Learning from Label Proportions with Generative Adversarial Network

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Outline

Outline

Problem Description (1)

From supervised learning to weakly supervised learning:

- Combating over-fitting issue: e.g., big data
- The lack of fully supervised data: infeasible or labor-intensive[1]
- Certain constraints: e.g., privacy[2]
- The ubiquity of weakly labeled learning (WeLL): Semi-supervised learning (SSL) and Multi-instance Learning (MIL)
- Learning with bags: MIL and learning from label proportions (LLP)

[1] Z. Wang and J. Feng. "Multi-class learning from class proportions". In: *Neurocomputing* 119.16 (2013), pp. 273–280.

[2] Z. Qi, B. Wang, F. Meng, et al. "Learning with label proportions via NPSVM". In: *IEEE Transactions on Cybernetics* 47.10 (2017), pp. 3293–3305.

Problem Description (2)

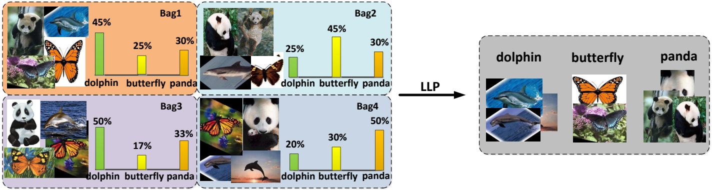

Figure: An illustration of multi-class LLP.

- The data belongs to three categories and is partitioned into four non-overlapping groups.
- The sizes of green, blue, and orange rectangles respectively denote available label proportions in different categories.
- We only know feature information and class proportions.

Challenges

- The uncertainty in label inference (proportional information in bags)
- Strict assumption on data distribution (statistical approaches, e.g., MeanMap[3] and Laplacian MeanMap[4])
- NP-hard combinatorial optimization issue (SVM-based methods, e.g., InvCal[5] and alter-$\propto$SVM[6])
- The lack of scalability (shallow models)

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[3] N. Quadrianto, A. J. Smola, T. S. Caetano, et al. "Estimating labels from label proportions". In: *Journal of Machine Learning Research* 10.Oct (2009), pp. 2349–2374.

[4] G. Patrini et al. "(Almost) no label no cry". In: *Advances in Neural Information Processing Systems*. 2014, pp. 190–198.

[5] S. Rueping. "SVM classifier estimation from group probabilities". In: *International Conference on Machine Learning*. 2010, pp. 911–918.

[6] F. X. Yu, D. Liu, S. Kumar, et al. "$\propto$-SVM for learning with label proportions". In: *International Conference on Machine Learning*. 2013, pp. 504–512.

Motivations

In this paper, we apply GANs to LLP in large scale scenarios.

- GAN is an elegant recipe for solving WeLL problem[7].
- Generative models offer explicit or implicit representations for WeLL[8].
- LLP-GAN is free of strict assumptions through the adversarial scheme.

[7] T. Salimans, I. Goodfellow, W. Zaremba, et al. "Improved techniques for training GANs". In: *Advances in Neural Information Processing Systems*. 2016, pp. 2234–2242.

[8] D. P. Kingma and M. Welling. "Auto-encoding variational bayes". In: *arXiv preprint arXiv:1312.6114* (2013).

Contributions

- We propose a simple improvement based on entropy regularization for the existing deep LLP solver.
- We reveal relationship between prior class proportions and posterior class likelihoods.
- We offer a decomposition representation of the class likelihood with respect to the prior class proportions, which verifies the existence of the final classifier.
- We empirically show that our method can achieve SOTA performance on large-scale LLP problems with a low computational complexity.

Outline

Problem Settings

- All the bags are disjoint and let $\mathcal{B}_i = \{\mathbf{x}_i^1, \mathbf{x}_i^2, \cdots, \mathbf{x}_i^{N_i}\}, i = 1, 2, \cdots, n$ be the bags in training set.
- Training data is $\mathcal{D} = \mathcal{B}_1 \cup \mathcal{B}_2 \cup \cdots \cup \mathcal{B}_n, \mathcal{B}_i \cap \mathcal{B}_j = \emptyset, \forall i \neq j$, where the total number of bags is n.
- Assuming we have K classes, for $\mathcal{B}_i$, let $\mathbf{p}_i$ be a K-element vector, where the k^{th} element p_i^k is the proportion of instances belonging to the class k, with the constraint $\sum_{k=1}^{K} p_i^k = 1$, i.e.,

$$p_i^k := \frac{|\{j \in [1 : N_i] | \mathbf{x}_i^j \in \mathcal{B}_i, y_i^{j*} = k\}|}{|\mathcal{B}_i|}. \tag{1}$$

Here, $[1 : N_i] = \{1, 2, \cdots, N_i\}$ and y_i^{j*} is the unaccessible ground-truth instance-level label of $\mathbf{x}_i^j$.

Deep LLP Appoach

- Suppose that $\tilde{\mathbf{p}}_i^j = p_\theta(\mathbf{y}|\mathbf{x}_i^j)$ is the vector-valued DNNs output for $\mathbf{x}_i^j$, where θ is the network parameter.
- The bag-level label proportion in the i^{th} bag is to incorporate the element-wise posterior probability:

$$\overline{\mathbf{p}}_i = \frac{1}{N_i} \bigoplus_{j=1}^{N_i} \tilde{\mathbf{p}}_i^j = \frac{1}{N_i} \bigoplus_{j=1}^{N_i} p_\theta(\mathbf{y}|\mathbf{x}_i^j). \tag{2}$$

- Entropy Regularization for DLLP[9]:

$$L = L_{prop} + \lambda E_{in} = -\sum_{i=1}^{n} \mathbf{p}_i^\intercal log(\overline{\mathbf{p}}_i) - \lambda \sum_{i=1}^{n} \sum_{j=1}^{N_i} (\tilde{\mathbf{p}}_i^j)^\intercal log(\tilde{\mathbf{p}}_i^j). \tag{3}$$

[9] E. M. Ardehaly and A. Culotta. "Co-training for demographic classification using deep learning from label proportions". In: *International Conference on Data Mining Workshops*. IEEE. 2017, pp. 1017–1024.

Outline

1. Introduction
   - Problem Description
   - Challenges
   - Motivation & Contribution
2. Preliminaries
   - Problem Settings
   - Deep LLP Appoach
3. Adversarial Learning for LLP
   - The Discriminator
   - The Generator
   - LLP-GAN Algorithm
4. Experimental Results
   - Algorithm Justification
   - Model Performance
5. Conclusion & Future Work

Adversarial Learning for LLP

We illustrate the LLP-GAN framework as follows.

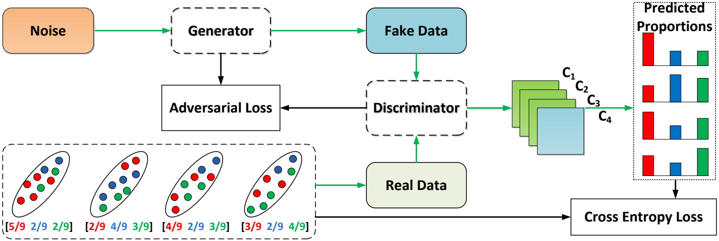


Figure: An illustration of our LLP-GAN framework.

The Objective of Discriminator (1)

- We normalize the first K classes in $P_D(\cdot|\mathbf{x})$ as instance-level posterior probability $\tilde{p}_D(\cdot|\mathbf{x})$ and compute $\overline{\mathbf{p}}$ based on (2).
- The *ideal* optimization problem for the discriminator of LLP-GAN is:

$$\max_D \quad V(G,D) = L_{unsup} + L_{sup} = L_{real} + L_{fake} - \lambda CE_{\mathcal{L}}(\mathbf{p}, \overline{\mathbf{p}})$$
$$= \sum_{i=1}^{n} E_{\mathbf{x}\sim p_d^i}\Big[logP_D(y \leq K|\mathbf{x})\Big] + E_{\mathbf{x}\sim p_g}\Big[logP_D(K+1|\mathbf{x})\Big] + \lambda \sum_{i=1}^{n} \mathbf{p}_i^\intercal log(\overline{\mathbf{p}}_i). \tag{4}$$

Here, $p_g(\mathbf{x})$ is the distribution of the synthesized data.

The Objective of Discriminator (2)

- The Lower Bound Approximation:

$$
\begin{aligned}
- CE_{\mathcal{L}}(\mathbf{p}, \overline{\mathbf{p}}) &= \sum_{i=1}^{n}\sum_{k=1}^{K} p_i(k) log\left[\frac{1}{N_i}\sum_{j=1}^{N_i}\tilde{p}_D(k|\mathbf{x}_i^j)\right] \\
&\backsimeq \sum_{i=1}^{n}\sum_{k=1}^{K} p_i(k) log\left[\int p_d^i(\mathbf{x})\tilde{p}_D(k|\mathbf{x})\mathrm{d}\mathbf{x}\right] \geqslant \sum_{i=1}^{n}\sum_{k=1}^{K} p_i(k) E_{\mathbf{x}\sim p_d^i}\left[log\,\tilde{p}_D(k|\mathbf{x})\right].
\end{aligned} \tag{5}
$$

- The expectation in the last term can be approximated by sampling. Similar to EM mechanism[10] for mixture models, by approximating $-CE_{\mathcal{L}}(\mathbf{p}, \overline{\mathbf{p}})$ with its lower bound, we can perform gradient ascend independently on every sample, e.g., SGD.

[10] T. K. Moon. "The expectation-maximization algorithm". In: *IEEE Signal processing magazine* 13.6 (1996), pp. 47–60.

The Optimity

Lemma

The maximization on lower bound in (5) induces optimal discriminator D^* with a posterior distribution $\tilde{p}_{D^*}(y|\mathbf{x})$, which is consistent with the prior distribution $p_i(y)$ in each bag.

Theorem

For fixed G, the optimal discriminator D^* for $\widetilde{V}(G, D)$ satisfies:

$$P_{D^*}(y=k|\mathbf{x}) = \frac{\sum_{i=1}^{n} p_i(k) p_d^i(\mathbf{x})}{\sum_{i=1}^{n} p_d^i(\mathbf{x}) + p_g(\mathbf{x})}, k=1,2,\cdots,K. \tag{6}$$

Beyond the Incontinuity of p_g

- The generator is a mapping from a low dimensional space to a high dimensional one.
- The density of $p_g(\mathbf{x})$ is infeasible[11].
- Based on the definition of $\tilde{p}_D(y|\mathbf{x})$, we have:

$$\tilde{p}_{D^*}(y|\mathbf{x}) = \frac{\sum_{i=1}^{n} p_i(y) p_d^i(\mathbf{x})}{\sum_{i=1}^{n} p_d^i(\mathbf{x})} = \sum_{i=1}^{n} w_i(\mathbf{x}) p_i(y). \tag{7}$$

- Our final classifier does not depend on $p_g(\mathbf{x})$.
- (7) explicitly expresses the normalized weights of the aggregation with $w_i(\mathbf{x}) = \frac{p_d^i(\mathbf{x})}{\sum_{i=1}^{n} p_d^i(\mathbf{x})}$.

[11] M. Arjovsky and L. Bottou. "Towards principled methods for training generative adversarial networks". In: *International Conference on Learning Representations*. 2016.

The Objective Function of Generator

- Normally, we should solve the following optimization problem with respect to p_g for the generator.

$$\min_G \widetilde{V}(G, D^*) = \min_G E_{\mathbf{x} \sim p_g} log P_{D^*}(K+1|\mathbf{x}). \qquad (8)$$

- However, a well-trained generator would lead to the inefficiency of supervised information.
- Hence, we apply feature matching (FM) to the generator and obtain its alternative objective by matching the expected value of features (statistics) on an intermediate layer of the discriminator:

$$L(G) = \| E_{\mathbf{x} \sim \frac{1}{n} p_d} f(\mathbf{x}) - E_{\mathbf{x} \sim p_g} f(\mathbf{x}) \|_2^2 \qquad (9)$$

LLP-GAN Algorithm

Algorithm 1: LLP-GAN Training Algorithm

Input: The training set $\mathcal{L} = \{(\mathcal{B}_i, \mathbf{p}_i)\}_{i=1}^{n}$; L: number of total iterations; λ: weight parameter.

Output: The parameters of the final discriminator D.

Set m to the total number of training data points.

for *i=1:L* **do**

  Draw m samples $\{\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \cdots, \mathbf{z}^{(m)}\}$ from a simple-to-sample noise prior $p(\mathbf{z})$ (e.g., $N(0, I)$).

  Compute $\{G(\mathbf{z}^{(1)}), G(\mathbf{z}^{(2)}), \cdots, G(\mathbf{z}^{(m)})\}$ as sampling from $p_g(\mathbf{x})$.

  Fix the generator G and perform gradient ascent on parameters of D in $\widetilde{V}(G, D)$ for one step.

  Fix the discriminator D and perform gradient descent on parameters of G in $L(G)$ for one step.

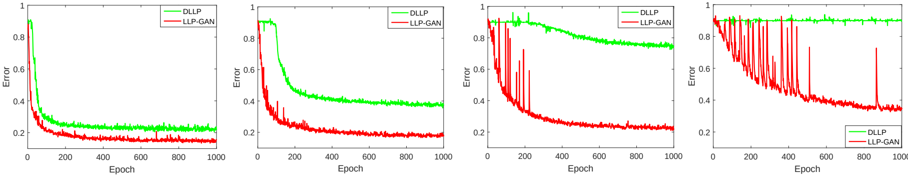
end

Return parameters of the discriminator D in the last step.

Outline

Convergence Analysis

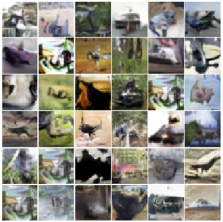
DLLP v.s. LLP-GAN (proposed)



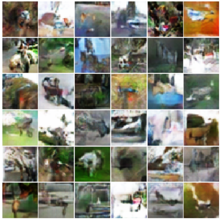
(a) Bag size: 16 (b) Bag size: 32 (c) Bag size: 64 (d) Bag size: 128

Figure: The convergence curves on CIFAR-10 w/ different bag sizes.

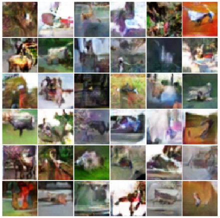
To validate the effectiveness of generator in LLP-GAN, we compare the generated samples of our model with that of the standard GAN with feature matching.



(a) GANs with FM



(b) 50 epochs (ours)

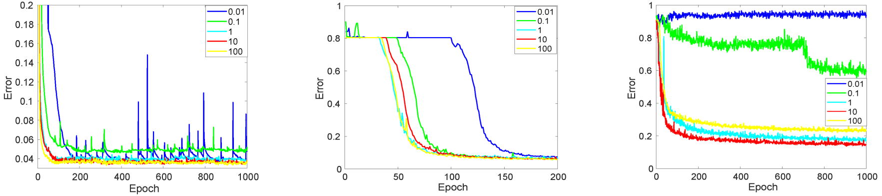


(c) 60 epochs (ours)

(d) 70 epochs (ours)

Figure: Generated samples on CIFAR-10.

Hyperparameter Analysis



(a) λ on MNIST (b) λ on SVHN (c) λ on CIFAR-10

Figure: Analysis on hyperparameter.

Error Rates Comparison(1)

The results are the average performances of four datasets: MNIST, SVHN, CIFAR-10, and CIFAR-100.

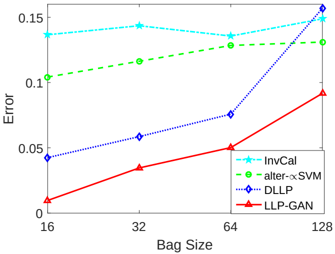


Figure: The average error rates w/ different bag sizes.

Error Rates Comparison (2)

Table: Test error rates (%) on benchmark datasets w/ different bag sizes.

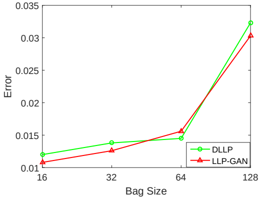
Dataset	Algorithm	Bag Size 16	32	64	128	Baseline CNNs
MNIST	DLLP	1.23 (0.100)	1.33 (0.094)	1.57 (0.088)	3.55 (0.27)	0.36
	LLP-GAN	**1.10** (0.026)	**1.23** (0.088)	**1.40** (0.089)	**3.49** (0.27)	
SVHN	DLLP	4.45 (0.069)	5.29 (0.54)	5.80 (0.91)	39.73 (1.60)	2.35
	LLP-GAN	**4.03**(0.021)	**4.83**(0.51)	**5.42**(0.59)	**11.17**(1.12)	
CIFAR-10	DLLP	19.70 (0.77)	34.39 (0.82)	68.32 (1.34)	82.89 (2.66)	9.27
	LLP-GAN	**13.68** (0.35)	**16.23** (0.43)	**21.03** (1.82)	**27.39** (4.31)	
CIFAR-100	DLLP	53.24(0.77)	98.38(0.11)	98.65(0.09)	98.98(0.08)	35.68
	LLP-GAN	**50.95**(0.67)	**56.44**(0.78)	**64.37**(1.52)	**85.01**(1.81)	

Error Rates Comparison (3)

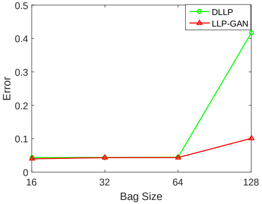
Table: Binary test error rates (%) on benchmark datasets w/ different bag sizes.

Dataset	Algorithm	Bag Size			
		16	32	64	128
MNIST	InvCal	0.50	0.55	1.25	0.1
	alter-pSVM	0.20	0.20	0.25	0.2
	DLLP	0.049	0.049	0.049	0.049
	LLP-GAN	**0.047**	**0.047**	**0.047**	**0.047**
CIFAR-10	InvCal	28.95	29.16	26.47	31.84
	alter-pSVM	24	26.74	30.32	27.95
	DLLP	11.31	15.83	18.96	22.59
	LLP-GAN	**1.39**	**1.61**	**11.59**	**18.29**
SVHN	InvCal	11.55	13.35	12.95	12.70
	alter-pSVM	7.05	7.95	7.95	11.15
	DLLP	**1.38**	**1.7**	3.77	24.45
	LLP-GAN	1.49	1.8	**3.46**	**9.23**

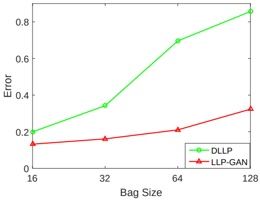
Error Rates Comparison (4)



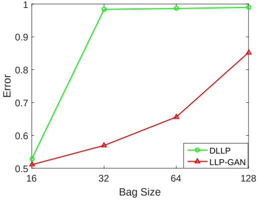
(a) MINST



(b) SVHN



(c) CIFAR-10



(d) CIFAR-100

Figure: Multi-class test error rates (%) on benchmark w/ different bag sizes.

Outline

Conclusion

- This paper proposed a new algorithm LLP-GAN for LLP problem in virtue of the adversarial learning based on GANs.
- Our method is superior to existing methods in three aspects.
    - Nice theoretical properties
    - A probabilistic classifier
    - Scalability: e.g., image data applications

Future Work

- Learning complexity in the sense of PAC is not involved in this study.
- There is no guarantee on algorithm robustness to data perturbations: e.g., imprecise proportions.
- Varying GANs are not considered in our current model and their performance is unknown: e.g. WGAN[12].
- The performance of LLP-GAN on tabular data and structured (non-random) data[13] is not included.

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[12] M. Arjovsky, S. Chintala, and L. Bottou. "Wasserstein generative adversarial networks". In: *ICML*. 2017, pp. 214–223.

[13] G. Patrini et al. "(Almost) no label no cry". In: *Advances in Neural Information Processing Systems*. 2014, pp. 190–198.

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