Is Complementary-Label Learning Realistic?

Hsuan-Tien Lin

林軒田

Professor, National Taiwan University

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The University of British Columbia

About Me

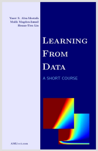
Hsuan-Tien Lin

Professor
National Taiwan University

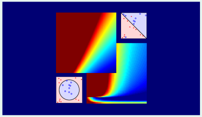
2025 Senior Program Chair
NeurIPS

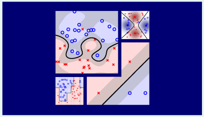
NEURAL INFORMATION PROCESSING SYSTEMS

Co-author
Learning from Data

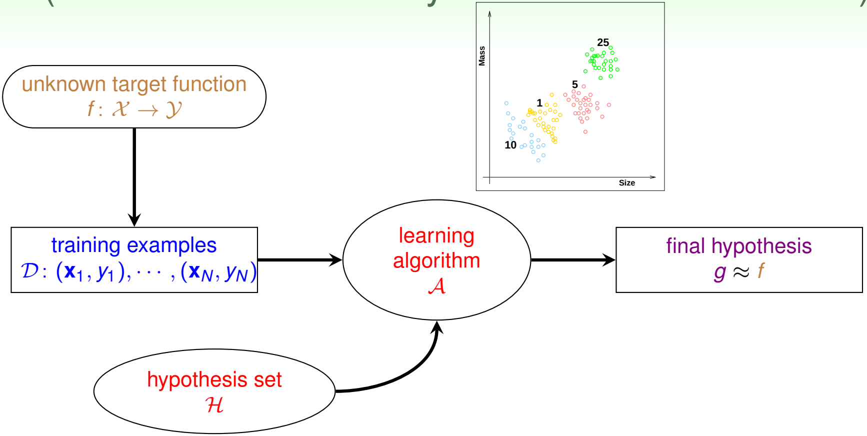


Instructor
NTU-Coursera Mandarin MOOCs
ML Foundations/Techniques



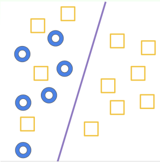


Supervised Learning (Slide Modified from My ML Foundations MOOC)



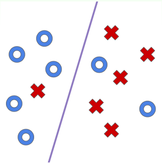
supervised learning:
every input vector $\mathbf{x}_n$ with
its (possibly expensive) label y_n,

Weakly-supervised: Learning without True y_n



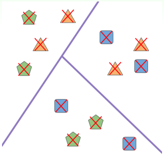
(a) Positive-unlabeled Learning [CE2008]

incomplete



(b) Learning with Noisy Labels [NN2013]

inaccurate



(c) Complementary-label Learning [TI2017]

inexact

- positive-unlabeled: **some** of true $y_n = +1$ revealed
- noisy: **possibly incorrect** label y'_n instead of true y_n
- complementary: **false label** $\overline{y}_n$ instead of true y_n

weakly-supervised: claimed to be a **realistic** route for reducing labeling burden

Complementary-Label Learning

complementary label $\overline{y}_n$ instead of true y_n

Figure 1 of [XY2018]

potential to reducing labeling burden [TI2017]

- 1 ordinary label per instance
- $(K-1)$ complementary labels per instance, **just need one of them**

complementary label: possibly **easier/cheaper** to obtain for some applications

Example: Fruit Labeling Task

→

(left: from 2020 AICup in Taiwan; right: `publicdomainvectors.org`)

hard: true label

- orange **?**
- mango **?**
- cherry
- banana

easy: complementary label

- orange
- mango
- cherry
- banana ✗

can also help improve other ML tasks,
like **semi-supervised learning** [QD2024]

Formal Setup of Complementary-Label Learning

input	complementary label
	banana

Given

size-N data $\mathcal{D} = \{(\text{input } \mathbf{x}_n \in \mathcal{X}, \text{complementary label } \overline{y}_n \in [K])\}_{n=1}^{N}$
such that $\overline{y}_n \neq y_n$ for some hidden ordinary label $y_n \in [K]$

Goal

a multi-class classifier $g(\mathbf{x})$ that **closely predicts the ordinary label** y associated with some unseen inputs $\mathbf{x}$ by $\text{argmax}_{k\in[K]}(g(\mathbf{x}))_k$

(**same goal** as ordinary learning, but **with different data**)

todo: two CLL models, **and more**!

Yu-Ting Chou, Gang Niu, Hsuan-Tien Lin, and Masashi Sugiyama. **Unbiased risk estimators can mislead: A case study of learning with complementary labels**. ICML 2020.

Review: Risk Minimization in Ordinary Learning

- goal: minimize **the 0/1 loss**

$$\ell_{01}(y, g(\mathbf{x})) = \left[\!\left[y \neq \operatorname*{argmax}_{k \in [K]} (g(\mathbf{x}))_k \right]\!\right]$$

with risk (average loss) $R_{01} = \mathbb{E}_{(\mathbf{x},y)} \{\ell_{01}(y, g(\mathbf{x}))\}$

- consider a surrogate loss ℓ that replaces ℓ_{01}

$$\ell \colon [K] \times \mathbb{R}^K \to \mathbb{R}_+$$

with risk $R_\ell = \mathbb{E}_{(\mathbf{x},y)} \{\ell(y, g(\mathbf{x}))\}$

Empirical Risk Minimization (ERM):
estimate R_ℓ **by training data** and minimize it

Unbiased Risk Estimation for CLL

Ordinary Learning

- ERM: minimizes

$$\hat{R}_\ell = \mathop{\mathbb{E}}_{(\mathbf{x}_n, y_n) \in \mathcal{D}} \{\ell(y_n, g(\mathbf{x}_n))\},$$

the empirical version of the surrogate risk $R_\ell = \mathbb{E}_{(\mathbf{x},y)}\{\ell(y, g(\mathbf{x}))\}$

Unbiased Risk Estimator for CLL [TI2019]

- [under assumption on $P(\overline{y} \mid y)$] rewrite ℓ to **some** $\overline{\ell}$ such that

$$\overline{R}_{\overline{\ell}} = \mathbb{E}_{(\mathbf{x},\overline{y})}\overline{\ell}(\overline{y}, g(\mathbf{x})) = \mathbb{E}_{(\mathbf{x},y)}\ell(y, g(\mathbf{x})) = R_\ell$$

- $\overline{R}_{\overline{\ell}}$ called **unbiased risk estimator** (URE)
- URE-CLL: minimize empirical version $\hat{\overline{R}}_{\overline{\ell}}$ of URE

URE-CLL: **pioneer model** for CLL, with **theoretical guarantees** like consistency

Example of URE-CLL

cross-entropy loss

for $g(\mathbf{x}) = \boldsymbol{p}(k \mid \mathbf{x})$,

- ℓ_{CE}: surrogate of ℓ_{01} derived by maximum likelihood, with risk

$$R_{CE} = \mathbb{E}_{(\mathbf{x},y)} \left\{ \underbrace{- \log \boldsymbol{p}(y \mid \mathbf{x})}_{\ell_{CE}} \right\}$$

URE for cross-entropy loss [TI2019]

$$\overline{R}_{CE} = \mathbb{E}_{(\mathbf{x},\overline{y})} \left\{ \overbrace{(K-1) \log \boldsymbol{p}(\overline{y} \mid \mathbf{x}) - \sum_{k=1}^{K} \log \boldsymbol{p}(k \mid \mathbf{x})}^{\overline{\ell}} \right\}$$

under **uniform $\overline{y}$ (that $\neq y$)** assumption

URE-CLL: $\min_{\boldsymbol{p}} \hat{\overline{R}}_{CE}$

Issue: URE-CLL Overfits Easily

$$\ell_{CE} = -\log \boldsymbol{p}(y \mid \mathbf{x})$$

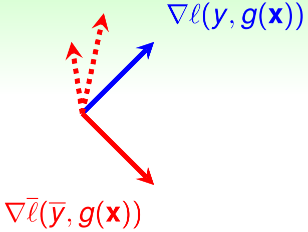
$$\bar{\ell}_{CE} = \underbrace{(K-1)\log \boldsymbol{p}(\bar{y} \mid \mathbf{x})}_{\text{negative}} - \sum_{k=1}^{K} \log \boldsymbol{p}(k \mid \mathbf{x})$$

ordinary risk and URE are very different

- $\ell_{CE} > 0$: ordinary risk R non-negative
- often small $\boldsymbol{p}(\bar{y} \mid \mathbf{x})$: $\bar{\ell}_{CE}$ **often very negative**
- **empirically**, negative $\hat{\bar{R}}_{\bar{\ell}}$
  —since only **some** $\bar{y}_n$ is observed
- **observation**: negative empirical URE $\rightarrow$ overfitting (but why?)

practical remedy NN-URE [TI2019]:
constrain empirical URE to be **non-negative**

Our Contributions



(to be discussed)

an analytical and algorithmic study of URE-CLL, which . . .

- constructs a **novel loss-design framework**
- results in **promising empirical performance**
- leads to **novel insights** on why negative empirical URE causes overfitting

will first describe **key idea**
behind our proposed framework

Key Idea: URE on 0/1 instead of ℓ

Minimize Complementary 0/1

- goal: minimize R_{01}, **not surrogate** R_ℓ
- URE of R_{01}: need

$$\overline{R}_{\overline{01}} = \mathbb{E}_{(\mathbf{x},\overline{y})} \overline{\ell}_{01}(\overline{y}, g(\mathbf{x})) = \mathbb{E}_{(\mathbf{x},y)} \underbrace{\ell_{01}(y, g(\mathbf{x}))}_{[\![y \neq \text{argmax}_k (g(\mathbf{x}))_k]\!]}$$

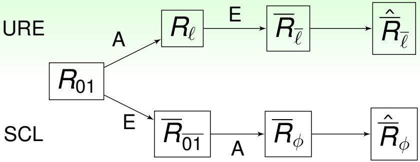
- simple solution:

$$\overline{\ell}_{01}(\overline{y}, g(\mathbf{x})) = [\![\overline{y} = \underset{k}{\text{argmax}} (g(\mathbf{x}))_k]\!]$$

- intuition: all we need is to discourage $g(\mathbf{x})$ from predicting $\overline{y}$ —minimum likelihood "principle"

Surrogate Complementary Loss (SCL): minimize (empirical) surrogate risk of $\overline{\ell}_{01}$

Illustrative Difference between URE and SCL



URE: ripple effect of error

- theoretical motivation [TI2017]
- estimation step (E) amplifies approximation error (A) in $\overline{\ell}$

SCL: "directly" minimize complementary likelihood

- non-negative surrogate loss ϕ for $\overline{\ell}_{01}$ to be minimized
- potentially preventing ripple effect
- unify previous studies as different ϕ [XY2018, YK2019]

SCL: swapping (E) and (A) for loss design

Example of Avoiding Negative Risk

Unbiased Risk Estimator (URE)

URE loss $\bar{\ell}_{CE}$ [TI2019] from ℓ_{CE},

$$\bar{\ell}_{CE}(\bar{y}, g(\mathbf{x})) = \underbrace{(K-1)\log \boldsymbol{p}(\bar{y} \mid \mathbf{x})}_{\text{negative}} - \sum_{j=k}^{K} \log \boldsymbol{p}(k \mid \mathbf{x})$$

Surrogate Complementary Loss (SCL)

[YK2019]

$$\phi_{\mathrm{NL}}(\bar{y}, g(\mathbf{x})) = -\log(1 - \boldsymbol{p}(\bar{y} \mid \mathbf{x}))$$

—a non-negative surrogate of $\bar{\ell}_{01}$

SCL opens new possibilities
on studying different ϕ

Experimental Results

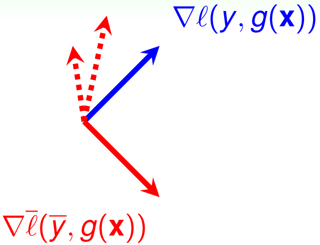
Models

1. Unbiased Risk Estimator (URE) with $\bar{\ell}_{CE}$ [TI2017]
2. Non-Negative Correction of URE (NN-URE) with $\bar{\ell}_{CE}$ [TI2019]
3. Surrogate Complementary Loss (SCL) with exponential ϕ (ours)

Dataset + Model	URE	NN-URE	SCL
MNIST + Linear	0.850	0.818	**0.902**
MNIST + MLP	0.801	0.867	**0.925**
CIFAR10 + ResNet	0.109	0.308	**0.492**
CIFAR10 + DenseNet	0.291	0.338	**0.544**

SCL is **significantly better**
than URE and NN-URE

Analysis Using Gradients



Gradient Direction of URE

- very diverse directions on each $\bar{y}$ to maintain unbiasedness
- low correlation to the target gradient

Gradient Direction of SCL

- targets towards minimum likelihood objective
- higher correlation to the target gradient

empirically quantified with **bias-variance decomposition** (see paper)

Some Issues for Mathematicians

minimize $\bar{\ell}_{01}$—hypothesis that **least matches** complementary data:

is this **minimum likelihood** principle well-justified? **Not yet.**

bias-variance decomposition of gradient based on **empirical findings**:

is there a theoretical guarantee to play with the trade-off? **Not yet.**

current results mostly based on **uniform** complementary labels:

do we understand the assumptions to make CLL 'learnable'? **Not yet.**

some (but not all) answered in the **next paper**

Mini-Summary

Explain Overfitting of URE

- URE only **expected** to do well
- fixed CLs cause **high variance (hence overfitting)**

Surrogate Complementary Loss (SCL)

- **avoids negative risk** issue by design
- **minimum likelihood** principle

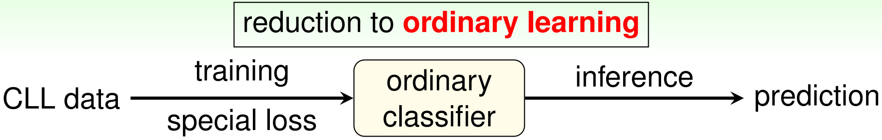
Experiment Results

- SCL **significantly outperforms** others
- trade small gradient bias for **lower variance**

"traditional" statistics tools
can be useful for **modern problem**

Wei-I Lin and Hsuan-Tien Lin.
Reduction from complementary-label learning to probability estimates. PAKDD 2023
Best Paper Runner-up Award.

Reflection on CLL Model Design



Inference: Easy

simply $\text{argmax}_k (g(\mathbf{x}))_k$

Training: Challenging

- indirect estimation from CLs
- prone to overfitting
- mostly only tested on deep models

can we make training **easier**?

Our Contributions

$$R_{01}(\text{dec}(\overline{g}, L_1)) \leq \frac{4\sqrt{2}}{\gamma}\sqrt{R(\overline{g}, \ell_{KL})}$$

(to be discussed)

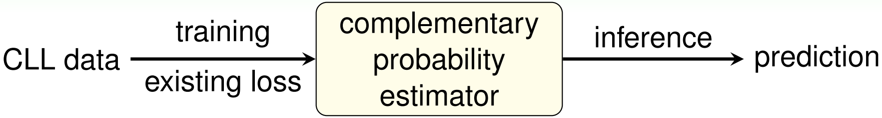
a principled study of CLL Model Design, which . . .

- promotes a **novel reduction framework**
- leads to **sound explanations** on several existing models
- results in **promising empirical performance** in some scenarios

again, will first describe **key idea**
behind our proposed framework

Key Idea: Complementary Probability Estimation

reduction to **complementary probability estimation (CPE)**



Training: Easy

learn complementary probability estimates $\overline{g}(\mathbf{x})$ with CLs

- **direct learning** from CLs
- many **existing deep/non-deep models**
- **easy to validate** too

inference: **how (under what assumption)?**

Assumption: How are CLs Generated?

uniform assumption

$$P(\overline{y} \mid y) = \frac{1}{K-1} [\![\overline{y} \neq y]\!]$$

conditional generation assumption

$$P(\overline{y} \mid \mathbf{x}, y) = P(\overline{y} \mid y) = T_{y,\overline{y}}$$

e.g. transition matrix

$$T = \begin{bmatrix} 0 & 0.3 & 0.3 & 0.4 \\ 0.4 & 0 & 0.3 & 0.3 \\ 0.3 & 0.4 & 0 & 0.3 \\ 0.4 & 0.3 & 0.3 & 0 \end{bmatrix}$$

how to do inference **with known T** after CPE?

Nearest Transition Vector Decoder

CLL data —training / existing loss→ complementary probability estimator —inference→ prediction

$$T = \begin{bmatrix} \color{red}{0} & \color{red}{0.3} & \color{red}{0.3} & \color{red}{0.4} \\ 0.4 & 0 & 0.3 & 0.3 \\ 0.3 & 0.4 & 0 & 0.3 \\ 0.4 & 0.3 & 0.3 & 0 \end{bmatrix}$$

looks like $y = 1$ if $\overline{g}(\mathbf{x}) = \color{red}{[0.03, 0.27, 0.25, 0.45]}$

proposed **nearest-transition-vector decoder** for inference:

$$\text{dec}(\overline{g}, d)\colon \mathbf{x} \to \operatorname*{argmin}_{y \in [K]} d(\overline{g}(\mathbf{x}), T_y)$$

Theoretical Guarantee of CPE

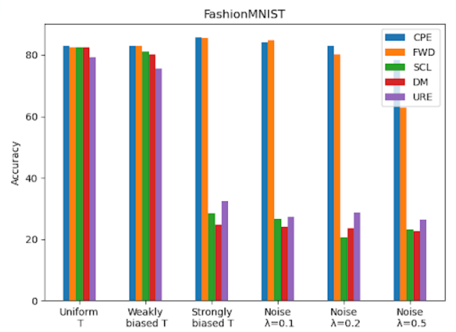
When using $d = L_1$ distance,

$$R_{01}(\text{dec}(\overline{g}, L_1)) \leq \frac{4\sqrt{2}}{\gamma}\sqrt{R_{KL}(\overline{g})}$$

- γ: **minimum L_1 distance** between rows of transition vectors
- smaller CPE error (KL divergence) $\rightarrow$ smaller R_{01}
- explains SCL as special case of L1 decoding under uniform assumption
- can be used to validate with CLs only

other distance measures possible
(but we did not study much)

Experimental Results



Models

1. Unbiased Risk Estimator (URE) [TI2017]
2. Discriminative model (DM*) [YG2021]
3. Surrogate Complementary Loss (SCL*, our previous work)
4. Forward (FWD*) [XY2018]
5. Complementary Probability Estimator (CPE, ours)

CPE **better than others & special cases(*)**, especially with noisy T

Some Issues for Mathematicians Revisited

minimize $\bar{\ell}_{01}$—hypothesis that **least matches** complementary data:

is **minimum likelihood** well-justified? **Yes, special case of CPE.**

bias-variance decomposition of gradient based on **empirical findings**:

is there a theoretical guarantee to play with the trade-off? **Not yet.**

current results mostly based on **uniform** complementary labels:

the assumptions to make CLL 'learnable'? **any known T with $\gamma > 0$.**

some answered in **this paper**

Mini-Summary

Explain SCL (and Others)

- via a **different reduction** route

Complementary Probability Estimation (CPE)

- **estimate complementary probabilities** during training (easy)
- **nearest transition vector decoding** (theoretical guarantees)

Experiment Results

- CPE **outperforms (?)** others
- potential for **noisy CLL and CL-only validation**

now, is CLL **realistic**?

Hsiu-Hsuan Wang, Tan-Ha Mai, Nai-Xuan Ye, Wei-I Lin, Hsuan-Tien Lin. **CLImage: Human-Annotated Datasets for Complementary-Label Learning**. TMLR 2025

Tan-Ha Mai, Nai-Xuan Ye, Yu-Wei Kuan, Po-Yi Lu, Hsuan-Tien Lin. **The Unexplored Potential of Vision-Language Models for Generating Large-Scale Complementary-Label Learning Data**. PAKDD 2025

Recall: Assumptions in CLL Model Design

noise-free assumption

$P(\bar{y} = y \mid y) = 0$

uniform assumption

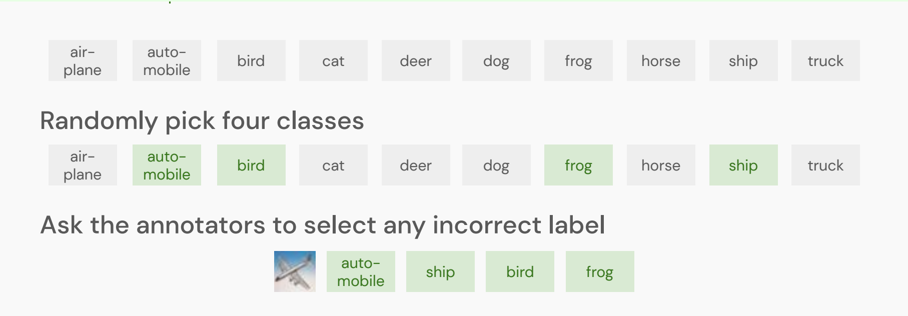
$$P(\bar{y} \mid y) = \frac{1}{K-1}[\![\bar{y} \neq y]\!]$$

conditional generation assumption

$$P(\bar{y} \mid \mathbf{x}, y) = P(\bar{y} \mid y) = T_{y,\bar{y}}$$

do they **hold in reality**?

CLImage: Protocol for Collecting CL from Annotators



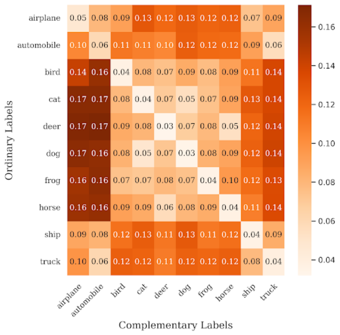
(courtesy of Wei-I Lin)

play here: `https://github.com/ntucllab/CLImage_Dataset/`

Analysis of Collected Data

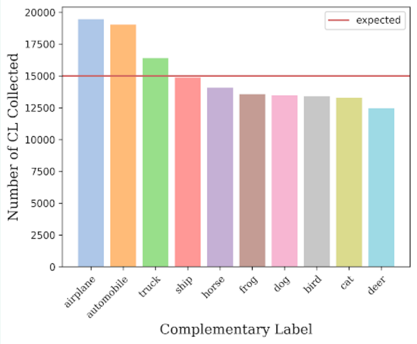
is it noise-free?

no (not surprisingly), and **it affects performance significantly**



is it uniform?

no (not surprisingly), and **it affects performance a bit**

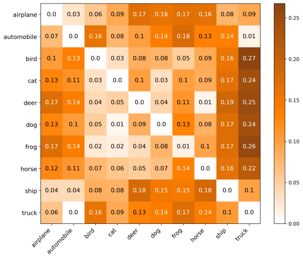


more studies on **noisy CLL** is needed

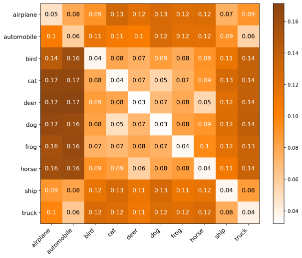
ACLImage: CLImage Protocol by VLMs

observations

- different from human annotators, more biased, less noisy



(ACLCIFAR10)



(CLCIFAR10)

- can systematically generate large-scale data **cheaply**

still potential of (V)LMs
on **weakly supervised learning**

An Insider Secret

CLImage

- CLCIFAR10
- CLCIFAR20 (20 meta-classes)
- CLMicroImageNet10 (10 random classes)
- CLMicroImageNet20 (20 random classes)

–why **only data of** 10 **or** 20 **classes**?

Truth

tried CIFAR100 **but failed**

- **higher accuracy than random guess**
- much lower than ordinary classification, **even after noise cleaning**

pure CLL **overly weak** and may not be realistic

Summary (Finally)

Surrogate Complementary Loss

run URE **before doing surrogate** instead

Complementary Probability Estimation

consider **probability estimation on CLs** instead

CLImage/ACLImage

attempt to benchmark how realistic CLL is, with **dataset collections** and a library in its beta version

`https://github.com/ntucllab/libcll`

Thank you and all my students/collaborators!

References

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