Learning Noise Transition Matrix from Only Noisy Labels via Total Variation Regularization

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Outline

Overview

Problem

- **Noise transition matrix** is important in **learning from noisy labels**.
- However, it is usually unavailable or hard to obtain.
- Existing methods often depend on unreliable noisy class-posterior estimation.

Contribution

- We characterized the class-conditional label corruption process.
- We proposed a conceptually novel method for transition matrix estimation.

Methodology

- **Make probabilities more distinguishable**: total variation regularization
- **Capture uncertainties during training**: Dirichlet posterior update

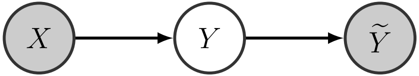
Outline

Learning from Noisy Labels

Notation

- X: input features
- Y: true labels
- $\widetilde{Y}$: noisy labels

Assumption



Class-conditional noise (CCN) assumes that the noisy label $\widetilde{Y}$ is independent of the input feature X given the true label Y: $p(\widetilde{Y}|Y, X) = p(\widetilde{Y}|Y)$.

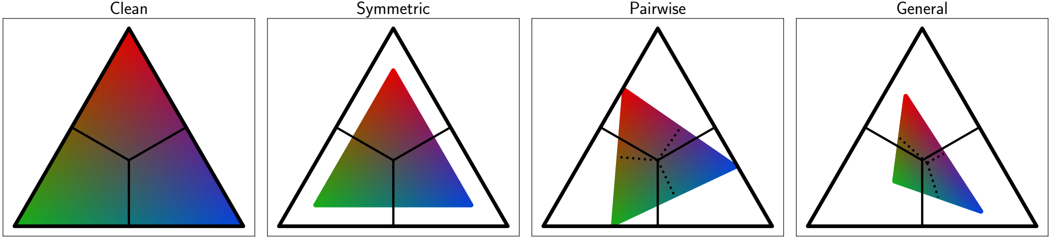
Noise transition matrix $\boldsymbol{T}_{ij} = p(\widetilde{Y} = j|Y = i)$

$$\begin{bmatrix} p(\widetilde{Y} = 1|X) \\ \vdots \\ p(\widetilde{Y} = K|X) \end{bmatrix} = \begin{bmatrix} p(\widetilde{Y} = 1|Y = 1) & \dots & p(\widetilde{Y} = 1|Y = K) \\ \vdots & \ddots & \vdots \\ p(\widetilde{Y} = K|Y = 1) & \dots & p(\widetilde{Y} = K|Y = K) \end{bmatrix} \begin{bmatrix} p(Y = 1|X) \\ \vdots \\ p(Y = K|X) \end{bmatrix}$$

$$\Downarrow$$

$$\boldsymbol{p}(\widetilde{Y}|X) = \boldsymbol{T}^{\mathsf{T}} \boldsymbol{p}(Y|X)$$

Noise Transition Matrix



Class-conditional label corruption maps the probability simplex Δ^{K-1} to a convex hull $\mathrm{Conv}(\boldsymbol{T})$ of the rows of the noise transition matrix $\boldsymbol{T}$.

- Outer black triangle: probability simplex Δ^2
- Inner colored triangle: convex hull $\mathrm{Conv}(\boldsymbol{T})$

Identifiability

Good news: if the ground-truth noise transition matrix $\boldsymbol{T}$ is known, $\boldsymbol{p}(Y|X)$ is **identifiable** based on observations of $\boldsymbol{p}(\widetilde{Y}|X)$ [Patrini et al., 2017].

Problem

Noise transition matrix is usually not available [Patrini et al., 2017].

Solution

Learn the noise transition matrix **from only noisy labels**.

Anchor Points

- An instance x is called an anchor point for class i if $p(Y = i|X = x) = 1$.
- Based on anchor points, we can estimate $\boldsymbol{p}(\widetilde{Y}|X)$ to obtain an estimate of $\boldsymbol{T}$.

$$\boldsymbol{p}(\widetilde{Y}|X = x) = \boldsymbol{T}^{\mathsf{T}}\boldsymbol{p}(Y|X = x) = \boldsymbol{T}_i$$

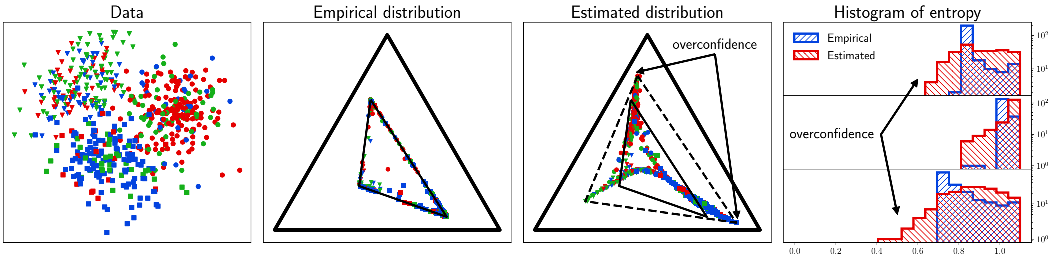
Problem

Anchor points are hard to obtain [Xia et al., 2019, Yao et al., 2020].

Solution

Do not rely on a separate set of anchor points.

Overconfidence



Problem

The estimation of the noisy class-posterior could be unreliable due to the **overconfidence** of deep neural networks [Guo et al., 2017, Hein et al., 2019].

Solution

Do not estimate the noisy class-posterior directly using neural networks.

Outline

Transition Matrix Equivalence

$$\boldsymbol{p}(\widetilde{Y}|X) = \widehat{\boldsymbol{T}}^\mathsf{T}\widehat{\boldsymbol{p}}(Y|X) = \boldsymbol{V}^\mathsf{T}(\boldsymbol{U}^\mathsf{T}\boldsymbol{p}(Y|X))$$

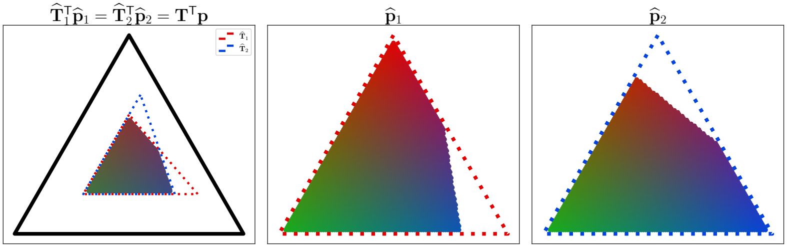
$$\begin{bmatrix} p(\widetilde{Y}_1|X) \\ p(\widetilde{Y}_2|X) \\ p(\widetilde{Y}_3|X) \end{bmatrix} = \begin{matrix} .64 & .14 & .07 \\ .27 & .70 & .24 \\ .09 & .16 & .69 \end{matrix} \left(\begin{matrix} 1.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 1.0 \end{matrix} \begin{bmatrix} p(Y_1|X) \\ p(Y_2|X) \\ p(Y_3|X) \end{bmatrix} \right) \quad \text{(best)}$$

$$\begin{bmatrix} p(\widetilde{Y}_1|X) \\ p(\widetilde{Y}_2|X) \\ p(\widetilde{Y}_3|X) \end{bmatrix} = \begin{matrix} 0.7 & 0.0 & 0.1 \\ 0.3 & 0.8 & 0.0 \\ 0.0 & 0.2 & 0.9 \end{matrix} \left(\begin{matrix} 0.9 & 0.2 & 0.0 \\ 0.0 & 0.8 & 0.3 \\ 0.1 & 0.0 & 0.7 \end{matrix} \begin{bmatrix} p(Y_1|X) \\ p(Y_2|X) \\ p(Y_3|X) \end{bmatrix} \right)$$

$$\begin{bmatrix} p(\widetilde{Y}_1|X) \\ p(\widetilde{Y}_2|X) \\ p(\widetilde{Y}_3|X) \end{bmatrix} = \begin{matrix} 1.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 1.0 \end{matrix} \left(\begin{matrix} .64 & .14 & .07 \\ .27 & .70 & .24 \\ .09 & .16 & .69 \end{matrix} \begin{bmatrix} p(Y_1|X) \\ p(Y_2|X) \\ p(Y_3|X) \end{bmatrix} \right) \quad \text{(worst)}$$

If the transition matrix can be written as a product of two transition matrices, then there could be **infinitely many wrong models** due to non-identifiability.

Transition Matrix Decomposition



- If anchor points exist in the dataset, then the **correct model is unique** and has nice properties.
- If such a condition does not hold, we do not have consistency guarantees, but the proposed method may still work empirically.
- Note that we do not need to detect anchor points from the dataset.

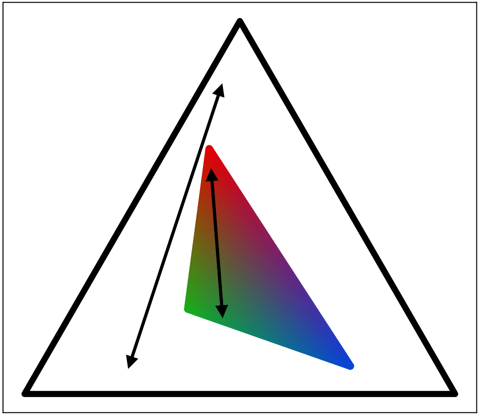
Transition Matrix as a Contraction Mapping

Key motivation 1

The mapping $\Delta \to \mathrm{Conv}(\boldsymbol{U})$ defined by $\boldsymbol{p} \mapsto \boldsymbol{U}^{\top}\boldsymbol{p}$ is a **contraction mapping** over the simplex Δ relative to the total variation distance [Del Moral et al., 2003]:

$$\forall \boldsymbol{U} \in \mathcal{T}, \forall \boldsymbol{p}, \boldsymbol{q} \in \Delta,$$
$$d_{\mathrm{TV}}(\boldsymbol{U}^{\top}\boldsymbol{p}, \boldsymbol{U}^{\top}\boldsymbol{q}) \leq d_{\mathrm{TV}}(\boldsymbol{p}, \boldsymbol{q})$$

Probabilities of the correct model are more **distinguishable** from each other.

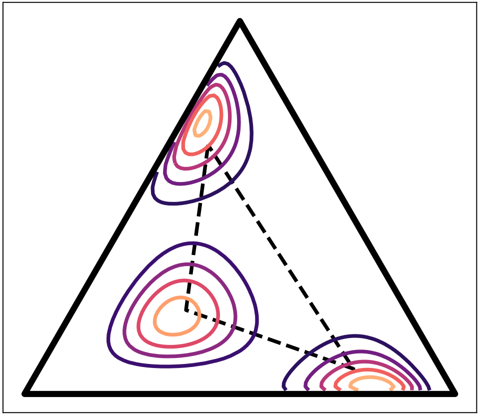


Transition Matrix Estimation

Key motivation 2

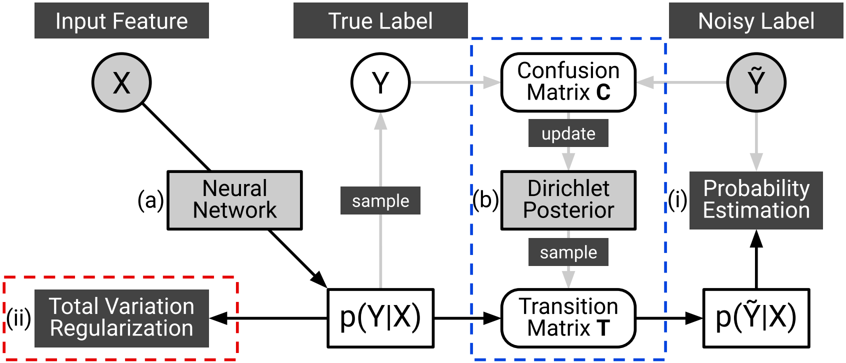
In addition to the gradient information, the **confusion matrix** is also helpful for estimating the transition matrix.

We have a **derivative-free** approach that uses Dirichlet distributions to model the transition matrix to capture uncertainties during training.



Outline

Overview



Our model has two modules:

- (a) a **neural network** for predicting $p(Y|X)$
- (b) a Dirichlet posterior for the noise transition matrix $\boldsymbol{T}$

The learning objective also contains two parts:

- (i) the usual **cross-entropy loss** for classification from noisy labels
- (ii) a **total variation regularization** term for the predicted probability

Total Variation Regularization

We sample a fixed number of pairs to reduce the additional computational cost.

$$d_{\mathrm{TV}}(\boldsymbol{p}, \boldsymbol{q}) := \frac{1}{2}\|\boldsymbol{p} - \boldsymbol{q}\|_1$$

$$R(W) := \mathop{\mathbb{E}}_{X_1 \sim p(X)} \mathop{\mathbb{E}}_{X_2 \sim p(X)} [d_{\mathrm{TV}}(\boldsymbol{p}_1, \boldsymbol{p}_2)]$$

$$\text{where } \boldsymbol{p}_i := \boldsymbol{p}(Y|X_i; W) \quad i = 1, 2$$

```
p = model(x)  # probability [batch_size, num_classes]
idx_1, idx_2 = randint(0, batch_size, (2, num_pairs))
tv = 0.5 * l1_norm(p[idx_1] - p[idx_2], dim=1).mean()
```

Dirichlet Posterior Update

Inspired by the closed-form posterior update rule for the Dirichlet-multinomial conjugate, we update the concentration parameters $\boldsymbol{A}$ during training using the confusion matrix $\boldsymbol{C}$, where (β_1, β_2) are fixed hyperparameters.

$$\boldsymbol{A}^{(\text{posterior})} = \boldsymbol{A}^{(\text{prior})} + \boldsymbol{C}^{(\text{observation})}$$

$$\boldsymbol{A} \leftarrow \beta_1 \boldsymbol{A} + \beta_2 \boldsymbol{C}$$

```
y = Categorical(p).sample()  # predicted labels
C = confusion_matrix(y, y_)  # confusion matrix
A = beta_1 * A + beta_2 * C  # update
```

Optimization

For each batch of data, we sample a transition matrix from the Dirichlet posterior.

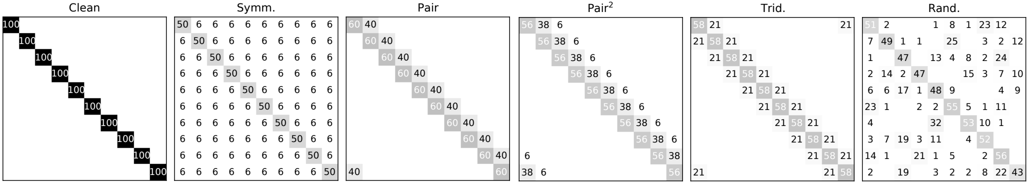
$$
\begin{aligned}
\boldsymbol{T}_i &\sim \mathrm{Dirichlet}(\boldsymbol{A}_i) \quad (i = 1, \ldots, K) \\
L_0(W, \boldsymbol{T}) &:= \mathop{\mathbb{E}}_{X \sim p(X)} \left[D_{\mathrm{KL}}\left(\boldsymbol{p}(\widetilde{Y} | X) \,\middle\|\, \boldsymbol{T}^{\mathsf{T}} \boldsymbol{p}(Y | X; W) \right) \right] \\
\mathcal{L}(W, \boldsymbol{T}) &:= L_0(W, \boldsymbol{T}) - \gamma R(W)
\end{aligned}
$$

```
T = Dirichlet(A).sample()  # transition matrix
loss = cross_entropy(p @ T, y_) - gamma * tv
```

Outline

Settings

Noise types



Baselines

- (Robust) loss functions:
  - (**CCE**) categorical cross-entropy loss
  - (**MAE**) mean absolute error [Ghosh et al., 2017]
  - (**GCE**) generalized cross-entropy loss [Zhang and Sabuncu, 2018]
- Transition matrix estimations:
  - (**Forward**) forward correction [Patrini et al., 2017]
  - (**T-Revision**) transition-revision [Xia et al., 2019]
  - (**Dual-T**) dual-T estimator [Yao et al., 2020]

Results

Improved classification performance, measured by **accuracy**.

		(a) Clean	(b) Symm.	(c) Pair	(d) Pair^2	(e) Trid.	(f) Rand.
CIFAR100	MAE	11.23(1.02)	7.89(0.67)	6.94(1.11)	6.60(0.74)	7.45(0.55)	7.15(0.98)
	CCE	**70.58(0.29)**	42.94(0.47)	44.00(0.71)	41.37(0.27)	46.55(0.54)	42.41(0.48)
	GCE	57.10(0.85)	48.66(0.58)	45.27(0.85)	43.67(0.94)	50.98(0.33)	48.66(0.63)
	Forward	**70.58(0.28)**	44.32(0.64)	44.17(0.57)	42.07(0.55)	47.48(0.40)	43.15(0.53)
	T-Revision	**70.47(0.26)**	46.52(0.57)	44.08(0.42)	42.01(0.52)	47.59(0.60)	45.33(0.40)
	Dual-T	**70.56(0.28)**	55.92(0.60)	46.22(0.72)	44.74(0.65)	61.68(0.51)	57.92(0.50)
	TVG	70.02(0.30)	**57.33(0.42)**	45.68(0.85)	44.38(0.72)	54.23(0.53)	**59.85(0.61)**
	TVD	69.93(0.21)	52.54(0.45)	**56.02(0.82)**	**49.18(0.53)**	**62.45(0.44)**	53.95(0.47)

Improved transition matrix estimation, measured by **average total variation**.

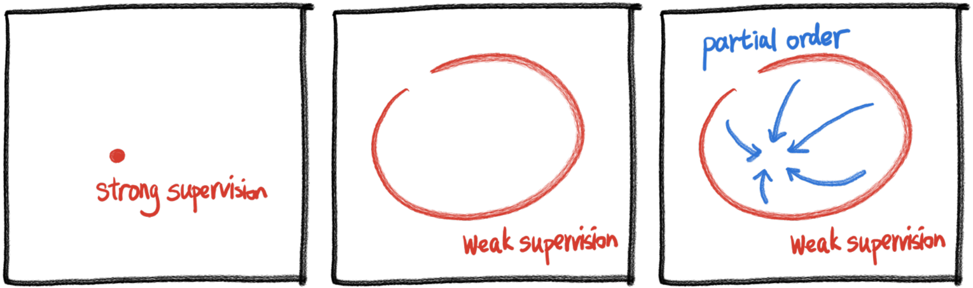
		(a) Clean	(b) Symm.	(c) Pair	(d) Pair^2	(e) Trid.	(f) Rand.
CIFAR-100	Forward	**0.00(0.00)**	48.62(0.11)	39.81(0.03)	43.57(0.04)	40.92(0.07)	49.06(0.10)
	T-Revision	0.46(0.05)	31.58(0.46)	39.45(0.03)	42.77(0.06)	40.01(0.09)	39.49(0.26)
	Dual-T	3.10(0.08)	17.10(0.18)	33.26(0.20)	33.79(0.26)	**23.56(0.43)**	22.59(0.23)
	TVG	1.59(0.02)	**13.11(0.10)**	37.79(0.30)	38.83(0.34)	30.80(0.51)	**16.47(0.18)**
	TVD	21.98(0.11)	26.46(0.15)	**29.47(0.26)**	**31.34(0.30)**	23.86(0.22)	35.37(0.30)

Outline

Summary

- **Total variation regularization** encourages the predicted probabilities to be more distinguishable from each other.
- The proposed method can estimate the transition matrix and learn a classifier **simultaneously**.
- Under mild assumptions, the proposed method yields a **consistent estimator** of the noise transition matrix.

Takeaway



- In this problem, the weak supervision is insufficient to identify the true model, i.e., we have a class of observationally equivalent models.
- We address this issue by finding characteristics of the true model under realistic assumptions and introducing a partial order as a regularization.
- Such an approach can be used in other weakly supervised learning problems.

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