Reduction from Complementary-Label Learning to Probability Estimates

Wei-I Lin National Taiwan University r10922076@csie.ntu.edu.tw Hsuan-Tien Lin National Taiwan University htlin@csie.ntu.edu.tw

Abstract

Complementary-Label Learning (CLL) is a weakly-supervised learning problem that aims to learn a multi-class classifier from only complementary labels, which indicate a class to which an instance does not belong. Existing approaches mainly adopt the paradigm of reduction to ordinary classification, which applies specific transformations and surrogate losses to connect CLL back to ordinary classification. Those approaches, however, face several limitations, such as the tendency to overfit or be hooked on deep models. In this paper, we sidestep those limitations with a novel perspective-reduction to probability estimates of complementary classes. We prove that accurate probability estimates of complementary labels lead to good classifiers through a simple decoding step. The proof establishes a reduction framework from CLL to probability estimates. The framework offers explanations of several key CLL approaches as its special cases and allows us to design an improved algorithm that is more robust in noisy environments. The framework also suggests a validation procedure based on the quality of probability estimates, leading to an alternative way to validate models with only complementary labels. The flexible framework opens a wide range of unexplored opportunities in using deep and non-deep models for probability estimates to solve the CLL problem. Empirical experiments further verified the framework's efficacy and robustness in various settings.

1 Introduction

In real-world machine learning applications, high-quality labels may be hard or costly to collect. To conquer the problem, researchers turn to the *weakly-supervised learning* (WSL) framework, which seeks to learn a good classifier with incomplete, inexact, or inaccurate data [27]. Several paradigms of WSL have been studied, including but not limited to semi-supervised learning [2], learning from partial labels [10], noisy labels [17], complementary labels [8], multiple complementary labels [6, 1], ordinary and complementary labels [11], positive-unlabeled data [5], and unlabeled-unlabeled data [16].

This paper focuses on a very weak type of WSL, called *complementary-label learning* (CLL) [8]. For the multi-class classification task, a complementary label designates a class to which a specific instance does not belong. The CLL problem assumes that the learner receives complementary labels rather than ordinary ones during training, while wanting the learner to correctly predict the ordinary labels of the test instances. Complementary labels can be cheaper to obtain. For example, when labeling with many classes, selecting the correct label is time-consuming for data annotators, while selecting a complementary label would be less costly [8]. In this case, fundamental studies on CLL models can potentially upgrade multi-class classification models and make machine learning more realistic. CLL's usefulness also attracts researchers to study its interaction with other tasks, such as generative-discriminative learning [23, 15] and domain-adaptation [26].

Table 1: Comparison of recent approaches to CLL. f(x) is the probability estimates of x, and ℓ is an arbitrary multi-class loss. labeltable:comp-recent

Method	TRANSFORMATION	Loss Function
URE [8, 9] SCL-NL [3] FwD [24] DM [7]	$\begin{split} \phi &= I \\ \phi &= I \\ \phi(f)(x) &= T^\top f(x) \\ \phi(f)(x) &= \operatorname{sm}(1 - f(x)) \end{split}$	$\begin{array}{c} -(K-1)\ell(f(x),\bar{y}) + \sum_{k=1}^{K} \ell(f(x),k) \\ -\log(1-f_{\bar{y}}(x)) \\ \ell(\phi(f)(x),\bar{y}) \\ \ell(\phi(f)(x),\bar{y}) \end{array}$

Ishida et al. [8, 9] proposed a pioneering model for CLL based on replacing the ordinary classification error with its unbiased risk estimator (URE) computed from only complementary labels under the assumption that the complementary labels are generated uniformly. Chou et al. [3] unveiled the overfitting tendency of URE and proposed the surrogate complementary loss (SCL) as an alternative design. Yu et al. [24] studied the situation where the complementary labels are not generated uniformly, and proposed a loss function that includes a transition matrix for representing the non-uniform generation. Gao & Zhang [7] argued that the non-uniform generation shall be tackled by being agnostic to the transition matrix instead of including the matrix in the loss function.

The methods mentioned above mainly focused on applying transformation and specific loss functions to the ordinary classifiers. Such a "reduction to ordinary classification" paradigm, however, faces some limitations and is not completely analyzed. For instance, so far most of the methods in the paradigm require differentiable models such as deep neural networks in their design. It is not clear whether non-deep models could be competitive or even superior to deep ones. It remains to be an important issue to correct the overfitting tendency caused by the stochastic relationship between complementary and ordinary labels, as repeatedly observed on URE-related methods [3]. More studies are also needed to understand the potential of and the sensitivity to the transition matrix in the non-uniform setting, rather than only fixing the matrix in the loss function [24] or dropping it [7].

The potential limitations from reduction to ordinary classification motivate us to sidestep them by taking a different perspective—reduction to complementary probability estimates. Our contribution can be summarized as follows.

- 1. We propose a framework that only relies on the probability estimates of complementary labels, and prove that a simple decoding method can map those estimates back to correct ordinary labels with theoretical guarantees.
- 2. The proposed framework offers explanations of several key CLL approaches as its special cases and allows us to design an improved algorithm that is more robust in noisy environments.
- 3. We propose a validation procedure based on the quality of probability estimates, providing a novel approach to validate models with only complementary labels along with theoretical justifications.
- 4. We empirically verify the effectiveness of the proposed framework under broader scenarios than previous works that cover various assumptions on complementary label generation (uniform and non-uniform; clean and noisy) and models (deep and non-deep). We find that the proposed framework improves the state-of-the-art methods in those scenarios, demonstrating the effectiveness and robustness of the framework.

The rest of the paper is organized as follows. We introduce the formulation of the ordinary and complementary label learning problem and discuss some recent approaches in Section 2. We describe the proposed framework in Section 3. In Section 4, we demonstrate the effectiveness of the proposed method under various scenarios. We then conclude in Section 5.

2 Problem Setup

In this section, we first introduce the problem of ordinary multi-class classification. Then, we will formulate the problem of complementary-label learning (CLL), and introduce the assumption and related works.

2.1 Ordinary-label learning

We start by reviewing the problem formulation of ordinary multi-class classification. In this problem, we let K with K > 2 denote the number of classes to be classified, and use $\mathcal{Y} = [K] = \{1, 2, \ldots, K\}$ to denote the label set. Let $\mathcal{X} \subset \mathbb{R}^d$ denote the feature space. Let D be an unknown joint distribution over $\mathcal{X} \times \mathcal{Y}$ with density function $p_D(x, y)$. Given N i.i.d. training samples $\{(x_i, y_i)\}_{i=1}^N$ and a hypothesis set \mathcal{H} , the goal of the learner is to select a classifier $f : \mathcal{X} \to \mathbb{R}^K$ from the hypothesis set \mathcal{H} that predicts the correct labels on unseen instances. The prediction \hat{y} of an unseen instance x is determined by taking the argmax function on f, i.e. $\hat{y} = \operatorname{argmax}_i f_i(x)$, where $f_i(x)$ denote the i-th output of f(x). The goal of the learner is to learn an f from \mathcal{H} that minimizes the following classification risk: $\mathbb{E}_{(x,y)\sim D} \left[\ell(f(x), e_y)\right]$, where $\ell \colon \mathbb{R}^K \times \mathbb{R}^K \to \mathbb{R}^+$ denotes the loss function, and e_y denote the one-hot vector of label y.

2.2 Complementary-label learning

In complementary-label learning, the goal for the learner remains the same—finding an f that minimizes the ordinary classification risk. The difference lies in the dataset to learn from. The complementary learner does not have access to the ground-truth labels y_i . Instead, for each instance x_i , the learner is given a complementary label \bar{y}_i . A complementary label is a class that x_i does not belong to; that is, $\bar{y}_i \in [K] \setminus \{y_i\}$. In CLL, it is assumed that the complementary dataset is generated according to an unknown distribution \bar{D} over $\mathcal{X} \times \mathcal{Y}$ with density function $\bar{p}_{\bar{D}}(x, y)$. Given access to i.i.d. samples $\{x_i, \bar{y}_i\}_{i=1}^N$ from \bar{D} , the complementary-label learner aims to find a hypothesis that classifies the correct ordinary labels on unseen instances.

Next, we introduce the *class-conditional complementary transition assumption*, which is used by many existing work [8, 9, 24, 7]. It assumes that the generation of complementary labels only depends on the ordinary labels; that is, $P(\bar{y} | y, x) = P(\bar{y} | y)$. The transition probability $P(\bar{y} | y)$ is often represented by a $K \times K$ matrix, called *transition matrix*, with $T_{ij} = P(\bar{y} = j | y = i)$. It is commonly assumed to be all-zeros on the diagonals, i.e., $T_{ii} = 0$ for all $i \in [K]$ in CLL because complementary labels are not ordinary. The transition matrix is further classified into two categories:

- Uniform: In uniform complementary generation, each complementary label is sampled uniformly from all labels except the ordinary one. The transition matrix in this setting is accordingly $T = \frac{1}{K-1}(\mathbf{1}_k \mathbf{I}_k)$. This is the most widely researched and benchmarked setting in CLL.
- *Biased:* A biased complementary generation is one that is not uniform. Biased transition matrices could be further classified as invertible ones and noninvertible ones based on its invertibility. The invertibility of a transition matrix comes with less physical meaning in the context of CLL; however, it plays an important role in some theoretical analysis in previous work [24, 3].

Following earlier approaches, we assume that the generation of complementary labels follows classconditional transition in the rest of the paper and that the transition matrix is given to the learning algorithms. What is different is that we do not assume the transition matrix to be uniform nor invertible. This allows us to make comparison in broader scenarios. In real-world scenario, the true transition matrix may be impossible to access. To loosen the assumption that the true transition matrix is given, we will analyze the case that the given matrix is *inaccurate* later. This analysis can potentially help us understand the CLL in a more realistic environment.

2.3 Recent Approaches towards CLL

Ishida et al. [8, 9] derived an *unbiased risk estimator* (URE) for arbitrary losses on the ordinary classifiers under uniform transition matrix. By setting the risk to classification error, URE can also serve as a surrogate metric for performance validation. Chou et al. [3] proposed the *surrogate complementary loss* (SCL) that employed the intuition of minimizing the likelihood of the complementary labels. They justified the principle by showing that SCL is an upper bound to a constant multiple of the ordinary classification error when the transition matrix is uniform. Yu et al. [24] proposed to use *Forward correction* (FwD) that employs the technique in noisy label learning [19, 18] to correct the softmax cross-entorpy loss by adding a transition layer to the end of the models outputs: $\bar{f}(x) = T^{\top} f(x)$, and applied cross-entorpy loss between $\bar{f}(x)$ and the complementary labels \bar{y} . Different from the methods

mentioned above, Gao & Zhang [7] did not assume class-conditional complementary transition, and directly used a *discriminative model* (DM) to estimate $P(\bar{y} | x)$. They parametrized the discriminative models by transforming the output of an ordinary classifier f as follows: $\bar{f}(x) = \operatorname{sm}(1 - f(x))$, where sm denotes the softmax function, then minimize the cross-entorpy loss between $\bar{f}(x)$ and \bar{y} .

Those methods share one common property – applying different transformation and surrogate loss functions to the ordinary classifier, as summarized in Table **??**. This paradigm, however, faces some limitations. For instance, as Chou et al. [3] points out, the URE approach suffers from the large variance in the gradients. Besides, it remains unclear how some of them behave when the transition matrix is biased. Also, those methods only studied using neural networks and linear models as base models. It is unclear how to easily cast other traditional models for CLL. These limitations motivate us to sidestep them with a different perspective—reduction to *complementary* probability estimates.

3 Proposed Framework

In this section, we propose a framework for CLL based on *complementary probability estimates* (CPE) and *decoding*. In Section 3.1, we describe the CPE framework and derive its theoretical properties. In Section 3.2, we explain how earlier approaches can be viewed as special cases in CPE. We further draw insights for earlier approaches through CPE and propose improved algorithms based on those insights.

3.1 Methodology

Overview The proposed method consists of two steps: In training phase, we aim to find a hypothesis \bar{f} that predicts the distribution of complementary labels well. That is, we want to find an \bar{f} that approximates $P(\bar{y} | x)$. This step is motivated by Yu et al. [24] and Gao & Zhang [7], which involve the idea of modeling the conditional distribution of complementary labels $P(\bar{y} | x)$, and Zhang et al. [25], which use similar idea on noisy-label learning. What is different in our framework is the decoding step during prediction. In inference phase, we propose to predict the label with closest transition vector to the predicted complementary probability estimates. Specifically, we propose to predict $\hat{y} = \operatorname{argmin}_{k \in [K]} d(\bar{f}(x), T_k)$ for an unseen instance x, where d denote a loss function. It is a natural choice to decode with respect to T because the transition vector $T_k = (P(\bar{y} = 1 | y = k), \ldots, P(\bar{y} = K | y = k))^{\top}$ is the ground-truth distribution of the complementary labels if the ordinary label is k. In the following paragraph, we provide further details of our framework. First, we discuss how to learn the distribution of the complementary labels with only one complementary label per sample. Next, we discuss the choice of the loss function for decoding and demonstrate that simply using L_1 distance can provide theoretical guarantee to the out-sample classification error.

Training Phase: Probability Estimates In this phase, we aim to find a hypothesis \overline{f} that predicts $P(\overline{y} | x)$ well. To do so, given a hypothesis \overline{f} from hypothesis set $\overline{\mathcal{H}}$, we set the following *complementary estimation loss* to optimize:

$$R(\bar{f};\ell) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\left(\ell(\bar{f}(x), P(\bar{y} \mid x, y))\right) \tag{1}$$

where ℓ can be any loss function defined between discrete probability distributions. By the assumption that complementary labels are generated with respect to the transition matrix T, the ground-truth distribution for $P(\bar{y} | x, y)$ is T_y , so we can rewrite Equation (1) as follows:

$$R(\bar{f};\ell) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\left(\ell(\bar{f}(x),T_y)\right)$$
(2)

The loss function above is still hard to optimize for two reasons: First, the presence of ordinary label y suggests that it cannot be accessed from the complementary dataset. Second, as we only have *one* complementary label per instance, it becomes questionable to directly use the empirical density, i.e., the one-hot vector of the complementary label $e_{\bar{y}}$ to approximate T_y as it may change the objective.

Here we propose to use the Kullback-Leibler divergence for the loss function to solve the two issues mentioned above with the following property:

Proposition 3.1. *There is a constant* C *such that*

$$\mathop{\mathbb{E}}_{(x,\bar{y})\sim\bar{\mathcal{D}}}\ell(\bar{f}(x),e_{\bar{y}}) + C = \mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}}\ell(\bar{f}(x),T_y)$$
(3)

holds for all hypothesis $\bar{f} \in \bar{\mathcal{H}}$ if ℓ is the KL divergence, i.e., $\ell(\hat{y}, y) = \sum_{k=1}^{K} -y_k (\log \hat{y}_k - \log y_k)$.

The result is well-known in the research of proper scoring rules [12, 21]. It allows us to replace the T_y by $e_{\bar{y}}$ in Equation (2) because the objective function only differs by a constant after the replacement. This suggests that the minimization of the two objective functions will be equivalent. Moreover, the replacement makes the objective function accessible through the complementary dataset because it only depends on the complementary label \bar{y} rather than ordinary ones.

Formally speaking, minimizing Equation (2) becomes equivalent to minimizing the following *surro-gate complementary estimation loss (SCEL)*:

$$\bar{R}(f;\ell) = \mathbb{E}_{(x,\bar{y})\sim\bar{\mathcal{D}}}\left(\ell(f(x), e_{\bar{y}})\right) \tag{4}$$

By using KL divergence as the loss function, we have that

$$\bar{R}(\bar{f};\ell) = \mathbb{E}_{(x,\bar{y})\sim\bar{\mathcal{D}}}\left(-\log\bar{f}_{\bar{y}}(x)\right)$$
(5)

with $\bar{f}_{\bar{y}}(x)$ being the \bar{y} -th output of $\bar{f}(x)$. Next, we can use the following empirical version as the training objective: $\frac{1}{N} \sum_{i=1}^{N} -\log \bar{f}_{\bar{y}_i}(x_i)$. According to the empirical risk minimization (ERM) principle, we can estimate the distribution of complementary labels $P(\bar{y} \mid x)$ by minimizing the log loss on the complementary dataset. That is, by choosing \bar{f}^* with $\bar{f}^* = \operatorname{argmin}_{\bar{f} \in \bar{\mathcal{H}}} \frac{1}{N} \sum_{i=1}^{N} -\log \bar{f}_{\bar{y}_i}(x_i)$, we can get an estimate of $P(\bar{y} \mid x)$ with \bar{f}^* .

In essence, we reduce the task of learning from complementary labels into learning probability estimates for multi-class classification (on the *complementary label space*). As the multi-class probability estimates is a well-researched problem, our framework becomes flexible on the choice of the hypothesis set. For instance, one can use K-Nearest Neighbor or Gradient Boosting with log loss to estimate the distribution of complementary labels. The flexibility is superior to the previous methods because previous methods rely on using neural networks to minimize specific surrogate losses, which would be hard to optimize for non-differentiable models. In contrast, the proposed methods enable existing ordinary models to learn from complementary labels.

Inference Phase: Decoding After finding a complementary probability estimator \overline{f}^* during the training phase, we propose to predict the ordinary label by decoding: Given an unseen example x, we predict the label \hat{y} whose transition vector $T_{\hat{y}}$ is closest to the predicted complementary probability estimates. That is, the label is predicted by

$$\hat{y} = \operatorname*{argmin}_{k \in [K]} d\left(\bar{f}^*(x), T_k\right) \tag{6}$$

where d could be an arbitrary loss function on the probability simplex and T_k is the k-th row vector of T. We use $dec(\bar{f};d)$ to denote the function that decodes the output from \bar{f} according to the loss function d. The next problem is whether the prediction of the decoder can guarantee a small out-sample classification error $R_{01}(f) = \mathbb{E}_{(x,y)\sim \mathcal{D}} I_{f(x)\neq y}$.

We propose to use a simple decoding step by setting L_1 distance as the loss function for decoding:

$$\det(\bar{f}; L_1)(x) = \underset{y \in [K]}{\operatorname{argmin}} \|T_y - \bar{f}(x)\|_1$$
(7)

This choice of L_1 distance makes the decoding step easy to perform and provides the following bound that quantifies the relationship between the error rate and the quality of probability estimator:

Proposition 3.2. For any $\overline{f} \in \overline{\mathcal{H}}$, and distance function d defined on the probability simplex Δ^K , it holds that

$$R_{01}\left(\operatorname{dec}(\bar{f};d)\right) \le \frac{2}{\gamma_d} R(\bar{f};d) \tag{8}$$

where $\gamma_d = \min_{i \neq j} d(T_i, T_j)$ is the minimal distance between any pair of transition vector. Moreover, if d is the L_1 distance and ℓ is the KL divergence, then with $\gamma = \min_{i \neq j} ||T_i - T_j||_1$, it holds that

$$R_{01}\left(\operatorname{dec}(\bar{f};L_1)\right) \le \frac{4\sqrt{2}}{\gamma}\sqrt{R(\bar{f};\ell)} \tag{9}$$

The proof is in Appendix A.2. In the realizable case, where there is a target function g that satisfies g(x) = y for all instances, the term $R(\bar{f}; \ell_{\text{KL}})$ can be minimized to zero with $\bar{f}^* : x \mapsto T_{g(x)}$. This indicates that for a sufficiently rich complementary hypothesis set, if the complementary probability estimator is consistent $(\bar{f} \to \bar{f}^*)$ then the L_1 decoded prediction is consistent $(R_{01}(\operatorname{dec}(\bar{f}; L_1)) \to T_{01})$

Table 2: A unifying view of earlier approaches and proposed algorithms through the lens of reduction to probability estimates, where U denote the uniform transition matrix. Two versions of Forward Correction are considered: General T denotes the original version in [24], and the Uniform denotes the case when the transition layer is fixed to be uniform. Proof of the equivalence is in Appendix B.

Метнор	Hypothesis set	DECODER
Fwd (general <i>T</i>) [24] Fwd (uniform) [24] SCL [3] DM [7]	$ \begin{split} & \{x \mapsto T^{\top}f(x;\theta): \theta \in \Theta\} \\ & \{x \mapsto U^{\top}f(x;\theta): \theta \in \Theta\} \\ & \{x \mapsto U^{\top}f(x;\theta): \theta \in \Theta\} \\ & \{x \mapsto \mathrm{sm}(1-f(x;\theta)): \theta \in \Theta\} \end{split} $	$\begin{split} & \operatorname{argmax}_k((T^\top)^{-1}\bar{f}(x))_k \\ & \operatorname{argmin}_k \ \bar{f}(x) - U_k\ _1 \\ & \operatorname{argmin}_k \ \bar{f}(x) - U_k\ _1 \\ & \operatorname{argmin}_k \ \bar{f}(x) - U_k\ _1 \end{split}$
CPE-I (NO TRANSITION LAYER) CPE-F (FIXED TRANSITION LAYER TO T) CPE-T (TRAINABLE TRANSITION LAYER)	$ \begin{aligned} & \{x \mapsto f(x;\theta) : \theta \in \Theta\} \\ & \{x \mapsto T^{\top}f(x;\theta) : \theta \in \Theta\} \\ & \{x \mapsto T(W)^{\top}f(x;\theta) : \theta \in \Theta, W \in \mathbb{R}^{K \times K}\} \end{aligned} $	$\begin{aligned} \operatorname*{argmin}_k \ \bar{f}(x) - T_k\ _1 \\ \operatorname*{argmin}_k \ \bar{f}(x) - T_k\ _1 \\ \operatorname*{argmin}_k \ \bar{f}(x) - T_k\ _1 \end{aligned}$

0). The result suggests that the performance of the L_1 decoder can be bounded by the accuracy of the probability estimates of complementary labels measured by the KL divergence. In other words, to obtain an accurate ordinary classifier, it suffices to find an accurate complementary probability estimator followed by the L_1 decoding. Admittedly, in the non-realizable case, $R(\bar{f}; \ell_{\rm KL})$ contains irreducible error. We leave the analysis of the error bound in this case for the future research.

Another implication of the Proposition 3.2 is related to the inaccurate transition matrix. Suppose the complementary labels are generated with respect to the transition matrix T', which may be different from T, the one provided to the learning algorithm. In the proposed framework, the only affected component is the decoding step. This allows us to quantify the effect of inaccuracy as follows:

Corollary 3.3. For any $\overline{f} \in \overline{\mathcal{H}}$, if d is the L_1 distance and ℓ is the KL divergence, then

$$R_{01}\left(\operatorname{dec}(f;L_1)\right) \le \frac{4\sqrt{2}}{\gamma}\sqrt{R(\bar{f};\ell)} + \frac{2\epsilon}{\gamma}.$$
(10)

where $\gamma = \min_{i \neq j} ||T_i - T_j||_1$ is the minimal L_1 distance between pairs of transition vectors, and $\epsilon = \max_{k \in [K]} ||T'_k - T_k||_1$ denotes the difference between T' and T.

Validation Phase: Quality of Probability Estimates The third implication of Proposition 3.2 is an alternative validation procedure to the unbiased risk estimation (URE) [8]. According to Proposition 3.2, selecting the best-performing parameter minimizes the RHS of Eq. (9) among all hyper-parameter choices minimizes the ordinary classification error. This suggests an alternative metric for parameter selection: using the surrogate complementary estimation loss (SCEL) on the validation dataset.

Although the proposed validation procedure does not directly estimate the ordinary classification error, it provides benefits in the scenarios where URE does not work well. For instance, when the transition matrix is non-invertible, the behavior of URE is ill-defined due to the presence of T^{-1} in the formula of URE: $\mathbb{E}_{x,\bar{y}} e_{\bar{y}} T^{-1} \ell(f(x))$. Indeed, replacing T^{-1} with T's pseudo-inverse can avoid the issue; however, it remains unclear whether the unbiasedness of URE still holds after using pseudo-inverse. In contrast, the quality of complementary probability estimates sidesteps the issue because it does not need to invert the transition matrix. This prevents the proposed procedure from the issue of an ill-conditioned transition matrix.

3.2 Connection to Previous Methods

The proposed method may seem different from the previous methods because the learning procedure is on the complementary label space rather than ordinarylabel space. Nonetheless, the proposed framework can explain several earlier approaches as its special cases, including (1) Forward Correction (FwD) [24], (2) Surrogate Complementary Loss (SCL) with log loss [3], and (3) Discriminative Model (DM) [7]. We summarize how they fit in our complementary probability estimates framework in Table 2, and provide the proof of equivalence in Appendix B. By viewing those earlier approaches in the proposed framework, we provide additional benefits for them. First, we can apply the novel validation process on them for parameter selection. This allows us to use an alternative way to validate those approaches. Also, we fill the gap on the theoretical explanation to help understand those approaches in the realizable case.

On the other hand, the success of FWD inspires us to reconsider the role of transition layers in the framework. As the base model's output $f(x;\theta)$ is in the probability simplex Δ^K , the model's output $T^{\top}f(x;\theta)$ lies in the convex hull formed by the row vectors of T. If the transition matrix T provided to the learning algorithm is accurate, then such transformation helps control the model's complexity by restricting its output. The restriction may be wrong, however, when the given transition matrix T is inaccurate. To address this issue, we propose to allow the transition layer to be *trainable*. This technique is also used in label-noise learning, such as [14]. Specifically, we propose three methods in our Complementary Probability Estimates framework: (a) **CPE-I** denotes a model *without* a transition layer (b) **CPE-F** denotes a model with a *fixed* additional layer to T (c) **CPE-T** denotes a model with a *trainable* transition layer. To make the transition layer trainable, we considered a $K \times K$ matrix W. A softmax function was applied to each row of W to transform it into a valid transition matrix $T(W) = (\operatorname{sm}(W_1), \operatorname{sm}(W_2), \ldots, \operatorname{sm}(W_K))^{\top}$. For a base model f, the complementary probability estimates of **CPE-T** for a given instance x would be $T(W)^{\top} f(x;\theta)$. Note that we use the L_1 decoder for **CPE-I**, **CPE-F**, and **CPE-T**.

We also draw the following observations by viewing earlier approaches with the proposed framework: *Remark* 3.4. By viewing FWD with the proposed framework, we can see in Table 2, the equivalent decoder is different from L_1 decoding. Intuitively, it converts the complementary probability estimates back to ordinary probability estimates and predicts the largest one. We name it MAX decoding for future reference.

Remark 3.5. If the transition matrix is uniform, then FWD and SCL with log loss match. The result suggests that they are exactly the same method, and explain why we see similar performances on the two methods in the Chou el al.'s experiment [2020]. The similarity between the two methods was also reproduced in our experiment in Section 4.1 and reported in Table 3.

Remark 3.6. DM was proposed to lift the generation assumption of complementary labels [7]. However, from the view of the proposed framework, DM implicitly assumes the complementary labels are generated uniformly, as we can see from the decoder. This provides an alternative explanation why its performance deteriorates as the transition matrix deviates from the uniform matrix, as shown in Gao and Zhang's experiment [2021].

4 **Experiments**

In Section 4.1 and 4.2, we benchmarked the proposed framework to state-of-the-art baselines and discussed the following questions through the experimental results: (a) Can the transition layers in the proposed CPE improve the model's performance? (b) Is the proposed L_1 decoding competitive to the more complex MAX? (c) Does the transition matrix provide information to the learning algorithms even if it is inaccurate? We further demonstrated the flexibility of incorporating traditional models in **CPE** in Section 4.3 and verified the effectiveness of the proposed validation procedure in Section 4.4.

4.1 Comparison on Clean Transition Matrix

Setup We first evaluated CPE and other baselines under the standard CLL setting where the correct transition matrix T is given to the learner. The baselines include the following state-of-the-art methods: (a) **URE-GA**: Gradient Ascent applied on the unbiased risk estimator [8, 9], (b) **Fwd**: Forward Correction [24], (c) **SCL**: Surrogate Complementary Loss with negative log loss [3], and (d) **DM**: Discriminative Models with Weighted Loss [7]. We did not include consistency regularization [20] in the experiment to prevent introducing extra factors and simplify the comparison. Three types of transition matrices are benchmarked in the experiment. Besides the uniform transition matrix, following Yu et al. [24], Gao & Zhang [7], we generated two biased ones as follows: For each class y, the complementary classes $\mathcal{Y} \setminus \{y\}$ are first randomly split into three subsets. Within each subset, the probabilities are set to p_1 , p_2 and p_3 , respectively. We consider two cases for (p_1, p_2, p_3) : (a) *Strong*: $(\frac{0.75}{3}, \frac{0.24}{3}, \frac{0.01}{3})$ to model stronger deviation from uniform transition matrix. (b) *Weak*: $(\frac{0.45}{3}, \frac{0.30}{3}, \frac{0.25}{3})$ to model milder deviation from uniform transition matrix.

Following the previous work, we test those methods on MNIST, Fashion-MNIST, and Kuzushiji-MNIST, and use the linear and one-layer mlp model (d-500-c) as base models. We report the performance of mlp models in this section and leave the results of linear models in the Appendix. All models are optimized using Adam with learning rate selected from {1e-3, 5e-4, 1e-4, 5e-5, 1e-5} and

	MNIST			FASHION-MNIST			KUZUSHIJI-MNIST		
	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG
URE-GA SCL DM FWD CPE-I CPE-F CPE-T	$90.3 \pm 0.2 94.3 \pm 0.4 91.9 \pm 0.6 94.4 \pm 0.2 90.2 \pm 0.2 94.4 \pm 0.2 92.8 \pm 0.6 93.8 \pm 0.6 94.4 \pm 0.2 94.4 \pm 0.2 94.4 \pm 0.2 94.4 \pm 0.2 95.8 \pm 0.6 \\95.8 \pm 0.6 \\$	87.8 ± 0.9 93.8 \pm 0.4 90.2 \pm 0.3 91.9 \pm 0.3 88.4 \pm 0.3 92.0 \pm 0.2 92.1 \pm 0.2	33.8±8.1 27.5±19.8 26.7±4.6 95.3±0.4 92.7±0.8 95.5±0.3 95.2±0.5	$79.4 \pm 0.7 \\82.6 \pm 0.4 \\82.5 \pm 0.3 \\82.6 \pm 0.6 \\81.1 \pm 0.3 \\83.0 \pm 0.1 \\83.0 \pm 0.1$	$75.7 \pm 2.0 \\ 81.2 \pm 0.1 \\ 80.3 \pm 1.1 \\ 83.0 \pm 1.0 \\ 79.2 \pm 0.5 \\ 83.0 \pm 0.3 \\ 83.$	32.3±4.5 28.5±10.8 24.8±5.0 85.5±0.3 81.9±1.4 85.8±0.3 85.8±0.3	$\begin{array}{c} 65.6 \pm 0.8 \\ \textbf{73.7} \pm \textbf{1.4} \\ 65.6 \pm 2.9 \\ 73.5 \pm 1.6 \\ 66.2 \pm 1.0 \\ 73.5 \pm 1.6 \\ 63.6 \pm 0.4 \end{array}$	$\begin{array}{c} 62.5 \pm 1.1 \\ \textbf{71.2} \pm 2.9 \\ 64.5 \pm 2.7 \\ 63.1 \pm 2.6 \\ 62.5 \pm 0.9 \\ 64.6 \pm 0.5 \\ 64.6 \pm 0.4 \end{array}$	$23.3 \pm 5.4 20.7 \pm 4.8 20.1 \pm 3.2 74.1 \pm 4.8 73.7 \pm 1.0 75.3 \pm 2.6 74.2 \pm 2.8 74.2 \pm 2.8 74.2 \pm 2.8 75.3 \pm 2.6 \75.3 \pm 2.6 \75$

Table 3: Comparison of the testing classification accuracies with different transition matrices.

Table 4: Comparison of the testing classification accuracies with different levels of noise.

	MNIST				FASHION-MNIST			KUZUSHIJI-MNIST		
	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	
URE-GA	31.8 ± 6.4	27.8 ± 8.2	28.1 ± 4.1	27.3 ± 5.5	28.6 ± 4.1	26.3 ± 2.0	24.5 ± 4.6	21.1 ± 2.2	19.8 ± 2.1	
SCL	25.1 ± 11.7	24.7 ± 8.9	23.8 ± 2.7	26.6 ± 9.2	20.6 ± 6.7	23.2 ± 5.7	20.4 ± 4.6	17.3 ± 2.9	16.8 ± 1.6	
DM	26.5 ± 9.1	24.6 ± 6.5	22.6 ± 1.3	24.1 ± 5.1	23.6 ± 6.7	22.6 ± 2.9	20.0 ± 3.0	19.2 ± 3.1	18.2 ± 1.6	
Fwd	88.3 ± 8.7	83.9 ± 10.7	71.6 ± 18.4	84.8 ± 0.6	80.2 ± 6.2	62.9 ± 20.1	72.8 ± 5.6	67.6 ± 7.5	54.7 ± 12.4	
CPE-I	92.4 ± 0.7	92.0 ± 0.8	87.6 ± 1.4	81.7 ± 1.4	81.3 ± 1.4	78.2 ± 1.5	73.0 ± 0.7	71.6 ± 0.9	62.7 ± 1.6	
CPE-F	94.3 ± 0.5	93.6 ± 0.5	89.0 ± 1.4	84.1 ± 0.8	83.0 ± 1.1	78.4 ± 2.5	76.1 ± 1.3	73.7 ± 1.5	63.7 ± 1.5	
CPE-T	$94.4{\pm}~0.5$	$93.7 {\pm}~0.5$	89.6 ± 0.9	84.1 ± 0.8	$83.2{\pm}~1.1$	78.9 ± 2.0	$76.1{\pm}~1.3$	$\textbf{73.9} \pm \textbf{1.6}$	64.2 ± 1.2	

a fixed weight decay 1e-4 for 300 epochs. The learning rate for **CPE** is selected with the Surrogate Complementary Estimation Loss (SCEL) on the validation dataset. For the baseline method, it is selected with unbiased risk estimator (URE) of the zero-one loss. It is worth noting that the validation datasets consist of only complementary labels, which is different from some previous works. Other experimental details are provided in Appendix D. The results are reported in Table 3.

Can Transition Layers Improve Performance? In Table 3, it is displayed that **CPE-F** and **CPE-T** outperform **CPE-I**, demonstrating that transition layers help achieve higher performances. Also, **CPE-F** achieve slightly better accuracies than **CPE-T**. To understand the reason behind the difference, we compared their training and validation loss in Figure 1 in Appendix D.2. In the figure, fixed or trainable transition layers achieve smaller training loss for linear models, demonstrating its ability in increasing the model's complexity. On the other hand, mlp model achieves small training loss without a transition layer but is prone to overfit. We conclude that transition layers improve model's ability to fit the distribution of complementary labels when the model is simple. Although the improvement becomes marginal when the model is complex enough, it provides better generalization performance. Overall, adding transition layers produce better testing accuracies when the transition matrix is clean.

Is L_1 competitive with MAX? As analyzed in Section 3.2, Fwd and CPE-F only differ in the decoding step, with the former using MAX and the latter using L_1 . In Table 3, Fwd and CPE-F have similar testing accuracies, suggesting the competitivity of L_1 decoding despite its simplicity. To eliminate the difference in the validation procedure, we provide testing accuracies when both methods use SCEL to select parameters in Table 8 in Appendix D.2. It is displayed that Fwd outperforms CPE-F only marginally, demonstrating that MAX has a small edge to L_1 but not much.

Discussion of T-**agnostic models** Among the baseline methods, **URE-GA**, **SCL** and **DM** are ones that does not take T as inputs or assumes T is uniform, which we called T-agnostic models. It is shown that those models perform well when the transition matrix is just slightly deviated from the uniform one. Their performances all dropped when the deviation from uniform becomes larger. As we discussed in Section 3.2, the result can be interpreted to be caused by their implicit assumption on uniform transition matrix, which brings great performance on uniform transition matrix but worse performance on biased ones. In contrast, we observed that all variations of CPE have similar testing accuracies across different transition matrices, demonstrating that CPE does exploit the information from the transition matrix that helps the models deliver better performance.

4.2 Robustness to Noisy Transition Matrix

Setup As in ordinary dataset, it is possible that the complementary labels are noisy. Such scenarios are explored in this experiment. Specifically, we consider the *Strong* deviation transition matrix T_{strong} to be the clean transition matrix, and a uniform noise transition matrix $\frac{1}{K} \mathbf{1}_K$ to model the

Table 5: Comparison of testing classification accuracies of CPE with traditional models.	Boldfaced
ones outperform the baseline methods based on single-layer deep models.	

		MNIST		F	FASHION-MNIS	Т	KUZUSHIJI-MNIST		
MODEL	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG
CPE-KNN CPE-GBDT	$\begin{array}{c} 93.1 {\pm}~0.1 \\ 86.9 {\pm}~0.4 \end{array}$	$\begin{array}{c} 92.6 \pm \ 0.1 \\ 86.0 \pm \ 0.3 \end{array}$	$\begin{array}{c} 94.5 \pm \ 0.4 \\ 90.3 \pm \ 0.9 \end{array}$	$\begin{array}{c} 79.1 \pm \ 0.4 \\ 79.8 \pm \ 0.4 \end{array}$	$\begin{array}{c} 77.8 \pm \ 0.6 \\ 78.0 \pm \ 0.4 \end{array}$	$\begin{array}{c} 79.0 \pm \ 1.7 \\ 81.4 \pm \ 1.1 \end{array}$	$\begin{array}{c} \textbf{74.9} \pm \textbf{0.8} \\ \textbf{60.6} \pm \textbf{0.4} \end{array}$	73.7±0.8 56.6±1.8	80.4 ± 1.3 68.4± 2.1
	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$
CPE-KNN CPE-GBDT	$\begin{array}{c} 93.7 {\pm}~0.4 \\ 89.7 {\pm}~1.0 \end{array}$	$\begin{array}{c} 93.4 {\pm}~0.4 \\ 88.6 {\pm}~1.2 \end{array}$	91.9± 1.1 84.0± 1.7	$\begin{array}{c} 78.7 \pm \ 1.9 \\ 80.6 \pm \ 1.7 \end{array}$	$\begin{array}{c} 78.5 \pm 1.9 \\ 80.0 \pm 1.6 \end{array}$	$\begin{array}{c} 76.6 {\pm}~1.9 \\ 76.0 {\pm}~2.2 \end{array}$	$\begin{array}{c} \textbf{77.2} \pm \textbf{1.1} \\ \textbf{66.7} \pm \textbf{2.4} \end{array}$	75.9±1.6 64.7±2.4	73.2 ± 1.7 55.8± 3.1

noisy complementary label generation. We generated complementary labels with the transition matrix $(1 - \lambda)T_{\text{strong}} + \lambda \frac{1}{K} \mathbf{1}_K$, but provided T_{strong} and the generated complementary dataset to the learners. The parameter λ controls the proportion of the uniform noise in the complementary labels. The testing accuracy is reported in Table 4.

Can Transition Layers Improve Performance? Table 4 displays that **CPE-F** and **CPE-T** outperform **CPE-I**, demonstrating that transition layers can improve the testing accuracies despite the provided transition matrix is inaccurate. When λ is large, we observe that **CPE-T** outperforms **CPE-F** in Table 4, and that **CPE-T** has smaller training loss than **CPE-F** in Figure 2. It suggests that by making transition layers trainable, the model can fit the distribution of complementary labels better by altering the transition layer. In contrast, **CPE-F** is restricted to a wrong output space, making it underperform **CPE-T**. The difference makes **CPE-T** a better choice for noisy environment.

Is L_1 competitive with MAX? Table 4 displays that CPE-F outperforms Fwd, especially when λ is larger. This results suggests that L_1 decoding employed by CPE-F is both simple and more tolerant than MAX decoding in noisy environments where the transition matrix becomes inaccurate. In Table 8 in Appendix D.2, we compare them using the same validation procedure. It is displayed that Fwd is better when λ is small whereas CPE-F is better when λ is large after fixing validation procedure. This result further confirms that L_1 decoding is more robust to an inaccurate transition matrix than MAX decoding.

Discussion of T-agnostic models Table 4 displays that T-agnostic models (**URE-GA**, **SCL**, **DM**) perform similarly under different levels of noise. This is expected because their prediction does not rely on the provided transition matrix and hence should not be affected by a wrong one. On the other hand, all variants of **CPE** show solid tolerance against noise. The testing accuracies deteriorate as the noise level rise, but overall they outperform T-agnostic methods by a large margin. We conclude that even if the provided transition matrix is inaccurate, **CPE** is still able to exploit its information and produce a better model.

4.3 Learn from CL with Traditional Methods

As discussed in Section 3, the proposed framework is not constrained by deep models. We explored the possibility of applying traditional methods to learn from CL, including (a) k-Nearest Neighbor (k-NN) and (b) Gradient Boosting Decision Tree (**GBDT**). We benchmarked those models in the same settings in Section 4.1 and 4.2. The testing accuracy reported in Table 5 displays that traditional models, specifically, k-NN, outperform than all the methods using deep models in Kuzushiji-MNIST, indicating the benefit of the proposed CPE's flexibility in using non-deep models.

4.4 Comparison of the validation procedure

Does SCEL Select Better Parameters for CPE? We conducted an additional validation procedure by selecting the parameters with the smallest URE on the validation dataset, compared the testing accuracies of the selected parameters, and reported the results in Table 9. It is displayed that the parameters selected by SCEL has better testing accuracies to the ones selected by URE in most scenarios. We further observed that as the noise level rises, the parameters selected by URE tended to be unstable and worse in testing accuracies, whereas SCEL did not exhibit such issue. The result demonstrated the superiority of SCEL over URE in terms of parameter selection even if it does not have the unbiased property as URE.

Does SCEL Select Better Parameters for Fwd? It is worth noting that SCEL could be applied to the earlier approaches by casting them in the proposed CPE framework. We explored whether SCEL selects better parameters for **Fwd** as we observed in the previous experiment and reported the results in Table 10. It is demonstrated that the parameters selected by SCEL outperform those selected by URE in almost all settings. Although SCEL is designed for the proposed CPE framework, the result demonstrated that SCEL can be applied to some earlier approaches and allows them to use a more robust approach to validate models.

5 Conclusion

In this paper, we view the CLL problem from a novel perspective, reduction to complementary probability estimates. Through this perspective, we propose a framework that only requires complementary probability estimates and prove that a simple decoding step can map the estimates to ordinary labels. The framework comes with a theoretically justified validation procedure, provable tolerance in noisy environment, and flexibility of incorporating non-deep models. Empirical experiments further verify the effectiveness and robustness of the proposed framework under broader scenarios, including non-uniform and noisy complementary label generation. We expect the realistic elements of the framework to keep inspiring future research towards making CLL practical.

References

- [1] Cao, Y., Liu, S., and Xu, Y. Multi-complementary and unlabeled learning for arbitrary losses and models. *Pattern Recognition*, 124:108447, 2022.
- [2] Chapelle, O., Schölkopf, B., and Zien, A. Semi-supervised learning. adaptive computation and machine learning series, 2006.
- [3] Chou, Y.-T., Niu, G., Lin, H.-T., and Sugiyama, M. Unbiased risk estimators can mislead: A case study of learning with complementary labels. In *International Conference on Machine Learning*, pp. 1929–1938. PMLR, 2020.
- [4] Clanuwat, T., Bober-Irizar, M., Kitamoto, A., Lamb, A., Yamamoto, K., and Ha, D. Deep learning for classical japanese literature, 2018.
- [5] Elkan, C. and Noto, K. Learning classifiers from only positive and unlabeled data. In Proceedings of the 14th ACM SIGKDD international conference on Knowledge discovery and data mining, pp. 213–220, 2008.
- [6] Feng, L., Kaneko, T., Han, B., Niu, G., An, B., and Sugiyama, M. Learning with multiple complementary labels. In *International Conference on Machine Learning*, pp. 3072–3081. PMLR, 2020.
- [7] Gao, Y. and Zhang, M.-L. Discriminative complementary-label learning with weighted loss. In International Conference on Machine Learning, pp. 3587–3597. PMLR, 2021.
- [8] Ishida, T., Niu, G., Hu, W., and Sugiyama, M. Learning from complementary labels. In Proceedings of the 31st International Conference on Neural Information Processing Systems, pp. 5644–5654, 2017.
- [9] Ishida, T., Niu, G., Menon, A., and Sugiyama, M. Complementary-label learning for arbitrary losses and models. In *International Conference on Machine Learning*, pp. 2971–2980. PMLR, 2019.
- [10] Jin, R. and Ghahramani, Z. Learning with multiple labels. In NIPS, volume 2, pp. 897–904. Citeseer, 2002.
- [11] Katsura, Y. and Uchida, M. Bridging ordinary-label learning and complementary-label learning. In Asian Conference on Machine Learning, pp. 161–176. PMLR, 2020.
- [12] Kull, M. and Flach, P. Novel decompositions of proper scoring rules for classification: Score adjustment as precursor to calibration. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pp. 68–85. Springer, 2015.

- [13] LeCun, Y., Cortes, C., and Burges, C. Mnist handwritten digit database. ATT Labs [Online]. Available: http://yann.lecun.com/exdb/mnist, 2, 2010.
- [14] Li, X., Liu, T., Han, B., Niu, G., and Sugiyama, M. Provably end-to-end label-noise learning without anchor points. In Meila, M. and Zhang, T. (eds.), *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pp. 6403–6413. PMLR, 18–24 Jul 2021.
- [15] Liu, J., Hang, H., Wang, B., Li, B., Wang, H., Tian, Y., and Shi, Y. Gan-cl: Generative adversarial networks for learning from complementary labels. *IEEE Transactions on Cybernetics*, 2021.
- [16] Lu, N., Niu, G., Menon, A. K., and Sugiyama, M. On the minimal supervision for training any binary classifier from only unlabeled data. In *International Conference on Learning Representations*, 2018.
- [17] Natarajan, N., Dhillon, I. S., Ravikumar, P. K., and Tewari, A. Learning with noisy labels. *Advances in neural information processing systems*, 26:1196–1204, 2013.
- [18] Patrini, G., Rozza, A., Krishna Menon, A., Nock, R., and Qu, L. Making deep neural networks robust to label noise: A loss correction approach. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 1944–1952, 2017.
- [19] Sukhbaatar, S., Bruna, J., Paluri, M., Bourdev, L., and Fergus, R. Training convolutional networks with noisy labels. *arXiv preprint arXiv:1406.2080*, 2014.
- [20] Wang, D.-B., Feng, L., and Zhang, M.-L. Learning from complementary labels via partial-output consistency regularization. In Zhou, Z.-H. (ed.), *Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence, IJCAI-21*, pp. 3075–3081. International Joint Conferences on Artificial Intelligence Organization, 8 2021. doi: 10.24963/ijcai.2021/423. Main Track.
- [21] Williamson, R. C., Vernet, E., and Reid, M. D. Composite multiclass losses. Journal of Machine Learning Research, 17(222):1-52, 2016. URL http://jmlr.org/papers/v17/ 14-294.html.
- [22] Xiao, H., Rasul, K., and Vollgraf, R. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms. arXiv preprint arXiv:1708.07747, 2017.
- [23] Xu, Y., Gong, M., Chen, J., Liu, T., Zhang, K., and Batmanghelich, K. Generative-discriminative complementary learning. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pp. 6526–6533, 2020.
- [24] Yu, X., Liu, T., Gong, M., and Tao, D. Learning with biased complementary labels. In *Proceedings of the European conference on computer vision (ECCV)*, pp. 68–83, 2018.
- [25] Zhang, M., Lee, J., and Agarwal, S. Learning from noisy labels with no change to the training process. In *International Conference on Machine Learning*, pp. 12468–12478. PMLR, 2021.
- [26] Zhang, Y., Liu, F., Fang, Z., Yuan, B., Zhang, G., and Lu, J. Learning from a complementarylabel source domain: Theory and algorithms. *IEEE Transactions on Neural Networks and Learning Systems*, 2021.
- [27] Zhou, Z.-H. A brief introduction to weakly supervised learning. *National science review*, 5(1): 44–53, 2018.

Checklist

- 1. For all authors...
 - (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes] See Abstract and Section 1
 - (b) Did you describe the limitations of your work? [Yes] For instance, see Section 3.1
 - (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Appendix C

- (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
- 2. If you are including theoretical results...
 - (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Section 2.2 and Section 3.1
 - (b) Did you include complete proofs of all theoretical results? [Yes] see Appendix A
- 3. If you ran experiments...
 - (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] see Appendix D
 - (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] see Appendix D
 - (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes]
 - (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] see Appendix D
- 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...(a) If your work uses existing assets, did you cite the creators? [Yes] See Appendix D
 - (a) If your work uses existing assets, did you cite the creators? [Yes] See Appendix I
 - (b) Did you mention the license of the assets? [Yes] See Appendix D
 - (c) Did you include any new assets either in the supplemental material or as a URL? [Yes]
 - (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
 - (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
- 5. If you used crowdsourcing or conducted research with human subjects...
 - (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
 - (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
 - (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

A Proofs

This section provides the proofs for the propositions, theorems claimed in the main text.

A.1 Proof of Proposition 3.1

First, set $C = \mathbb{E}_{(x,y)\sim \mathcal{D}} \sum_{k=1}^{K} T_{yk} \log(T_{yk})$, then

$$\mathbb{E}_{(x,y)\sim\mathcal{D}}\ell(\bar{f}(x),T_y) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\sum_{k=1}^K -T_{yk}\log\left(\frac{\bar{f}_k(x)}{T_{yk}}\right) = C + \mathbb{E}_{(x,y)\sim\mathcal{D}}\sum_{k=1}^K -T_{yk}\log(\bar{f}_k(x))$$
(11)

Next, as $P(\bar{y} | y) = T_{y\bar{y}}$, then

$$\mathbb{E}_{(x,y)\sim\mathcal{D}}\sum_{k=1}^{K} -T_{yk}\log(\bar{f}_k(x)) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\left(\mathbb{E}_{\bar{y}\mid y} - \log(\bar{f}_{\bar{y}}(x))\right) = \mathbb{E}_{(x,\bar{y})\sim\bar{\mathcal{D}}}\ell(\bar{f}(x), e_{\bar{y}})$$
(12)

Hence, $\mathbb{E}_{(x,y)\sim\mathcal{D}} \ell(\bar{f}(x), T_y) = C + \mathbb{E}_{(x,\bar{y})\sim\bar{\mathcal{D}}} \ell(\bar{f}(x), e_{\bar{y}}).$

A.2 Proof of Proposition 3.2

Let I_A denote the indicator function of event A, then using Markov's inequality on the random variable $d(\bar{f}(x), T_y)$, we have

$$R_{01}\left(\operatorname{dec}(\bar{f};d)\right) \le P\left(d(\bar{f}(x),T_y) \ge \frac{\gamma_d}{2}\right) \le \frac{2}{\gamma_d} \mathbb{E}\left[d(\bar{f}(x),T_y)\right] = \frac{2}{\gamma_d} R(\bar{f};d)$$
(13)

To see the first inequality holds, note that if $d(\bar{f}(x), T_y) < \frac{\gamma_d}{2}$, then for any incorrect class $y' \neq y$, we have

$$d(\bar{f}(x), T_{y'}) \ge d(T_y, T_{y'}) - d(T_y, \bar{f}(x)) \ge \frac{\gamma_d}{2}$$
(14)

by triangular inequality and the definition of γ_d . As a result, the decoder decodes $\bar{f}(x)$ to the correct class y if $d(\bar{f}(x), T_y) < \frac{\gamma_d}{2}$. This completes the first part of the Proposition.

Next, by Pinsker's inequality and Jensen's inequality, we have that

$$R(\bar{f};L_1) = \mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}} \left\| \bar{f}(x) - T_y \right\|_1$$
(15)

$$\leq 2 \mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}} \sqrt{2\ell_{\mathrm{KL}}(\bar{f}(x), T_y)} \tag{16}$$

$$\leq 2\sqrt{2\mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}}\ell_{\mathrm{KL}}(\bar{f}(x),T_y)} = 2\sqrt{2R(\bar{f};\ell_{\mathrm{KL}})}$$
(17)

According to the above inequality and the results of the first part, the proof for the second part is now complete.

A.3 Proof of Corollary 3.3

The decoding step remains the same when $T' \neq T$ because the decoder uses the same transition matrix T to decode. The only difference is in the complementary probability estimates. Specifically, we have that the complementary estimation loss becomes $R(\bar{f}; \ell) = \mathbb{E}_{(x,y)\sim \mathcal{D}} \left(\ell(\bar{f}(x), T'_y)\right)$ as the complementary labels are generated with respect to T'.

Hence, the last equality in Equation (13) is no longer correct. Instead, we use the following:

$$\mathbb{E}\left[d(\bar{f}(x), T_y)\right] \le \mathbb{E}\left[d(\bar{f}(x), T'_y) + d(T'_y, T_y)\right] \le \mathbb{E}\left[d(\bar{f}(x), T'_y)\right] + \epsilon$$
(18)

to obtain that $R_{01}(\operatorname{dec}(\bar{f};d)) \leq \frac{2}{\gamma_d}R(\bar{f};d) + \frac{2\epsilon}{\gamma_d}$. Then, we can use Pinsker's inequality and Jensen's inequality as in (15) to get

$$R_{01}\left(\operatorname{dec}(f;L_1)\right) \le \frac{4\sqrt{2}}{\gamma}\sqrt{R(\bar{f};\ell)} + \frac{2\epsilon}{\gamma}.$$
(19)

B **Details of the Connections between Proposed Framework and Previous Methods**

In this section, we provide further details about how our framework can explain several previous methods as its special cases. Across this section, we let $f(\cdot; \theta)$ denote the base model parametrized by $\theta \in \Theta$.

Forward Correction In the training phase, Forward Correction optimizes the following loss functions:

$$L_{\text{Fwd}}(\theta) = \frac{1}{N} \sum_{i=1}^{N} -\log\left(T^{\top} f(x_i; \theta)\right)_{\bar{y}_i}$$
(20)

In the inference phase, Forward Correction predicts $\hat{y} = \operatorname{argmax}_k f_k(x)$ for an unseen instance x. We claim that Forward Correction is equivalent to CPE with the following parameters when T is invertible:

- Hypothesis Set: {x → T^T f(x; θ) : θ ∈ Θ}
 Decoder: argmax_k ((T^T)⁻¹ f(x; θ))_k.

Proof. First, by setting the hypothesis set as above and plugging in the surrogate complementary estimation loss, we get the training objective function for CPE:

$$L_{\text{CPE}}(\theta) = \frac{1}{N} \sum_{i=1}^{N} -\log\left(T^{\top} f(x_i; \theta)\right)_{\bar{y}_i}$$
(21)

Equation (21) matches Equation (20), implying that in the training phase they select the same parameter θ . Next, in the inference phase, it is clear that $(T^{\top})^{-1}\overline{f(x;\theta)} = (T^{\dagger})^{-1}T^{\top}f(x;\theta) =$ $f(x; \theta)$, so both methods predict the same label for an instance x.

Next, we further show that when T is the uniform transition matrix U, the decoder is equivalent to the L_1 decoder, i.e., $\operatorname{argmax}_k((U^{\top})^{-1}\bar{f}(x))_k = \operatorname{argmin}_k ||U_k - \bar{f}(x)||_1$:

Proof. First, as

$$((U^{\top})^{-1}\bar{f}(x))_k = -(K-1)\bar{f}_k(x) + \sum_{k=1}^K \bar{f}_k(x) = -(K-1)\bar{f}_k(x) + 1,$$

we have that $\operatorname{argmax}_k((U^{\top})^{-1}\bar{f}(x))_k = \operatorname{argmin}_k \bar{f}_k(x)$. Next, set $\hat{y} = \operatorname{argmin}_k \bar{f}_k(x)$. For any $y \neq \hat{y}$, we want to show

$$|U_{y\hat{y}} - \bar{f}_{\hat{y}}(x)| + |U_{yy} - \bar{f}_{y}(x)| \ge |U_{\hat{y}\hat{y}} - \bar{f}_{\hat{y}}(x)| + |U_{\hat{y}y} - \bar{f}_{y}(x)|.$$
(22)

As
$$\overline{f}_{\hat{y}}(x) \leq \frac{1}{K} \leq \frac{1}{K-1} = U_{y\hat{y}}$$
,

$$|U_{y\hat{y}} - \bar{f}_{\hat{y}}(x)| + |U_{yy} - \bar{f}_{y}(x)| = |U_{y\hat{y}} - \bar{f}_{\hat{y}}(x)| + \bar{f}_{\hat{y}}(x) + |U_{yy} - \bar{f}_{y}(x)| - f_{\hat{y}}(x)$$
(23)
$$= |U_{\hat{x}\hat{x}} - \bar{f}_{\hat{x}}(x)| + |U_{x\hat{x}} - \bar{f}_{\hat{x}}(x)| + |U_{yy} - \bar{f}_{y}(x)| - \bar{f}_{\hat{x}}(x)| - \bar{f}_{\hat{x}}(x)$$
(24)

$$|U_{\hat{y}\hat{y}} - f_{\hat{y}}(x)| + |U_{y\hat{y}} - f_{\hat{y}}(x)| + |U_{yy} - f_{y}(x)| - f_{\hat{y}}(x)$$
(24)

$$= |U_{\hat{y}\hat{y}} - \bar{f}_{\hat{y}}(x)| + \frac{1}{K-1} - \bar{f}_{\hat{y}}(x) + \bar{f}_{y}(x) - \bar{f}_{\hat{y}}(x)$$
(25)

If $\bar{f}_y(x) \leq \frac{1}{K-1}$, as $\bar{f}_{\hat{y}}(x) \leq \bar{f}_y(x)$,

$$\frac{1}{K-1} - \bar{f}_{\hat{y}}(x) + \bar{f}_{y}(x) - \bar{f}_{\hat{y}}(x) \ge \frac{1}{K-1} - \bar{f}_{\hat{y}}(x) \ge \frac{1}{K-1} - \bar{f}_{y}(x) = |U_{\hat{y}y} - \bar{f}_{y}(x)|$$

Otherwise, as $\bar{f}_{\hat{y}}(x) \leq \frac{1}{K}$,

$$\frac{1}{K-1} - \bar{f}_{\hat{y}}(x) + \bar{f}_{y}(x) - \bar{f}_{\hat{y}}(x) \ge \bar{f}_{y}(x) - \bar{f}_{\hat{y}}(x) \ge \frac{1}{K-1} - \bar{f}_{y}(x) = |U_{\hat{y}y} - \bar{f}_{y}(x)|.$$

Hence, Equation (22) holds. Now,

$$\sum_{k=1}^{K} \left| U_{yk} - \bar{f}_k(x) \right| = \left| U_{y\hat{y}} - \bar{f}_{\hat{y}}(x) \right| + \left| U_{yy} - \bar{f}_y(x) \right| + \sum_{k \neq y, \hat{y}} \left| U_{yk} - \bar{f}_k(x) \right|$$
(26)

$$\geq \left| U_{\hat{y}y} - \bar{f}_y(x) \right| + \left| U_{\hat{y}\hat{y}} - \bar{f}_{\hat{y}}(x) \right| + \sum_{k \neq y, \hat{y}} \left| U_{\hat{y}k} - \bar{f}_k(x) \right| = \sum_{k=1}^{K} \left| U_{\hat{y}k} - \bar{f}_k(x) \right|$$
(27)

As a result, \hat{y} minimizes $k \mapsto ||U_k - \bar{f}(x)||_1$. Hence, we conclude that $\operatorname{argmin}_k \bar{f}_k(x) = \bar{y} =$ $\operatorname{argmin}_k \|U_k - \bar{f}_k(x)\|_1$. Then the proof is complete.

As the two decoders are equivalent, we have that Forward Correction is equivalent to CPE with

- Hypothesis Set: {x → U^T f(x; θ) : θ ∈ Θ}
 Decoder: argmin_k || f(x; θ) − U_k ||₁.

when the transition layer is fixed to the uniform transition matrix.

Surrogate Complementary Loss In the training phase, Surrogate Complementary Loss with Log Loss optimizes the following loss functions:

$$L_{\text{SCL}}(\theta) = \frac{1}{N} \sum_{i=1}^{N} -\log(1 - f(x_i; \theta))_{\bar{y}_i}$$
(28)

In the inference phase, this method predicts the ordinary labels by $\hat{y} = \operatorname{argmax}_k f_k(x)$ for an unseen instance x. We claim that this method is equivalent CPE with:

- Hypothesis Set: {x → U^T f(x; θ) : θ ∈ Θ}
 Decoder: argmin_k || f(x; θ) − U_k ||₁.

Proof. Observe that the training objective function for CPE with the hypothesis set has the following property:

$$L_{\text{CPE}}(\theta) = \frac{1}{N} \sum_{i=1}^{N} -\log\left(U^{\top} f(x_i; \theta)_{\bar{y}_i}\right) = \frac{1}{N} \sum_{i=1}^{N} -\log\left(\frac{1}{K-1} \sum_{k \neq \bar{y}_i} f_k(x_i; \theta)\right)$$
(29)

$$= \frac{1}{N} \sum_{i=1}^{N} -\log\left(1 - f_{\bar{y}_i}(x_i;\theta)\right) + \log(K-1) = L_{\text{SCL}}(\theta) + \log(K-1)$$
(30)

That is, the objective function only differs by a constant. As a result, the two methods match during the training phase.

In inference phase, SCL predicts $\hat{y} = \operatorname{argmax}_k f(x; \theta)$ for unseen instance x as in Forward Correction. In addition, they have the same hypothesis set $\{x \mapsto U^{\top} f(x; \theta) : \theta \in \Theta\}$ if the transition layer of Forward Correction is fixed to uniform. Hence, SCL is equivalent to Forward Correction with uniform transition layer. It implies that they have the same decoder: $\hat{y} = \operatorname{argmin}_{k} \|\bar{f}(x) - U_{k}\|_{1}$.

Discriminative Model In the training phase, Discriminative Model with unweighted loss optimizes the following loss functions:

$$L_{\rm DM}(\theta) = \frac{1}{N} \sum_{i=1}^{N} -\log\left(\,{\rm sm}(1 - f(x_i;\theta))\right)_{\bar{y}_i} \tag{31}$$

In the inference phase, this method predicts the ordinary labels by $\hat{y} = \operatorname{argmax}_k f_k(x)$ for an unseen instance x. We claim that this method is equivalent CPE with:

- Hypothesis Set: {x → sm(1 f(x; θ)) : θ ∈ Θ}
 Decoder: argmin_k || f(x; θ) U_k ||₁.

Proof. The equivalence in the training phase is clear by plugging in the hypothesis to the surrogate complementary estimation loss. During inference phase, first observe that

$$\bar{f}_k(x) = \frac{1}{Z} \exp\left(1 - f_k(x_i;\theta)\right) = \frac{e}{Z} \exp\left(-f_k(x_i;\theta)\right),\tag{32}$$

where $Z = \sum_{k=1}^{K} \exp(1 - f_k(x_i; \theta))$ is the normalization term. As $x \mapsto \exp(-x)$ is monotonic decreasing, we have that $\operatorname{argmin}_k \bar{f}_k(x; \theta) = \operatorname{argmax}_k f_k(x; \theta)$. Next, as we have shwon $\operatorname{argmin}_k \bar{f}_k(x) = \operatorname{argmin}_k ||U_k - \bar{f}_k(x)||_1$, so $\operatorname{argmax}_k f_k(x; \theta) = \operatorname{argmin}_k ||U_k - \bar{f}_k(x)||_1$, implying that both methods predict the same label for all instances.

C Broader Impact

This paper proposed a new approach to better utilizing the information from complementary labels. This may potentially make personal data less private because in some sense CLL algorithms enable recovery ordinary labels from only complementary ones.

D Experiment Details

In this section, we provide missing details of the experiments in Section 4.

D.1 Setup

Datasets Across the experiments, we use the following datasets:

- MNIST [13] (CC BY-SA 3.0 license)
- Fashion-MNIST [22] (MIT license)
- Kuzushiji-MNIST [4] (CC BY-SA 4.0 license)

For the above dataset, the size of the training set is 60000, and the size of the testing set is 10000. To perform the hyperparameter selection, in each trial, we split 10 percent of the training dataset randomly as the validation dataset. We performed five trials with different random seeds for all the experiments in this paper.

Models We implemented the deep models in PyTorch. The base models considered in the experiment are linear and one-layer mlp model (d-500-c) with 500 hidden units. In CPE-T, the parameter of the transition layer is initialized such that it matches the provided transition matrix, i.e. it is initialized to W_0 such that $T(W_0) = T$. All models are optimized using Adam with learning rate selected from {1e-3, 5e-4, 1e-4, 5e-5, 1e-5} and a fixed weight decay 1e-4 for 300 epochs. We used the default parameters in PyTorch for other parameters in Adam. The experiments are run with Nvidia Tesla V100 GPUs.

For the two traditional models, we used the K nearest neighbor (KNN) classifier from scikit-learn with the number of neighbors selected from $\{10, 20, \ldots, 250\}$ based on the complementary estimation loss on the validation dataset. We performed PCA on the dataset to map the feature to a 32-dimension space for KNN to reduce the training/inference time. We used Gradient Boosting Decision Tree from LightGBM, and set the objective to "multiclass" to optimize the log loss. The hyperparameters include the number of trees $\{5, 10, \ldots, 500\}$ and learning rate $\{0.01, 0.025, 0.05, 0.1\}$. Those parameters are also selected based on the complementary estimation loss on the validation dataset.

D.2 Additional Results

This section provides figures and tables that are helpful in analyzing the experiment results.

	MNIST			FASHION-MNIST			KUZUSHIJI-MNIST		
	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG
URE-GA SCL DM FwD CPE-I CPE-F	81.7 ± 0.5 90.5 ± 0.2 89.7 ± 0.5 90.5 ± 0.2 80.4 ± 0.3 90.5 ± 0.2	$73.4 \pm 1.4 90.2 \pm 0.2 89.1 \pm 0.2 90.6 \pm 0.4 73.5 \pm 1.3 90.7 \pm 0.1$	$23.7 \pm 2.9 25.0 \pm 17.9 22.7 \pm 8.5 91.6 \pm 0.7 76.1 \pm 1.6 91.8 \pm 0.4 \\91.8 \pm 0.4 \\91.$	$76.2 \pm 0.3 \\ 82.0 \pm 0.4 \\ 81.8 \pm 0.3 \\ 82.0 \pm 0.4 \\ 74.6 \pm 0.5 \\ 82.2 \pm 0.3 \\ 82.0 \pm 0.4 \\ 82.2 \pm 0.3 \\ 82.0 \pm 0.4 \\ 82.0 \pm 0.3 \\ 82.0 \pm 0.0 \\ 82.$	$70.8 \pm 1.5 79.6 \pm 2.2 78.2 \pm 3.1 81.6 \pm 1.2 71.0 \pm 1.5 82.4 \pm 0.4 92.4 \pm 0.4 92.5 92$	21.3 ± 5.5 26.2 ± 8.7 23.6 ± 5.5 83.4 \pm 0.7 74.7 ± 2.3 83.1 ± 1.0	51.0 ± 1.0 59.9 ± 0.9 61.0 \pm 1.5 59.9 ± 0.9 49.7 ± 0.6 60.4 ± 0.6 60.2 ± 0.5	$43.7 \pm 1.0 \\ 58.9 \pm 0.7 \\ 59.4 \pm 1.4 \\ 60.4 \pm 0.9 \\ 42.8 \pm 0.8 \\ 60.8 \pm 0.4 \\ 60.8 \pm 0.4 \\ 60.5 \\ 100000000000000000000000000000000000$	$16.7 \pm 2.5 \\ 16.4 \pm 2.2 \\ 17.7 \pm 3.0 \\ 62.6 \pm 0.7 \\ 46.8 \pm 1.4 \\ 62.8 \pm 0.2 \\ 22.4 \pm 0.2 \\ 62.4 \pm 0.2 \\ 62.4 \pm 0.2 \\ 62.4 \pm 0.2 \\ 63.4 \pm 0.2 \\ 63.$

Table 6: Comparison of the testing classification accuracies with different transition matrices.

Table 7: Comparison of the testing classification accuracies with different levels of noise.

		MNIST			FASHION-MNIST			Kuzushiji-MNIST		
	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	
URE-GA SCL DM	$\begin{array}{c} 22.8 \pm 2.0 \\ 25.6 \pm 13.8 \\ 23.3 \pm 7.4 \end{array}$	21.1 ± 4.4 23.9 ± 10.3 22.4 ± 8.7	21.4 ± 1.6 23.7 ± 4.3 23.4 ± 2.9	20.2 ± 6.7 23.9 ± 7.8 24.1 ± 7.1	23.5 ± 3.9 24.5 ± 5.2 24.3 ± 5.0	22.6 ± 3.1 26.0 ± 3.2 25.6 ± 3.9	16.8 ± 2.1 17.8 ± 2.5 18.1 ± 2.6	16.4 ± 2.8 17.8 ± 3.2 17.6 ± 2.4	15.2 ± 2.2 17.4 ± 1.3 16.5 ± 1.4	
Fwd CPE-I CPE-F CPE-T	$\begin{array}{c} 91.1 \pm 0.7 \\ 75.7 \pm 2.0 \\ 91.2 \pm 0.7 \\ \textbf{91.3} \pm \textbf{0.7} \end{array}$	89.6 ± 1.0 75.4 ± 2.0 90.2 ± 1.0 90.5 ± 0.8	$\begin{array}{c} 82.5 \pm 3.6 \\ 73.8 \pm 2.2 \\ 85.2 \pm 1.7 \\ \textbf{85.7} \pm \textbf{1.6} \end{array}$	$\begin{array}{c} 82.4 \pm \ 0.9 \\ 74.6 \pm \ 2.3 \\ 82.2 \pm \ 1.2 \\ \textbf{82.6} \pm \ \textbf{1.3} \end{array}$	81.4 ± 0.9 73.9 ± 2.2 81.0 ± 1.5 81.6 ± 1.3	$\begin{array}{c} 72.0 \pm 7.5 \\ 71.1 \pm 2.0 \\ 75.4 \pm 3.3 \\ \textbf{78.0} \pm \textbf{1.6} \end{array}$	$\begin{array}{c} \textbf{62.7} \pm \textbf{1.0} \\ 47.0 \pm 1.4 \\ 61.9 \pm 0.9 \\ 62.2 \pm 0.8 \end{array}$	60.9 ± 0.9 46.5 ± 1.3 61.1 ± 2.2 61.7 ± 1.7	$52.1 \pm 6.2 \\ 43.4 \pm 1.1 \\ 53.4 \pm 1.5 \\ 55.0 \pm 1.1$	

Benchmark results of linear models Table 6 and 7 provide the the noiseless and noisy benchmark results using linear models as base models, as introduced in Section 4.1 and Section 4.2, respectively. We can see that the proposed CPE performs slightly better or is competitive with the baseline methods in most scenarios. When the transition matrix is highly inaccurate ($\lambda = 0.5$), CPE outperforms the baselines and is more stable in terms of testing accuracies. These are consistent with our observation when using mlp as base models.

Table 8: Comparison of testing accuracies of decoders when the baseline models use fixed transition layers. The parameters are selected from the one with smallest SCEL on the validation dataset. Note that L_1 and MAX correspond to CPE-F and Fwd, respectively.

		MNIST		F	FASHION-MNIST			KUZUSHIJI-MNIST		
	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG	
LINEAR										
MAX	90.5 ± 0.2	90.7 ± 0.2	91.9 ± 0.4	82.2 ± 0.3	82.6 ± 0.3	83.8 ± 0.2	60.4 ± 0.6	61.2 ± 0.3	63.2 ± 0.2	
L_1	90.5 ± 0.2	90.7 ± 0.1	91.8 ± 0.4	82.2 ± 0.3	82.4 ± 0.4	83.1 ± 1.0	60.4 ± 0.6	60.8 ± 0.4	62.8 ± 0.2	
MLP										
MAX	94.4 ± 0.2	92.0 ± 0.2	95.5 ± 0.2	83.0 ± 0.1	83.3 ± 0.2	86.1 ± 0.5	73.5 ± 1.6	64.8 ± 0.5	75.3 ± 2.6	
L_1	94.4 ± 0.2	92.0 ± 0.2	95.5 ± 0.3	83.0 ± 0.1	83.0 ± 0.3	85.8 ± 0.3	73.5 ± 1.6	64.6 ± 0.5	75.3 ± 2.6	
		MNIST		FASHION-MNIST			KUZUSHIJI-MNIST			
	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	
LINEAR										
MAX	91.4 ± 0.5	90.5 ± 0.5	83.9 ± 2.6	83.2 ± 0.3	82.4 ± 0.4	76.3 ± 2.8	62.5 ± 0.9	62.5 ± 1.6	55.6 ± 2.0	
L_1	91.2 ± 0.7	90.2 ± 1.0	85.2 ± 1.7	82.2 ± 1.2	81.0 ± 1.5	75.4 ± 3.3	61.9 ± 0.9	61.1 ± 2.2	53.4 ± 1.5	
MLP										
MAX	94.4 ± 0.3	93.5 ± 0.3	84.5 ± 4.1	85.0 ± 0.3	84.0 ± 0.5	76.5 ± 2.5	76.4 ± 1.1	73.8 ± 1.2	59.9 ± 3.4	
L_1	94.3 ± 0.5	93.6 ± 0.5	$\textbf{89.0} \pm \textbf{1.4}$	84.1 ± 0.8	83.0 ± 1.1	78.4 ± 2.5	76.1 ± 1.3	73.7 ± 1.5	$63.7 {\pm}~1.5$	

Comparison of decoders Table 8 provide the comparison of L_1 decoder and MAX decoder under the same the validation procedure (SCEL). It is displayed that the MAX decoder outperform L_1 in most noiseless settings; however, when the transition matrix is highly inaccurate ($\lambda = 0.5$), we observe that the L_1 decoder outperform the MAX decoder when using mlp. This suggests that L_1 could be more tolerant to an inaccurate transition matrix when the models are complex. These results reveal that a deeper sensitivity analysis of different decoders, both empirically and theoretically, would be desired. We leave this as future studies.

		MNIST		I	FASHION-MNIS	Т	KUZUSHIJI-MNIST		
	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG
LINEAR									
URE	90.3 ± 0.6	90.4 ± 0.3	91.8 ± 0.5	82.1 ± 0.3	81.5 ± 1.2	82.6 ± 1.3	59.9 ± 0.4	60.0 ± 0.9	62.5 ± 0.5
SCEL	90.5 ± 0.2	90.6 ± 0.1	91.8 ± 0.4	82.0 ± 0.3	82.1 ± 0.5	83.2 ± 1.2	60.3 ± 0.5	60.6 ± 0.5	63.0 ± 0.3
MLP									
URE	92.7 ± 0.5	91.8 ± 0.7	90.4 ± 6.5	82.9 ± 0.1	83.0 ± 0.3	84.3 ± 1.5	63.8 ± 0.7	63.8 ± 1.9	74.5 ± 2.7
SCEL	92.8 ± 0.6	92.1 ± 0.2	95.2 ± 0.5	83.0 ± 0.1	83.0 ± 0.3	85.8 ± 0.3	63.6 ± 0.4	64.6 ± 0.4	74.2 ± 2.8
		MNIST		FASHION-MNIST			KUZUSHIJI-MNIST		
	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$
LINEAR									
URE	90.9 ± 1.0	90.2 ± 0.8	86.1 ± 1.3	82.2 ± 1.3	81.2 ± 1.4	77.1 ± 1.8	62.3 ± 0.8	60.6 ± 0.9	55.3 ± 2.3
SCEL	91.3 ± 0.7	90.5 ± 0.8	85.7 ± 1.6	82.6 ± 1.3	81.6 ± 1.3	78.0 ± 1.6	62.2 ± 0.8	61.7 ± 1.7	55.0 ± 1.1
MLP									
URE	83.7 ± 9.7	90.8 ± 4.7	82.9 ± 9.4	83.0 ± 3.2	74.8 ± 10.1	74.3 ± 10.1	68.5 ± 11.4	67.1 ± 7.7	57.2 ± 16.3
SCEL	94.4 ± 0.5	93.7 ± 0.5	89.6 ± 0.9	84.1 ± 0.8	83.2 ± 1.1	78.9 ± 2.0	$\textbf{76.1}{\pm}~\textbf{1.3}$	$\textbf{73.9} \pm \textbf{1.6}$	64.2 ± 1.2

Table 9: Comparison of CPE-T's testing accuracies using different validation procedures.

Table 10: Comparison of Fwd's testing accuracies using different validation procedures.

		MNIST		FASHION-MNIST			KUZUSHIJI-MNIST		
	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG	UNIF.	WEAK	STRONG
LINEAR									
URE	90.5 ± 0.2	90.6 ± 0.4	91.6 ± 0.7	82.0 ± 0.4	81.6 ± 1.2	83.4 ± 0.7	59.9 ± 0.9	60.4 ± 0.9	62.6 ± 0.7
SCEL	90.5 ± 0.2	90.7 ± 0.2	91.9 ± 0.4	82.2 ± 0.3	82.6 ± 0.3	83.8 ± 0.2	60.4 ± 0.6	61.2 ± 0.3	63.2 ± 0.2
MLP									
URE	94.4 ± 0.2	91.9 ± 0.3	95.3 ± 0.4	82.6 ± 0.6	83.0 ± 1.0	85.5 ± 0.3	73.5 ± 1.6	63.1 ± 2.6	74.1 ± 4.8
SCEL	94.4 ± 0.2	$\textbf{92.0}{\pm 0.2}$	95.5 ± 0.2	83.0 ± 0.1	83.3 ± 0.2	86.1 ± 0.5	73.5 ± 1.6	64.8 ± 0.5	75.3 ± 2.6
		MNIST			FASHION-MNI	ST	KUZUSHIJI-MNIST		
	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 0.5$
LINEAR									
URE	91.1 ± 0.7	89.6 ± 1.0	82.5 ± 3.6	82.4 ± 0.9	81.4 ± 0.9	72.0 ± 7.5	62.7 ± 1.0	60.9 ± 0.9	52.1 ± 6.2
SCEL	91.4 ± 0.5	90.5 ± 0.5	83.9 ± 2.6	83.2 ± 0.3	82.4 ± 0.4	76.3 ± 2.8	62.5 ± 0.9	62.5 ± 1.6	55.6 ± 2.0
MLP									
URE	88.3 ± 8.7	83.9 ± 10.7	71.6 ± 18.4	84.8 ± 0.6	80.2 ± 6.2	62.9 ± 20.1	72.8 ± 5.6	67.6 ± 7.5	54.7 ± 12.4
SCEL	94.4 ± 0.3	93.5 ± 0.3	$84.5{\pm}~4.1$	85.0 ± 0.3	84.0 ± 0.5	76.5 ± 2.5	76.4 ± 1.1	73.8 ± 1.2	59.9 ± 3.4

Comparison of validation processes Table 9 and 10 provide comparison of validation process using URE and the proposed SCEL. In Table 9, we observe that SCEL selects better parameters in most cases. We also observe that when the transition matrix is inaccurate, the parameters selected by SCEL tends to be more stable, especially when the base models are mlp. This demonstrates the superiority of SCEL despite not being an unbiased estimator of the classification accuracies. In Table 10, we further apply SCEL to Fwd. Similarly, we observe that SCEL selects better parameters in most cases. This suggests that the proposed validation procedure can not only be applied to CPE but also earlier approaches. It enables a more robust approach to validate earlier methods.

Training and validation loss curves



Figure 1: Comparison of the training and validation loss of CPE with different transition layers in MNIST under different transition matrices. CPE-F and CPE-T perform almost identically, so the red lines and blue lines overlap in the figures. The shaded area denotes the standard deviation of five random trials.



Figure 2: Comparison of the training and validation loss of CPE with different transition layers in MNIST under different noise level. CPE-F and CPE-T perform almost identically when λ is small, so the red lines and blue lines overlap in those figures. The shaded area denotes the standard deviation of five random trials.