU}[\langle \Theta_{c,h}, \mathbf{x}_n^p \rangle] \mathbf{x}_n^p$$
(12)

Assume that the given sample has a major feature  $\mathbf{v}_{c,l}$ , taking dot product with respect to  $\mathbf{v}_{c,l}$  on both side of (12) leads

$$\langle -\nabla_{\Theta_{c,h}} l(\Theta; \mathbf{x}_n, y_n), \mathbf{v}_{c,l} \rangle = [1 - \text{SOFT}_c(F(\mathbf{x}_n))] \sum_{p \in [P]} \langle \text{ReLU}[\langle \Theta_{c,h}, \mathbf{x}_n^p \rangle] \mathbf{x}_n^p, \mathbf{v}_{c,l} \rangle$$
(13)

Let's further assume that the feature set is orthonormal:  $\forall c, c', \forall l \in [L], ||\mathbf{v}_{c,l}||_2 = 1 \text{ and } \mathbf{v}_{c,l} \perp \mathbf{v}_{c',l'}$ when  $(c, l) \neq (c', l')$ . Using  $\mathbf{x}^p = a^p \mathbf{v}_{c,l} + \sum_{\mathbf{v}' \in \cup \setminus \mathbf{v}_c} \alpha^{p, \mathbf{v}'} \mathbf{v}' + \epsilon^p$  given in (4), we have

$$\langle -\nabla_{\Theta_{c,h}} l(\Theta; \mathbf{x}_n, y_n), \mathbf{v}_{c,l} \rangle = [1 - \texttt{SOFT}_c(F(\mathbf{x}_n))] \left( \sum_{p \in \mathcal{P}_{v,l}(\mathbf{x}_n)} \texttt{ReLU}[\langle \Theta_{c,h}, \mathbf{x}_n^p \rangle a^p] + \sum_{p \in [P]} \langle \epsilon^p, \mathbf{v}_{c,l} \rangle \right)$$
(14)

It should be noted that the term *i.e.*,  $\sum_{v' \in \cup \setminus \mathbf{v}_c} \alpha^{p,v'} \langle \mathbf{v}', \mathbf{v}_{c,l} \rangle$  becomes zero due to the orthogonal properties of the feature set. Let us represent the second term by  $\kappa$ :  $\sum_{p \in [P]} \langle \epsilon^p, \mathbf{v}_{c,l} \rangle = \kappa$ . Then, we have

$$\langle -\nabla_{\Theta_{c,h}} l(\Theta; \mathbf{x}_n, y_n), \mathbf{v}_{c,l} \rangle = (1 - \texttt{SOFT}_c(F(\mathbf{x}_n))) \left( \sum_{p \in \mathcal{P}_{v,l}(\mathbf{x}_n)} \texttt{ReLU}[\langle \Theta_{c,h}, \mathbf{x}_n^p \rangle a^p] + \kappa \right)$$
(15)

Furthermore, let us define  $V_{c,h,l}(\mathbf{x}_j) = \sum_{p \in \mathcal{P}_{\mathbf{v}_{c,l}}(\mathbf{x}_j)} \text{ReLU}(\langle \Theta_{c,h}, \mathbf{x}_j^p \rangle a^p)$  then above equation further reduces to following

$$\langle -\nabla_{\Theta_{c,h}} l(\Theta; \mathbf{x}_n, y_n), \mathbf{v}_{c,l} \rangle = (1 - \texttt{SOFT}_c(F(\mathbf{x}_n)))(V_{c,h,l}(\mathbf{x}_n) + \kappa)$$
(16)

Recall the above equation is the gradient with respect to the  $n^{th}$  data sample. Considering the gradient with respect to all data samples with  $y_n = c$ , and let us consider the total loss, where the weight  $z_n$  of each loss is assigned according to a distribution specified by the uncertainty set  $\mathcal{U}$ . Then, the total gradient is

$$\langle -\nabla_{\Theta_{c,h}} l(\Theta; \mathbf{X}, \mathbf{Y}), \mathbf{v}_{c,l} \rangle = \max_{\mathbf{z} \in \mathcal{U}} \sum_{n=1}^{N} z_n \left[ \mathbb{1}_{y_j = c} (V_{c,h,l}(\mathbf{x}_n) + \kappa) (1 - \mathsf{SOFT}_c(F(\mathbf{x}_n))) \right]$$
(17)

Now using the standard gradient update rule with  $\beta$  being the learning rate, we have

$$\langle \Theta_{c,h}^{t+1}, \mathbf{v}_{c,l} \rangle = \langle \Theta_{c,h}^{t}, \mathbf{v}_{c,l} \rangle + \beta \max_{\mathbf{z} \in \mathcal{U}} \sum_{n=1}^{N} z_n \left[ \mathbb{1}_{y_j=c} (V_{c,h,l}(\mathbf{x}_n) + \kappa) (1 - \mathsf{SOFT}_c(F(\mathbf{x}_n))) \right]$$
(18)

Let  $\mathbf{x}_k \in \mathcal{D}_N^S$  be the most difficult sample having  $\mathbf{v}_{c,l}$  as the main feature. Also, consider  $\mathbf{x}_n \in \mathcal{D}_N^M$ to be the easy sample with  $y_n = c, y_k = c$ . Then, we have

$$[1 - \operatorname{SOFT}_c(F(\mathbf{x}_k))] \ge [(1 - \operatorname{SOFT}_c(F(\mathbf{x}_n))], \ \forall n \in [1, N], n \neq k, y_n = c$$
(19)

<sup>545</sup> Using above property, we can write the following using (18)

$$\langle \Theta_{c,h}^{t}, \mathbf{v}_{c,l} \rangle + \beta \max_{\mathbf{z} \in \mathcal{U}} \sum_{n=1}^{N} z_{n} \left[ \mathbb{1}_{y_{j}=c} (V_{c,h,l}(\mathbf{x}_{n}) + \kappa) (1 - \mathsf{SOFT}_{c}(F(\mathbf{x}_{n}))) \right]$$

$$\leq \langle \Theta_{c,h}^{t}, \mathbf{v}_{c,l} \rangle + \beta N z_{k} (1 - \mathsf{SOFT}_{c}(F(\mathbf{x}_{k})))$$

$$(20)$$

On the r.h.s., we have  $z_n = \frac{1}{N}$  for ERM, which assigns equal weights to all samples. Under the assumption of  $N_{\mathbf{v}_{c,l}} \ll N_{\cup \setminus \mathbf{v}_{c,l}}$ , the contribution of the  $N_{\mathbf{v}_{c,l}}$  on overall gradient will be negligible. In contrast, for the DRO framework, using (11), we have

$$z_k = \frac{1}{\sum_{j=1, j \neq k}^{N} \exp\left(\frac{l_j(\Theta) - l_k(\Theta)}{\lambda}\right) + 1}$$
(21)

Since  $l_k(\Theta) > l_j(\Theta), \forall \lambda > 0, \lambda \neq \infty$ , we have  $z_k > \frac{1}{N}$ . Using r.h.s. of (20) and incorporating  $z_k = \frac{1}{N}$  for ERM and  $z_k > \frac{1}{N}$ , we have

$$\{\langle \Theta_{c,h}^t, \mathbf{v}_{c,l} \rangle + \beta (1 - \mathsf{SOFT}_c(F(\mathbf{x}_k)))\}_{ERM} \le \{\langle \Theta_{c,h}^t, \mathbf{v}_{c,l} \rangle + \beta (1 - \mathsf{SOFT}_c(F(\mathbf{x}_k)))\}_{Robust}$$
(22)

<sup>551</sup> This subsequently leads to the following:

$$\{\langle \Theta_{c,h}^t, \mathbf{v}_{c,l} \rangle\}_{Robust} > \{\langle \Theta_{c,h}^t, \mathbf{v}_{c,l} \rangle\}_{ERM}; \forall t > 0$$
(23)

<sup>552</sup> which completes the proof of Lemma 1.

#### 553 C.2 Proof of Theorem 2

Let  $\mathbf{x} \in \mathcal{D}_S^N$  from class c with  $\mathbf{v}_{c,l}$  as the main feature and  $\mathbf{v}'$  as the dominant feature learned through the memorization. Also consider  $\mathbf{v}'$  to be the main feature characterizing class k. Then for any class c', we can define the following

$$\text{SOFT}_{c'}(\mathbf{x}) = \frac{\exp(F_{c'}(\mathbf{x}))}{\sum_{j \in [C]} \exp(F_j(\mathbf{x}))}$$
(24)

In the above equation,  $F_{c'}(\mathbf{x})$  can be written as

$$F_{c'}(\mathbf{x}) = \sum_{h \in [H]} \sum_{p \in [P]} \operatorname{ReLU}[\langle \Theta_{c',h}, \mathbf{x}^p \rangle]$$
(25)

558 Substituting  $\mathbf{x}^p$  from (4), we have

$$F_{c'}(\mathbf{x}) = \sum_{h \in [H]} \sum_{p \in [P]} \operatorname{ReLU} \left[ a^p \langle \Theta_{c',h}, \mathbf{v}_{c,l} \rangle + \sum_{\mathbf{v}' \in \cup \backslash \mathbf{v}_c} \alpha^{p,\mathbf{v}'} \langle \Theta_{c',h}, \mathbf{v}' \rangle + \langle \Theta_{c',h}, \epsilon^p \rangle \right]$$
(26)

559 Substituting c' by k, we have

$$F_{k}(\mathbf{x}) = \sum_{h \in [H]} \sum_{p \in [P]} \operatorname{ReLU} \left[ a^{p} \langle \Theta_{k,h}, \mathbf{v}_{c,l} \rangle + \sum_{\mathbf{v}' in \cup \backslash \mathbf{v}_{c}} \alpha^{p,\mathbf{v}'} \langle \Theta_{k,h}, \mathbf{v}' \rangle + \langle \Theta_{k,h}, \epsilon^{p} \rangle \right]$$
(27)

In case of ERM, the  $\mathbf{v}_{c,l}$  signal is fairly weak during the training process due to  $N_{\mathbf{v}_{c,l}} \ll N_{\cup \setminus \mathbf{v}_{c,l}}$ . Therefore, the term  $\langle \Theta_{k,h}, \mathbf{v}_{c,l} \rangle$  is negligible. Also, the last term  $\langle \Theta_{k,h}, \epsilon^p \rangle$  is also small as this corresponds to the Gaussian noise. For the second term  $\exists \mathbf{v}'$  for which  $\langle \Theta_{k,h}, \mathbf{v}' \rangle$  is very high because of the spurious correlation. In contrast, for the robust loss, using Lemma 1, the model learns a stronger correlation with the true class parameter and therefore  $\langle \Theta_{c,h}, \mathbf{v}_{c,l} \rangle$  is high. As such, both terms  $\langle \Theta_{k,h}, \mathbf{v}_{c,l} \rangle$  as well as  $\langle \Theta_{k,h}, \mathbf{v}' \rangle$ ,  $\forall v'$  becomes low. As a result, we have

$$\{F_k(\mathbf{x})\}_{ERM} > \{F_k(\mathbf{x})\}_{Robust}$$
(28)

566 Substituting this inequality to (24), we have

$$\{\text{SOFT}_k(\mathbf{x})\}_{Robust} < \{\text{SOFT}_k(\mathbf{x})\}_{ERM}$$
(29)

<sup>567</sup> This completes the proof of Theorem 2.

## 568 D Experimental Details and Additional Results

In this section, we first provide a detailed description of datasets used in our experimentation followed 569 by hardware description of our experimentation. Consequently, we provide examples of single-570 view and multi-view data samples. Next, we provide additional experimental results on Cifar10 571 and Cifar100 datasets with a 15% density. After that, we provide additional baselines results on 572 573 TinyImageNet. We also compare our model performance with different calibration techniques commonly used in dense networks. Then, we perform an in-depth ablation study. Parameter size and 574 inference speed are discussed in the subsequent subsection. We also further investigate the diversity 575 of the sparse subnetworks. Finally, we provide detailed qualitative analysis to support our proposed 576 claim. 577

#### 578 D.1 Detailed Dataset Description

585

586

587

For general classification setting, we consider Cifar10, Cifar100 [12], and TinyImageNet [14] datasets.
For the out of distribution setting, we consider corrupted version of Cifar10 and Cifar100, which are
named as Cifar10-C and Cifar100-C [10], respectively. Finally, for open-set detection, we leverage
SVHN [19] as the open-set dataset. The detailed description of each dataset is given below:

- *Cifar10*. This dataset consists of total 10 classes, each consisting of 5,000 training samples and 1,000 testing (evaluation) samples. Each image is a colored image with size 32 × 32.
  - *Cifar100.* This dataset consists of 20 super classes where each super-class consists of 5 classes resulting into total 100 classes. Each class consists of 500 training samples and 100 testing samples. Each image is a colored image with size  $32 \times 32$ .
- *TinyImageNet.* The original dataset consists of 200 classes with 1,000,000 samples where each class has 500 training images, 50 validation images, and 50 test images. Each image is a colored image with size  $64 \times 64$ .
- Cifar10-C. Fifteen different types of corruptions are applied on the Cifar10 clean testing
   dataset where each corruption has 5 severity levels, ranging from 1 to 5 with 1 being least
   severe and 5 being most severe. The corruptions include Gaussian noise, shot noise, impulse
   noise, defocus blur, forsted glass blur, motion blur, zoom blur, snow, frost, fog, brightness,
   contrast, elastic, pixelate, and JPEG.



Single View (Present: Headlight, Missing: Tire, Door handle)

Headlight

O Tire

handle)



Door handle

Figure 4: Examples of single-view and multi-view samples.

(Present: Headlight, Tire, Door

- *Cifar100-C.* Similar to Cifar10-C, fifteen different corruptions are applied on the Cifar100 clean testing dataset.
- SVHN. The Street View House Numbers (SVHN) dataset consists of 10 classes with digit 1 as class 1, digit 9 as class 9 and digit 0 as class 10. These are original, variable-resolution, colored house-number images with character level bounding boxes. We use this dataset as the open-set dataset in our experimentation.

## 602 D.2 Hardware Details for Experimentation

All experimentations are conducted using NVIDIA RTX A6000 GPU with 48GB memory requiring 300 Watt power. For GPU, CUDA Version: 11.6, Driver Version: 510.108.03, and NVIDIA-SMI: 510.108.03 is used. In terms of CPU, our experimentation uses an Intel(R) Xeon(R) Gold 6326 CPU @ 2.90GHz with a 64-bit system and an x86\_64 architecture.

## 607 D.3 Single-view and Multi-view Examples

Figure 4 show the three example images, where the first image is a representative single-view data sample whereas the last two are multi-view samples. In this example, we consider three major features for cars: *i.e.*, Tire, Headlight, and Door handle. As only headlight feature is present in the first image, it belongs to the single-view category. For the second and third images, multiple features are presented and therefore we regard those images as multi-view data samples.

## 613 D.4 Additional Result on Cifar10 and Cifar100

Table 5 shows the experimental result on Cifar10 and Cifar100 datasets with a 15% density. As shown, the proposed technique has a far superior performance in terms of the ECE score compared to the competitive baselines. This is consistent with the results with a 9% density as presented in the main paper, which further justifies the effectiveness of our proposed technique.

## 618 D.5 Additional Baseline Results on TinyImageNet

As mentioned in the main paper, the computational 619 issue (i.e., memory overflow) makes it impossible to 620 run sparse learning techniques *i.e.*, CigL [15], DST 621 Ensemble [17], and Sup-ticket [30] on the ResNet101 622 and WideResNet101 architectures to make a fair com-623 parison. Therefore, in this section, we pick a lower 624 capacity model (ResNet50) and compare the perfor-625 mance. Even for the ResNet50 architecture, CigL 626 still runs into the memory overflow issue with a batch 627

Table 6: Additional baseline results on Tiny-ImageNet using ResNet50 with  $\mathcal{K} = 15\%$ .

Training Type	Approach	$\mathcal{ACC}$	ECE
Sparse Training	DST Ensemble Sup-ticket	72.00 68.68	2.94 10.96
Mask Training	DRE	71.57	1.51

size of 128. Furthermore, lowering the batch size (*e.g.*, 16) makes the training process extremely

		Cif	ar10	Cifar100			
Training Type	Approach	ResNet50	ResNet101	ResNet101	ResNet152		
		ACC ECE	ACC ECE	ACC ECE	ACC ECE		
	Dense <sup>†</sup>	94.82 5.87	95.12 5.99	76.40 16.89	77.97 16.73		
Dense Training	L1 Pruning LTH DLTH Mixup	93.88 5.69 92.97 4.03 95.15 6.21 93.22 4.02	94.23 5.88 93.15 5.69 95.65 6.96 93.38 5.68	75.5315.5274.3615.1377.9816.2474.4815.10	75.8315.7874.7715.2278.2316.5474.6815.16		
Sparse Training	CigL DST Ensemble Sup-ticket	92.25 4.67 89.57 2.10 94.65 3.20	93.34 4.59 88.64 1.34 94.95 3.09	77.88 10.16 64.57 9.76 78.68 10.16	77.27 10.62 64.75 9.27 78.95 10.32		
Mask Training	AdaBoost EP SNE <b>DRE</b>	94.07 5.65 94.41 3.90 94.85 3.05 94.87 <b>1.71</b>	94.76 5.14 94.42 4.07 94.96 3.18 94.74 <b>1.34</b>	75.9823.5575.6614.7976.8211.12 <b>75.864.90</b>	76.2824.2776.0514.7977.2311.6376.46 <b>5.81</b>		

Table 5: Accuracy and ECE performance with 15% density for Cifar10 and Cifar100 Dataset.

slow even using a 48*Gb* GPU, where each training epoch takes more than half an hour, making model training extremely difficult. Therefore, we did not report the performance of CigL. It should be noted that CigL can be trained on Cifar10 and Cifar100 because of lower dimension of the input images and we have already reported its performance in the main paper. Table 6 shows the performance of DRE along with those from DST Ensemble and Sup-ticket on ResNet50. It is clear that DRE achieves better performance compared to these baselines.

#### 635 D.6 Performance from Ensemble Members

Table 7: Different subnetworks performance on Cifar100 Dataset.

We investigate how performance varies in different 636 sparse sub-networks. We use Cifar100 as an example 637 and Table 7 report the individual sub-network perfor-638 mance on both accuracy and ECE. While each sparse 639 sub-network is a relatively weaker learner (which 640 is expected), they contribute to the final ensemble 641 model in a complementary way, leading to a better 642 ECE score as well as accuracy. 643

Subnetworks	Resl	Net101	ResNet152		
	$\mathcal{ACC}$	ECE	$\mathcal{ACC}$	ECE	
Subetwork 1 (3%)	68.22	14.35	69.65	13.31	
Subetwork 2 (3%)	69.03	1.39	70.00	3.39	
Subetwork 3 (3%) DRE	72.86 74.68	11.96 <b>1.20</b>	70.24 74.37	14.78 2.09	

#### 644 D.7 Comparison with Common Calibration Techniques

In this section, we investigate whether existing calibration techniques designed for training dense 645 networks can be leveraged to further improve the calibration performance of sparse networks. How-646 647 ever, most of these techniques (e.g., temperature scaling and mix-n-match) are post hoc techniques, 648 which require a separate validation set to fine-tune the parameters. This means we need to further divide the training data into training and validation sets, which may negatively impact the general-649 ization capability of the trained model (due to less training data). To make a comparison, we pick 650 Temperature Scaling (TS) [9], Label Smoothing (LS) [27], and a few other techniques proposed in 651 [31], including Ensemble Temperature Scaling (ETS) and Isotonoic Regression One vs All combined 652 with Temperature Scaling (IROvA-TS). We apply these calibration techniques on the top of the EP 653 algorithm. Specifically, as LS does not require a separate validation set, we train it on the full training 654 dataset using the LS loss (with  $\epsilon = 0.1$ ). Other calibration techniques require a separate validation 655 set and therefore we divide training data into training and validation with a 80:20 ratio. EP (No 656 Validation) uses the full training dataset whereas EP (Validation) is trained using 80% of the training 657 data. Once the model is trained with 80% of training data using EP, we further calibrate it using the 658 aforementioned calibration techniques. Table 8 shows the results. There are two key observations: 659 (i) the classification accuracy decreases for all calibration techniques at the expense of improving 660 calibration performance as they require a separate validation set, and (ii) DRE achieves the best ECE 661 in all cases, which further justifies its strong calibration performance. 662

	Ci	far10	Cifar100			
Approach	ResNet50	ResNet101	ResNet101	ResNet152		
	ACC ECE	ACC ECE	ACC ECE	ACC ECE		
TS	93.42 0.96	93.42 1.37	73.06 1.72	73.40 2.45		
ETS	93.42 0.97	93.42 1.37	73.06 1.76	73.40 2.40		
IROvA-TS	89.90 1.45	88.69 0.89	60.87 1.56	60.77 2.86		
LS	94.06 7.56	94.21 7.41	75.96 9.36	76.40 7.71		
EP (No Validation)	94.20 3.97	94.35 4.03	75.05 14.62	75.68 14.41		
EP (Validation)	93.42 4.46	93.42 4.83	73.06 15.56	73.40 15.88		
DRE	94.60 <b>0.7</b>	94.28 <b>0.7</b>	74.68 1.20	74.37 2.09		

Table 8: Different calibration techniques on the top of EP Algorithm with  $\mathcal{K} = 9\%$ .



Figure 5: (a-b) Impact of  $\lambda$  on ECE using ResNet101 architecture on Cifar100 dataset.

Table 9: ACC and ECE with different: (a) backbones and (b) number of subnetworks.

Approach	WideResNet28-10	ViT	
- pprouein	ACC ECE	ACC ECE	
EP	94.12 4.53	86.16 10.01	
DRE	93.98 <b>1.93</b>	85.53 <b>4.18</b>	

(a) Different backbones on Cifar10 Dataset.

(b) Different M values on Cifar10 with  $\mathcal{K} = 15\%$ .

#### 663 D.8 Ablation Study

In this section, we first show the impact of  $\lambda$  values on the prediction and calibration performance. We then investigate how the size of the ensemble affects it calibration performance. Finally, we show the effectiveness of the proposed technique as we vary the backbones. In addition to the backbones used in the main paper, we will further evaluate two other commonly used backbones, including WideResNet28 and Vision Transformer (ViT) [5] as backbones.

**Impact of the uncertainty set size.** For simplicity, we always keep one sparse sub-network in our framework to be with  $\lambda_1 \rightarrow \infty$ . The ECE performance with respect to different sets of  $\lambda$  value for the remaining sub-networks is shown using the heatmap given in Figure 5 (a-b). As can be seen, it is important to choose  $\lambda_2$  and  $\lambda_3$  with very distinct values to achieve a low calibration error.

**Performance analysis of different backbones.** Table 9 (a) reports the performance of Cifar10 from 673 both DRE and EP using different backbone architectures. In case of WideResNet28-10, the calibration 674 error is low without sacrificing the accuracy. It also demonstrates that the superior performance of 675 DRE is not limited to a specific backbone. In case of ViT, DRE still achieves a much lower calibration 676 error than EP. However, using ViT as a backbone, the accuracy from both EP and DRE is lower and 677 ECE is higher than other backbones. Existing studies show that without pretraining, the lack of useful 678 inductive biases for ViT can cause performance drop [1]. Since no pretraining is conducted in both 679 EP and DRE, it causes a lower accuracy (and a higher ECE). 680

Impact of number of sparse-sub-networks. In this analysis, we study the impact of number of sparse sub-networks. It should be noted that our work is not limited only for M = 3. We can instead increase the M value. For example, Table 9 (b) shows the performance for ensemble model with M = 5, where each sub-network is trained with  $\mathcal{K} = 3\%$  leading to a total  $\mathcal{K} = 15\%$ . We also show the performance with M = 3, where each sub-network is trained with  $\mathcal{K} = 5\%$ . As can be seen, if there is a sufficient learning capacity for each sub-network, the ECE score can further improve with the increase of M.

#### 688 D.9 Parameter Size and Inference Speed

Table 10: Parameter size and inference speed.

We compare parameter size and inference speed of different types of sparse networks. Table 10 shows the FLOPS along with number of parameters associated with each technique. As can be seen, the proposed DRE has a comparable parameter size as that of the sparse network en-

Approach	F	ResNet50	ResNet101		
	Params	Flops ( $\times 10^9$ )	Params	Flops ( $\times 10^9$ )	
Dense <sup>†</sup>	23.6M	4.14	42.5M	7.88	
SNE	3.5M	1.31	6.3M	2.53	
DRE	3.5M	1.31	6.3M	2.53	

semble. In terms of computational times, our approach is comparable to the sparse network ensemble.

<sup>696</sup> Compared to a dense network, our technique has a much smaller parameter size with less FLOPS.

#### 697 D.10 Diversity on Sparse Sub-networks

To justify our claim that our technique ensures the diverse sparse sub-networks, we adapt the disagreement metric  $(d_{dist})$  from [17]. This metric measures the disagreement among sub-networks in terms of class label prediction. Table 11 below shows the results for Cifar10 and Cifar100 datasets. As shown, compared to Sparse Network Ensemble, DRE achieves higher disagreement which implies that the sparse sub-networks are more diverse.

Table 11: Accuracy, ECE, and prediction disagreement performance with a  $\mathcal{K} = 15\%$  density.

	Cifar10					Cifar100						
Approach	ResNet50		ResNet101		ResNet101		ResNet152		52			
	$\mathcal{ACC}$	ECE	$d_{dist}$	$\mathcal{ACC}$	ECE	$d_{dist}$	ACC	ECE	$d_{dist}$	$\mathcal{ACC}$	ECE	$d_{dist}$
SNE	94.85	3.05	0.048	94.96	3.18	0.049	76.82	11.12	0.20	77.23	11.63	0.20
DRE (Ours)	94.87	1.71	0.088	94.74	1.34	0.069	75.86	4.90	0.24	76.46	5.81	0.24

#### 703 D.11 Qualitative Analysis

In this section, we provide illustrative examples to further justify the proposed DRE is better calibrated 704 compared to existing baselines. Figure 6 (a)-(d) show the confidence values for the wrongly classified 705 samples using different baselines. As can be seen, all of the baselines suffer from the overfitting 706 issue, resulting into the incorrect predictions with high confidence. In contrast, as shown in Figure 6 707 (e)-(f), the sparse sub-networks provide the confidence values in different ranges, where sub-network 708 in (a) is learned from representative samples and (c) from the difficult ones. As these sub-networks 709 are complementary with each other, the DRE has a much better confidence distribution for both the 710 correct as well as incorrect samples. Figure 7 shows the confidence score of correctly classified 711 data samples from the CIFAR100 dataset with different techniques. As shown, our DRE technique 712 remains confident on the correct data samples while being not confident on the incorrect data samples. 713 This result shows our approach is well calibrated and trustworthy compared with the competitive 714

baselines. In summary, our proposed technique remains uncertain for incorrect samples while being
 confident on the correct samples resulting in a much improved calibration.



(e) DRO sparse Network 1 (f) DRO sparse network 2 (g) DRO sparse network 3 (h) DRE

Figure 6: Confidence scores of incorrectly classified samples in CIFAR100 with ResNet101



(1) D RO sparse network 1 (1) D RO sparse network 2 (g) D RO sparse network 3 (1) D RE

Figure 7: Confidence scores of correctly classified samples in CIFAR100 with ResNet101

## 717 E Broader Impact, Limitations, and Future Work

In this section, we first describe the potential broader impacts of our work. We then discuss the limitations and identify some possible future directions.

## 720 E.1 Broader Impact

Sparse network training provides a highly promising way to significantly reduce the computational cost for training large-scale deep neural networks without sacrificing their predictive power. Besides energy savings, it also opens the gate for deploying deep neural networks to lightweight computing or edge devices that can further broaden the applications of AI in more diverse and resource constrained settings. The proposed robust ensemble framework provides a general solution to achieve calibrated

training of deep learning models. As a result, the trained model is expected to provide more reliable uncertainty predictions, which could be an important step towards using AI in safety-critical domains.

### 728 E.2 Limitations and Future Works

As an ensemble model, DRE involves multiple base learners (*i.e.*, sparse sub-networks). Consequently, 729 it may lead to more computational overhead. This could create issues for real-time application as 730 during the inference time, the input needs to be passed through all base learners to get the final 731 output, which can slow down the prediction speed. A straightforward way to speed up the inference 732 process is to execute all the base learners in parallel, which still incurs additional computational 733 overhead. One interesting future direction is to investigate knowledge distillation and train a single 734 sparse network from the ensemble model. Theoretical evidence [1] shows that knowledge distillation 735 has the potential to largely maintain the ensemble performance while providing a promising way to 736 train a single sparse network with an even higher sparsity level and improved inference speed. 737

## 738 F Source Code

<sup>739</sup> For the source code of this paper, please click here.

## 740 G References

- [1]. Dosovitskiy et al. An Image is Worth 16x16 Words: Transformers for Image Recognition at
- 742 Scale. ICLR2021.
- 743