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anyvision.

Paper Reading: deep feature space (without retraining/fine-tuning)

1. Detection of abnormal testing samples (OOD) &

2. Robust inference (removing noisy training examples)

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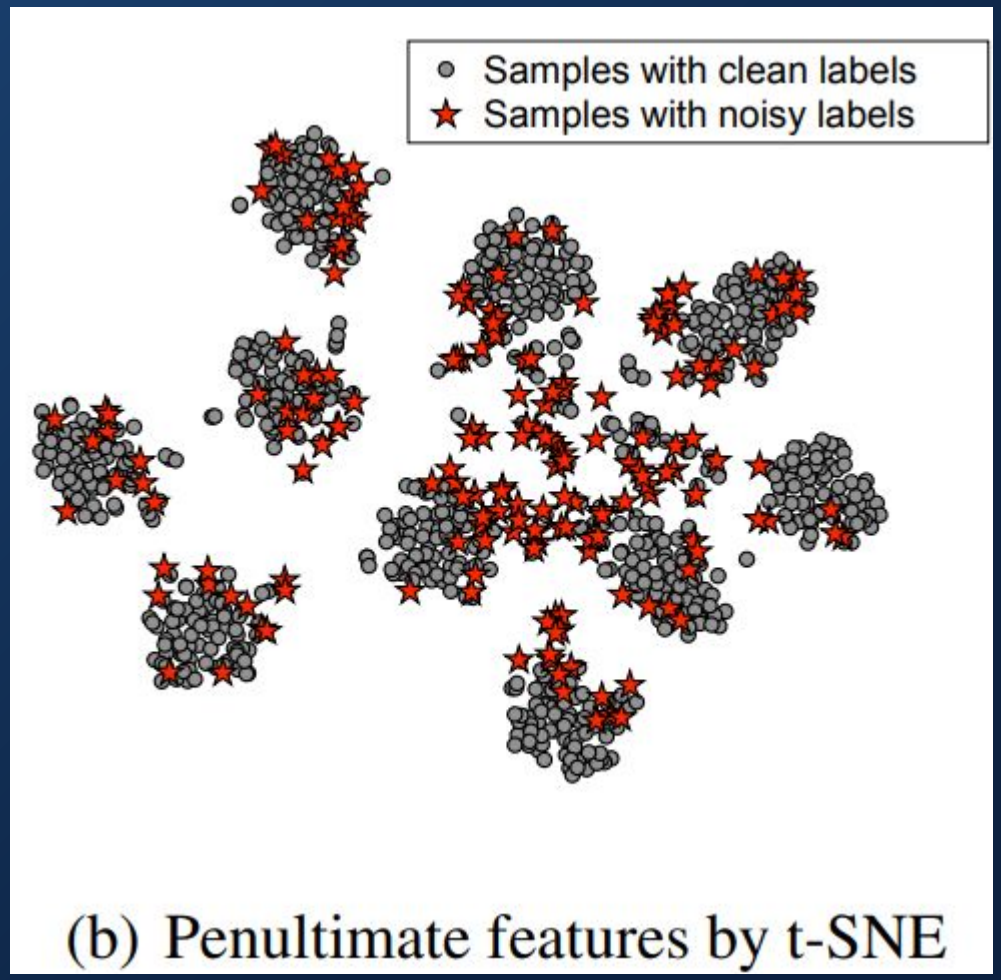
09/08/2019

Papers

NeurIPS-18: A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks

ICML-19: Robust Inference via Generative Classifiers for Handling Noisy Labels

Abnormal/OOD/Adversarial/Noisy examples are related



- Without fitting/using noisy training samples:
  Robust training/learning, i.e., without fitting those abnormal examples, outliers, examples with noisy labels, etc.
  Robust Inference: without relying on them for predicting, e.g., generative classifier, ICML-19.

- Without predicting abnormal testing samples:
  Predictive uncertainty (maximum value of posterior distribution).
  Know the unknown: abstain from predicting (Out-of-distribution detection)

Objective & Challenge of OOD Detection

- Objective: Detecting test samples drawn sufficiently far away from the training distribution statistically or adversarially is a fundamental requirement for deploying a good classifier in many real-world machine learning applications.

- Challenge: Deep neural networks with the softmax classifier are known to produce highly overconfident posterior distributions even for such abnormal samples.

Lee et al. A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks. NeurIPS, 2018

Contributions of Lee et al. NeurIPS 2018

- Contribution 1: most prior methods have been evaluated for detecting either out-of-distribution or adversarial samples, but not both.
- Contribution 2: more robust in harsh cases, e.g., when the training dataset has noisy labels or small number of samples.
- Contribution 3: broader usage by applying it to class-incremental learning
- More robust in the choice of its hyperparameters as well as against extreme scenarios

Lee et al. A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks. NeurIPS, 2018

Introduction: basic idea, metric, empirical results

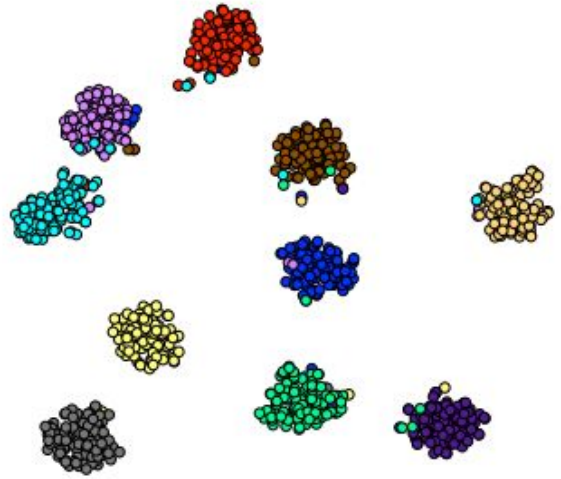
- High-level idea: the probability density of test sample on feature spaces (low- and upper-level) using the concept of a “generative” (distance-based) classifier.

- We define the confidence score using the Mahalanobis distance with respect to the closest class conditional distribution, where its parameters are chosen as empirical class means and tied empirical covariance of training samples.

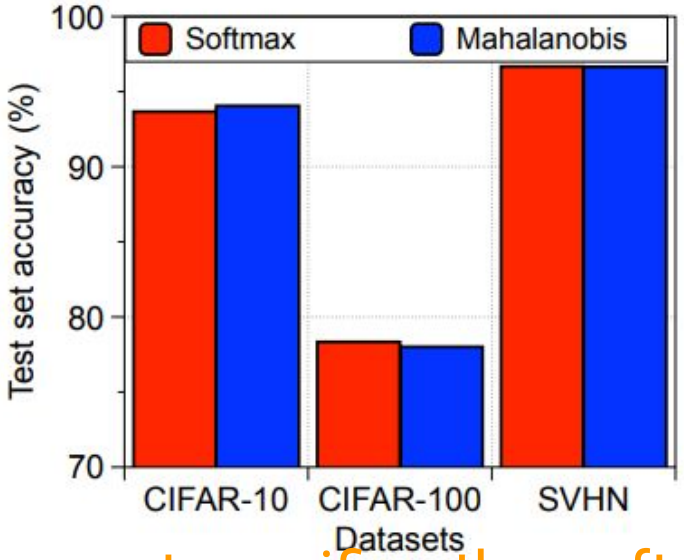
- Empirical Results: 1) generative classifier does not sacrifice the softmax classification accuracy; 2) its confidence score outperforms softmax-based ones very strongly across multiple other tasks: detecting OOD samples, detecting adversarial samples and class-incremental learning.

Lee et al. A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks. NeurIPS, 2018

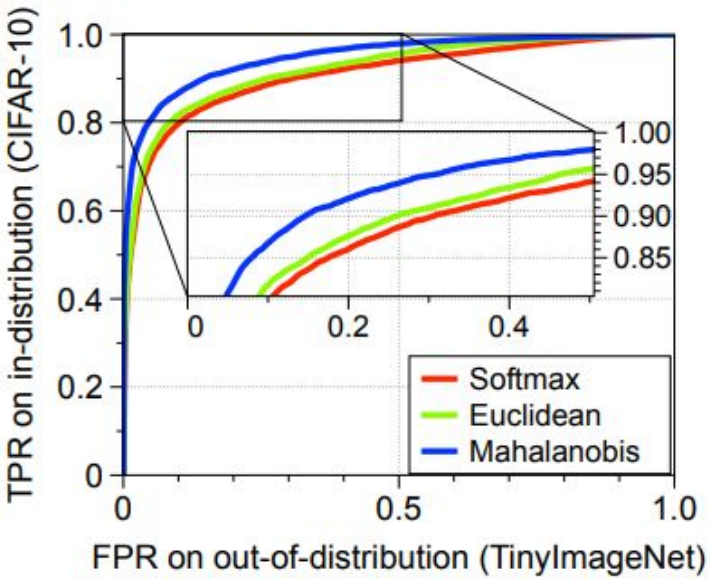
Comparison of classification accuracy & ROC curve



(a) Visualization by t-SNE



(b) Classification accuracy



(c) ROC curve

does not sacrifice the softmax classification accuracy

Figure 1: Experimental results under the ResNet with 34 layers. (a) Visualization of final features from ResNet trained on CIFAR-10 by t-SNE, where the colors of points indicate the classes of the corresponding objects. (b) Classification test set accuracy of ResNet on CIFAR-10, CIFAR-100 and SVHN datasets. (c) Receiver operating characteristic (ROC) curves: the x-axis and y-axis represent the false positive rate (FPR) and true positive rate (TPR), respectively.

Lee et al. A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks. NeurIPS, 2018

Algorithm 1: Confidence score of positive (in-distribution) examples

- Class-conditional Gaussian distributions with a tied covariance:

$$P\left(f(\mathbf{x})|y=c\right) = \mathcal{N}\left(f(\mathbf{x})|\mu_c, \mathbf{\Sigma}\right)$$

$$\widehat{\mu}_c = \frac{1}{N_c}\sum_{i:y_i=c} f(\mathbf{x}_i), \quad \widehat{\mathbf{\Sigma}} = \frac{1}{N}\sum_{c}\sum_{i:y_i=c}\left(f(\mathbf{x}_i)-\widehat{\mu}_c\right)\left(f(\mathbf{x}_i)-\widehat{\mu}_c\right)^\top$$

Algorithm 1 Computing the Mahalanobis distance-based confidence score.

Input: Test sample $\mathbf{x}$, weights of logistic regression detector α_ℓ, noise ε and parameters of Gaussian distributions $\{\widehat{\mu}_{\ell,c}, \widehat{\mathbf{\Sigma}}_\ell : \forall \ell, c\}$

Initialize score vectors: $\mathbf{M}(\mathbf{x}) = [M_\ell : \forall \ell]$

for each layer $\ell \in 1, \ldots, L$ **do**

Find the closest class: $\widehat{c} = \arg\min_c \left(f_\ell(\mathbf{x}) - \widehat{\mu}_{\ell,c}\right)^\top \widehat{\mathbf{\Sigma}}_\ell^{-1} \left(f_\ell(\mathbf{x}) - \widehat{\mu}_{\ell,c}\right)$

Add small noise to test sample: $\widehat{\mathbf{x}} = \mathbf{x} - \varepsilon \text{sign}\left(\nabla_{\mathbf{x}} \left(f_\ell(\mathbf{x}) - \widehat{\mu}_{\ell,\widehat{c}}\right)^\top \widehat{\mathbf{\Sigma}}_\ell^{-1} \left(f_\ell(\mathbf{x}) - \widehat{\mu}_{\ell,\widehat{c}}\right)\right)$

Computing confidence score: $M_\ell = \max_c -\left(f_\ell(\widehat{\mathbf{x}}) - \widehat{\mu}_{\ell,c}\right)^\top \widehat{\mathbf{\Sigma}}_\ell^{-1} \left(f_\ell(\widehat{\mathbf{x}}) - \widehat{\mu}_{\ell,c}\right)$

end for

return Confidence score for test sample $\sum_\ell \alpha_\ell M_\ell$

Input pre-processing

Feature ensemble

The performance of features from different levels

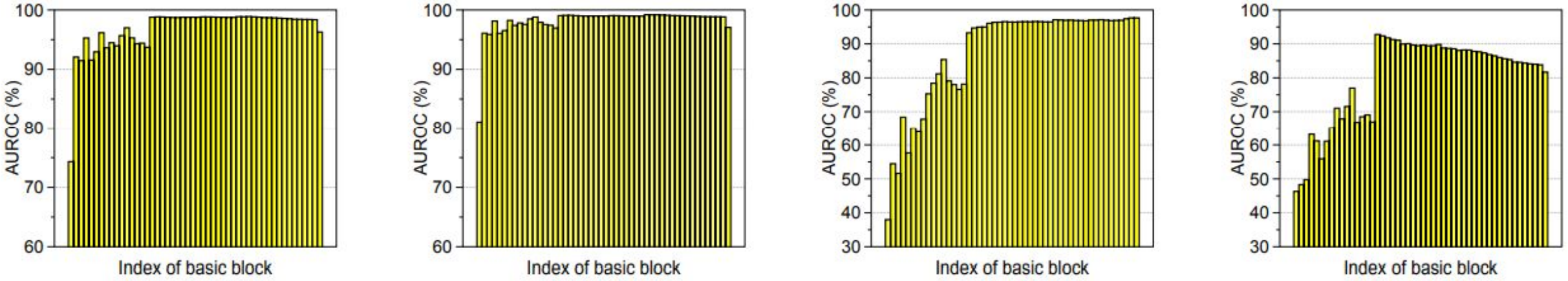


Figure 2: AUROC (%) of threshold-based detector using the confidence score in (2) computed at different basic blocks of DenseNet trained on CIFAR-10 dataset. We measure the detection performance using (a) TinyImageNet, (b) LSUN, (c) SVHN and (d) adversarial (DeepFool) samples.

Lee et al. A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks. NeurIPS, 2018

Feature ensemble strategy motivated by Figure 2

- We choose the weight of each layer by training a logistic regression detector using validation samples.

- We remark that such weighted averaging of confidence scores can prevent the degradation on the overall performance even in the case when the confidence scores from some layers are not effective: the trained weights (using validation) would be nearly zero for those ineffective layers.

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OOD Detection Results and ablation study

Method	Feature ensemble	Input pre-processing	TNR at TPR 95%	AUROC	Detection accuracy	AUPR in	AUPR out
Baseline [13]	-	-	32.47	89.88	85.06	85.40	93.96
ODIN [21]	-	-	86.55	96.65	91.08	92.54	98.52
Mahalanobis (ours)	-	-	54.51	93.92	89.13	91.56	95.95
	-	✓	92.26	98.30	93.72	96.01	99.28
	✓	-	91.45	98.37	93.55	96.43	99.35
	✓	✓	**96.42**	**99.14**	**95.75**	**98.26**	**99.60**

Table 1: Contribution of each proposed method on distinguishing in- and out-of-distribution test set data. We measure the detection performance using ResNet trained on CIFAR-10, when SVHN dataset is used as OOD. All values are percentages and the best results are indicated in bold.

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Robustness against validation data for hyper-params optimisation

In-dist (model)	OOD	Validation on OOD samples			Validation on adversarial samples		
		TNR at TPR 95%	AUROC	Detection acc.	TNR at TPR 95%	AUROC	Detection acc.
		Baseline [13] / ODIN [21] / Mahalanobis (ours)			Baseline [13] / ODIN [21] / Mahalanobis (ours)		
CIFAR-10 (DenseNet)	SVHN	40.2 / 86.2 / **90.8**	89.9 / 95.5 / **98.1**	83.2 / 91.4 / **93.9**	40.2 / 70.5 / **89.6**	89.9 / 92.8 / **97.6**	83.2 / 86.5 / **92.6**
	TinyImageNet	58.9 / 92.4 / **95.0**	94.1 / 98.5 / **98.8**	88.5 / 93.9 / **95.0**	58.9 / 87.1 / **94.9**	94.1 / 97.2 / **98.8**	88.5 / 92.1 / **95.0**
	LSUN	66.6 / 96.2 / **97.2**	95.4 / 99.2 / **99.3**	90.3 / 95.7 / **96.3**	66.6 / 92.9 / **97.2**	95.4 / 98.5 / **99.2**	90.3 / 94.3 / **96.2**
CIFAR-100 (DenseNet)	SVHN	26.7 / 70.6 / **82.5**	82.7 / 93.8 / **97.2**	75.6 / 86.6 / **91.5**	26.7 / 39.8 / **62.2**	82.7 / 88.2 / **91.8**	75.6 / 80.7 / **84.6**
	TinyImageNet	17.6 / 42.6 / **86.6**	71.7 / 85.2 / **97.4**	65.7 / 77.0 / **92.2**	17.6 / 43.2 / **87.2**	71.7 / 85.3 / **97.0**	65.7 / 77.2 / **91.8**
	LSUN	16.7 / 41.2 / **91.4**	70.8 / 85.5 / **98.0**	64.9 / 77.1 / **93.9**	16.7 / 42.1 / **91.4**	70.8 / 85.7 / **97.9**	64.9 / 77.3 / **93.8**
SVHN (DenseNet)	CIFAR-10	69.3 / 71.7 / **96.8**	91.9 / 91.4 / **98.9**	86.6 / 85.8 / **95.9**	69.3 / 69.3 / **97.5**	91.9 / 91.9 / **98.8**	86.6 / 86.6 / **96.3**
	TinyImageNet	79.8 / 84.1 / **99.9**	94.8 / 95.1 / **99.9**	90.2 / 90.4 / **98.9**	79.8 / 79.8 / **99.9**	94.8 / 94.8 / **99.8**	90.2 / 90.2 / **98.9**
	LSUN	77.1 / 81.1 / **100**	94.1 / 94.5 / **99.9**	89.1 / 89.2 / **99.3**	77.1 / 77.1 / **100**	94.1 / 94.1 / **99.9**	89.1 / 89.1 / **99.2**
CIFAR-10 (ResNet)	SVHN	32.5 / 86.6 / **96.4**	89.9 / 96.7 / **99.1**	85.1 / 91.1 / **95.8**	32.5 / 40.3 / **75.8**	89.9 / 86.5 / **95.5**	85.1 / 77.8 / **89.1**
	TinyImageNet	44.7 / 72.5 / **97.1**	91.0 / 94.0 / **99.5**	85.1 / 86.5 / **96.3**	44.7 / 69.6 / **95.5**	91.0 / 93.9 / **99.0**	85.1 / 86.0 / **95.4**
	LSUN	45.4 / 73.8 / **98.9**	91.0 / 94.1 / **99.7**	85.3 / 86.7 / **97.7**	45.4 / 70.0 / **98.1**	91.0 / 93.7 / **99.5**	85.3 / 85.8 / **97.2**
CIFAR-100 (ResNet)	SVHN	20.3 / 62.7 / **91.9**	79.5 / 93.9 / **98.4**	73.2 / 88.0 / **93.7**	20.3 / 12.2 / **41.9**	79.5 / 72.0 / **84.4**	73.2 / 67.7 / **76.5**
	TinyImageNet	20.4 / 49.2 / **90.9**	77.2 / 87.6 / **98.2**	70.8 / 80.1 / **93.3**	20.4 / 33.5 / **70.3**	77.2 / 83.6 / **87.9**	70.8 / 75.9 / **84.6**
	LSUN	18.8 / 45.6 / **90.9**	75.8 / 85.6 / **98.2**	69.9 / 78.3 / **93.5**	18.8 / 31.6 / **56.6**	75.8 / 81.9 / **82.3**	69.9 / 74.6 / **79.7**
SVHN (ResNet)	CIFAR-10	78.3 / 79.8 / **98.4**	92.9 / 92.1 / **99.3**	90.0 / 89.4 / **96.9**	78.3 / 79.8 / **94.1**	92.9 / 92.1 / **97.6**	90.0 / 89.4 / **94.6**
	TinyImageNet	79.0 / 82.1 / **99.9**	93.5 / 92.0 / **99.9**	90.4 / 89.4 / **99.1**	79.0 / 80.5 / **99.2**	93.5 / 92.9 / **99.3**	90.4 / 90.1 / **98.8**
	LSUN	74.3 / 77.3 / **99.9**	91.6 / 89.4 / **99.9**	89.0 / 87.2 / **99.5**	74.3 / 76.3 / **99.9**	91.6 / 90.7 / **99.9**	89.0 / 88.2 / **99.5**

Table 2: Distinguishing in- and out-of-distribution test set data for image classification under various validation setups. All values are percentages and the best results are indicated in bold.

Robustness against harsh training data

(Since our method utilizes empirical class mean and covariance of training samples, there is a caveat such that it can be affected by the properties of training data.)

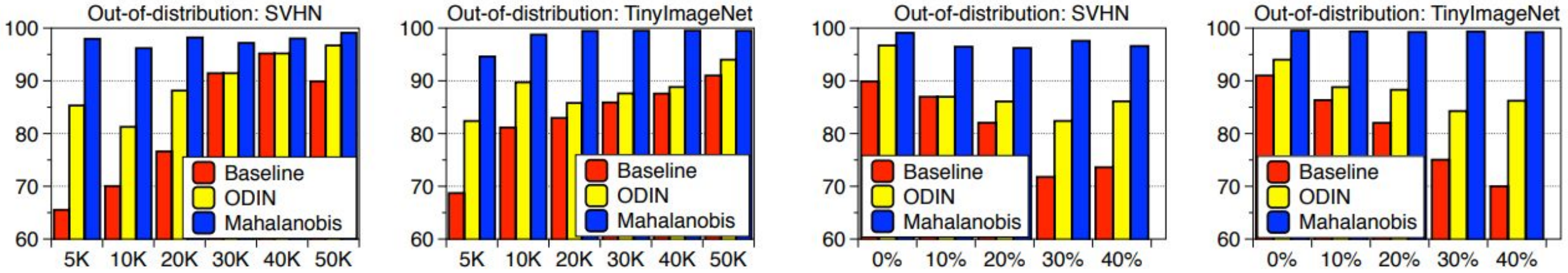

Figure 3: Comparison of AUROC (%) under extreme scenarios: (a) small number of training data, where the x-axis represents the number of training data. (b) Random label is assigned to training data, where the x-axis represents the percentage of training data with random label.

Lee et al. A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks. NeurIPS, 2018

Detecting adversarial samples

Model	Dataset (model)	Score	Detection of known attack				Detection of unknown attack			
			FGSM	BIM	DeepFool	CW	FGSM (seen)	BIM	DeepFool	CW
DenseNet	CIFAR-10	KD+PU [7]	85.96	96.80	68.05	58.72	85.96	3.10	68.34	53.21
		LID [22]	98.20	99.74	**85.14**	80.05	98.20	94.55	70.86	71.50
		Mahalanobis (ours)	**99.94**	**99.78**	83.41	**87.31**	**99.94**	**99.51**	**83.42**	**87.95**
	CIFAR-100	KD+PU [7]	90.13	89.69	68.29	57.51	90.13	66.86	65.30	58.08
		LID [22]	99.35	98.17	70.17	73.37	99.35	68.62	69.68	72.36
		Mahalanobis (ours)	**99.86**	**99.17**	**77.57**	**87.05**	**99.86**	**98.27**	**75.63**	**86.20**
	SVHN	KD+PU [7]	86.95	82.06	89.51	85.68	86.95	83.28	84.38	82.94
		LID [22]	99.35	94.87	91.79	94.70	99.35	92.21	80.14	85.09
		Mahalanobis (ours)	**99.85**	**99.28**	**95.10**	**97.03**	**99.85**	**99.12**	**93.47**	**96.95**
ResNet	CIFAR-10	KD+PU [7]	81.21	82.28	81.07	55.93	83.51	16.16	76.80	56.30
		LID [22]	99.69	96.28	88.51	82.23	99.69	95.38	71.86	77.53
		Mahalanobis (ours)	**99.94**	**99.57**	**91.57**	**95.84**	**99.94**	**98.91**	**78.06**	**93.90**
	CIFAR-100	KD+PU [7]	89.90	83.67	80.22	77.37	89.90	68.85	57.78	73.72
		LID [22]	98.73	96.89	71.95	78.67	98.73	55.82	63.15	75.03
		Mahalanobis (ours)	**99.77**	**96.90**	**85.26**	**91.77**	**99.77**	**96.38**	**81.95**	**90.96**
	SVHN	KD+PU [7]	82.67	66.19	89.71	76.57	82.67	43.21	**84.30**	67.85
		LID [22]	97.86	90.74	92.40	88.24	97.86	84.88	67.28	76.58
		Mahalanobis (ours)	**99.62**	**97.15**	**95.73**	**92.15**	**99.62**	**95.39**	72.20	**86.73**

Table 3: Comparison of AUROC (%) under various validation setups. For evaluation on unknown attack, FGSM samples denoted by "seen" are used for validation. For our method, we use both feature ensemble and input pre-processing. The best results are indicated in bold.

Algorithm 2: Class-incremental learning using Mahalanobis distance

Algorithm 2 Updating Mahalanobis distance-based classifier for class-incremental learning.

Input: set of samples from a new class $\{\mathbf{x}_i : \forall i = 1 \dots N_{C+1}\}$, mean and covariance of observed classes $\{\widehat{\mu}_c : \forall c = 1 \dots C\}, \widehat{\mathbf{\Sigma}}$

Compute the new class mean: $\widehat{\mu}_{C+1} \leftarrow \frac{1}{N_{C+1}} \sum_i f(\mathbf{x}_i)$

Compute the covariance of the new class: $\widehat{\mathbf{\Sigma}}_{C+1} \leftarrow \frac{1}{N_{C+1}} \sum_i (f(\mathbf{x}_i) - \widehat{\mu}_{C+1})(f(\mathbf{x}_i) - \widehat{\mu}_{C+1})^\top$

Update the shared covariance: $\widehat{\mathbf{\Sigma}} \leftarrow \frac{C}{C+1}\widehat{\mathbf{\Sigma}} + \frac{1}{C+1}\widehat{\mathbf{\Sigma}}_{C+1}$

return Mean and covariance of all classes $\{\widehat{\mu}_c : \forall c = 1 \dots C+1\}, \widehat{\mathbf{\Sigma}}$

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Papers

NeurIPS-18: A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks

ICML-19: Robust Inference via Generative Classifiers for Handling Noisy Labels

Robust Inference via Robust Generative classifier

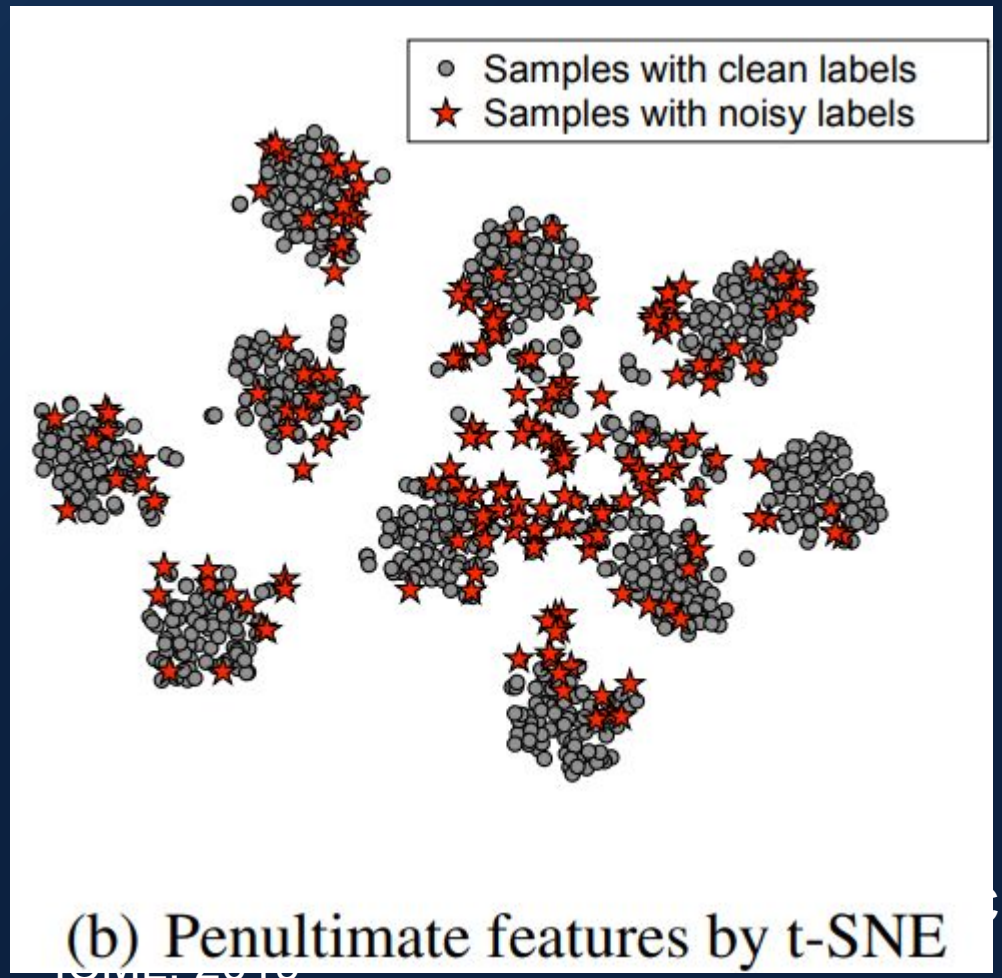
- Robust Generative classifier (RoG) = LDA (GDA) + MCD
  LDA (GDA): Linear/Gaussian Discriminant Analysis
  MCD: minimum covariance determinant
- Complementary to the prior works: one can combine ours and a prior training method for the best performance

- Belief/Assumption: the softmax DNNs can learn meaningful feature patterns shared by multiple training examples even under datasets with noisy labels.

Lee et al. Robust Inference via Generative Classifiers for Handling Noisy Labels. ICML, 2019

Assumption/Observation: Clustering properties of DNN representations even when trained with noisy labels

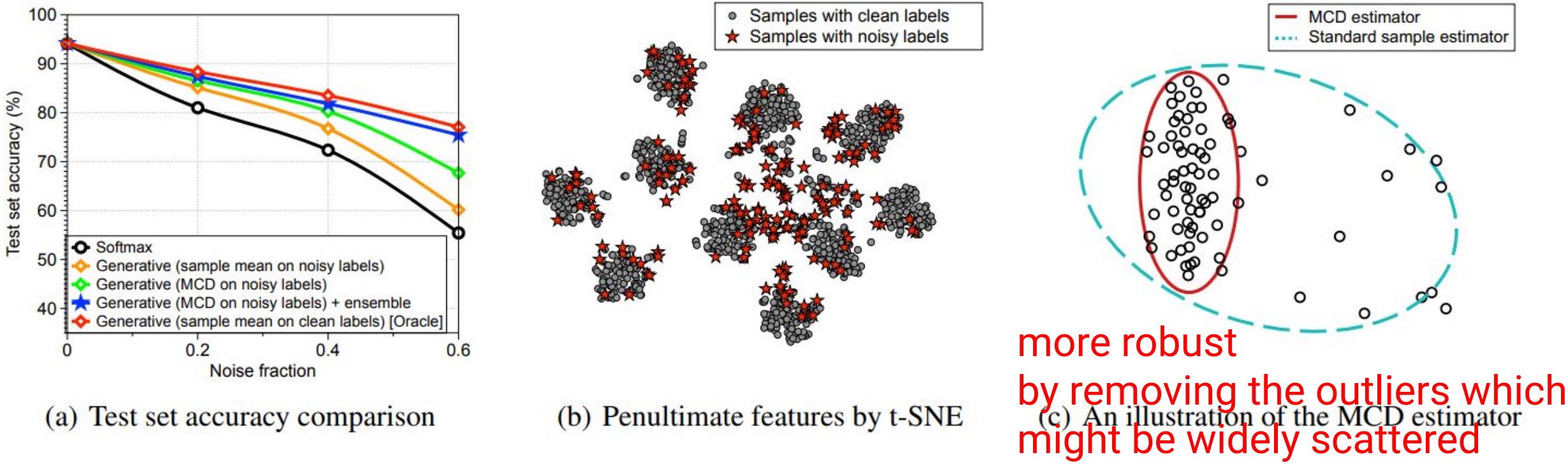
- DNN learns embedding that tend to group clean examples of the same class into the clusters while pushing away the examples with corrupt labels outside these clusters.



(b) Penultimate features by t-SNE

lassifiers for Handling Noisy Labels.

Overview



(a) Test set accuracy comparison (b) Penultimate features by t-SNE (c) An illustration of the MCD estimator

more robust
by removing the outliers which might be widely scattered

Figure 1. Experimental results under DenseNet-100 and CIFAR-10 with uniform noise, i.e., the labels of a given proportion of training samples are flipped to other labels uniformly at random. (a) Test set accuracy of softmax and generative classifiers with various parameter estimations. (b) Visualization of features on the penultimate layer using t-SNE from training samples when the noise fraction is 20%. (c) An illustration of the MCD estimator: it is more robust against outliers by finding a subset with minimum covariance determinant.

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Generative classifier

- Generative classifier via LDA

$$P\left(f(\mathbf{x})|y=c\right)=\mathcal{N}\left(f(\mathbf{x})|\mu_c,\boldsymbol{\Sigma}\right) \quad P\left(y=c\right)=\beta_c$$

According to Bayesian rule:

$$P\left(y=c|f(\mathbf{x})\right)=\frac{P\left(y=c\right)P\left(f(\mathbf{x})|y=c\right)}{\sum_{c'}P\left(y=c'\right)P\left(f(\mathbf{x})|y=c'\right)}$$

$$=\frac{\exp\left(\mu_c^\top\boldsymbol{\Sigma}^{-1}f(\mathbf{x})-\frac{1}{2}\mu_c^\top\boldsymbol{\Sigma}^{-1}\mu_c+\log\beta_c\right)}{\sum_{c'}\exp\left(\mu_{c'}^\top\boldsymbol{\Sigma}^{-1}f(\mathbf{x})-\frac{1}{2}\mu_{c'}^\top\boldsymbol{\Sigma}^{-1}\mu_{c'}+\log\beta_{c'}\right)}.$$

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Naive and Robust MCD estimator

- Naive sample estimator (outliers/training examples with noisy labels are also used)

$$\bar{\mu}_c = \sum_{i:y_i=c} \frac{f(\mathbf{x}_i)}{N_c}, \quad \bar{\beta}_c = \frac{N_c}{N},$$

$$\bar{\Sigma} = \sum_c \sum_{i:y_i=c} \frac{(f(\mathbf{x}_i) - \bar{\mu}_c)(f(\mathbf{x}_i) - \bar{\mu}_c)^\top}{N}$$

- MCD estimator: For each class, finding a subset for which the determinant of the corresponding sample covariance is minimized => outliers are removed.

$$\min_{\mathcal{X}_{K_c} \subset \mathcal{X}_{N_c}} \det\left(\hat{\Sigma}_c\right) \quad \text{subject to } |\mathcal{X}_{K_c}| = K_c$$

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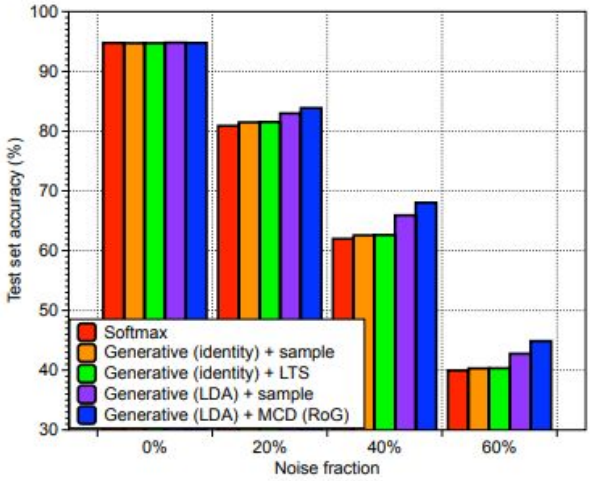
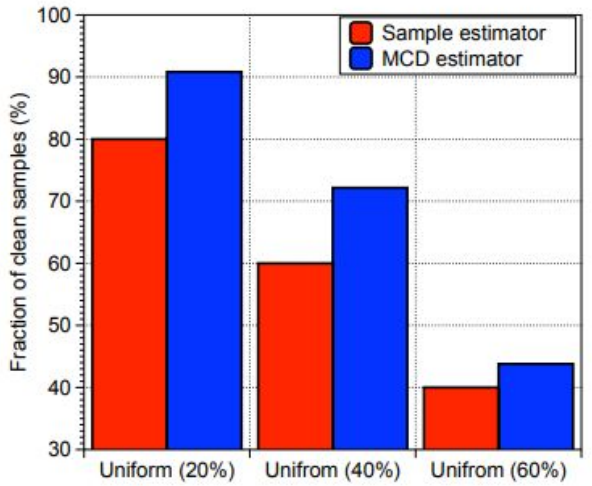
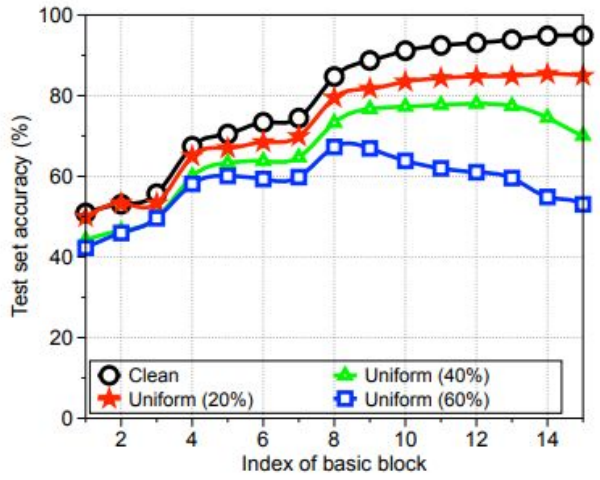
Results



(a) Model comparison



(b) Accuracy of the MCD estimator



(c) Layer-wise accuracy

Figure 2. Experimental results under ResNet-34 model and CIFAR-10 dataset. (a) Test accuracy of generative classifiers from penultimate features under various assumptions: identity covariance and tied covariance (LDA). (b) The number of clean samples among selected samples by the MCD estimator. (c) Test accuracy of generative classifiers computed at different basic blocks.

Model	Inference method	Ensemble	Clean	Uniform (20%)	Uniform (40%)	Uniform (60%)
DenseNet	Softmax	-	94.11	81.01	72.34	55.42
	Generative + sample	-	94.18	85.12	76.75	60.14
		✓	93.97	87.40	81.27	69.81
	Generative + MCD (ours)	-	94.22	86.54	80.27	67.67
		✓	94.18	**87.41**	**81.83**	**75.45**
ResNet	Softmax	-	94.76	80.88	61.98	39.96
	Generative + sample	-	94.80	82.97	65.92	42.76
		✓	94.82	83.36	68.57	46.45
	Generative + MCD (ours)	-	94.76	83.86	68.03	44.87
		✓	94.68	**84.62**	**75.28**	**54.57**

Table 1. Effects of an ensemble method. We use the CIFAR-10 dataset with various uniform noise fractions. All values are percentages and the best results are highlighted in bold if the gain is bigger than 1% compared to softmax classifier.

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Research Questions

- Why is RoG better than softmax classifiers?

1. **Naive Generative classifiers are generally at most competitively with softmax classifiers,** as shown in the first paper `A Simple Unified Framework for Detecting Out-of-Distribution Samples and Adversarial Attacks, NeurIPS-18'.

2. When noisy training examples exist, softmax classifiers tend to overfit (fit noisy ones), thus softmax ones degrade in this case.
   While with MCD to remove those noisy training examples, RoG > Naive Generative classifier > Softmax
3. RoG can use feature ensemble from different layers, while softmax can only use the penultimate-layer feature

Many Thanks !

Any Questions on these two papers?
e.g. merits and demerits