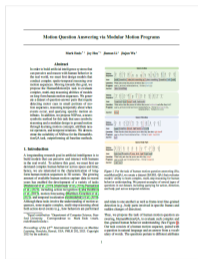

Training neural models using logic: results, challenges, and applications

Efi Tsamoura

Why neurosymbolic AI?

(Some of) our success stories

Applications in foundational models

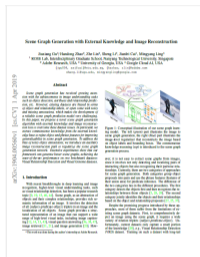


Ziyang Li, et al. **Relational Programming with Foundation Models.** In AAI, 2024.

Hanlin Zhang, et al. **Improved Logical Reasoning of Language Models via Differentiable Symbolic Programming.** In ACL, 2023.

Joy Hsu, et al. **What's Left? Concept Grounding with Logic-Enhanced Foundation Models.** In NeurIPS 2023.

Applications in computer vision



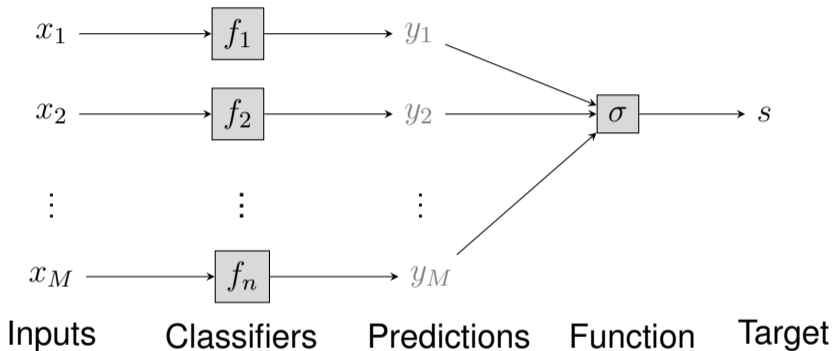
Ziwei Xu, et al. **Don't Pour Cereal into Coffee: Differentiable Temporal Logic for Temporal Action Segmentation**. In NeurIPS, 2022.
Jiuxiang Gu, et al. **Scene Graph Generation with External Knowledge and Image Reconstruction**. In CVPR, 2019.
Mark Endo, et al. **Motion Question Answering via Modular Motion Programs**. In ICML, 2023.
Davide Buffelli and Eftymia Tsamoura. **Scalable Theory-Driven Regularization of Scene Graph Generation Models**. In AAAI, 2023.
Leon Jonathan Feldstein, Jurčius Modestas, and Eftymia Tsamoura. **Parallel neurosymbolic integration with Concordia**. In ICML, 2023.

Weakly-supervised learning using logic

aka Multi-Instance Partial Label Learning (MI-PLL)

Kaifu Wang, **Efthymia Tsamoura**, and Dan Roth. **On learning latent models with multi-instance weak supervision**. In NeurIPS, 2023.

MI-PLL



MI-PLL

- **Given:**

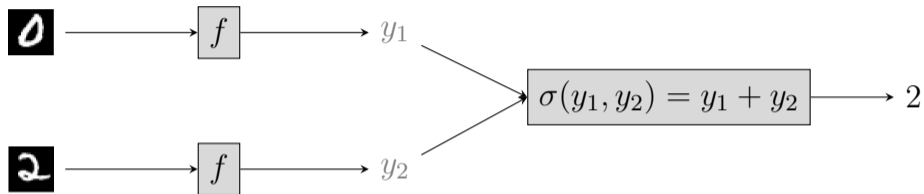
- $x_1, \dots, x_M,$

- trainable classifiers $f_1, \dots, f_n,$

- a target $s = \sigma(y_1, \dots, y_M),$ where y_i 's are the predictions of the classifiers on x_i 's,

- **learn** $f_1, \dots, f_n.$

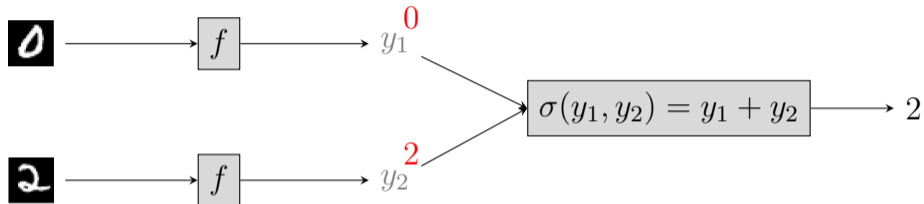
MI-PLL: 2SUM



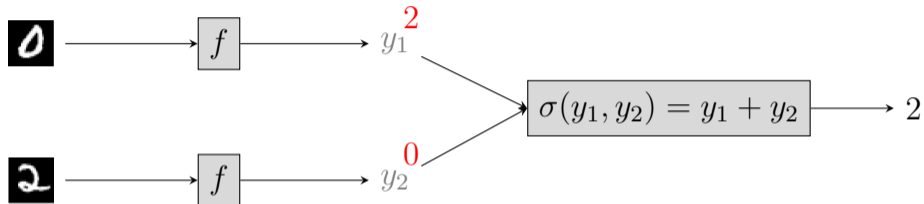
Challenges

- σ may not be 1-1.

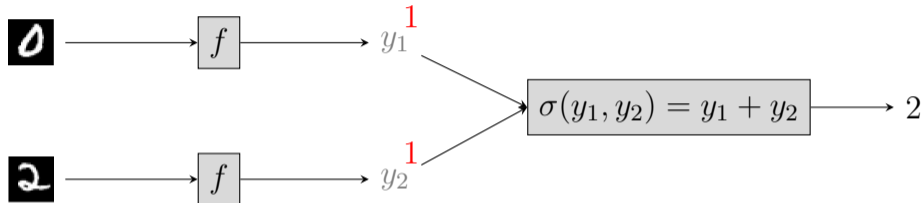
Challenges: σ may not be 1-1



Challenges: σ may not be 1-1



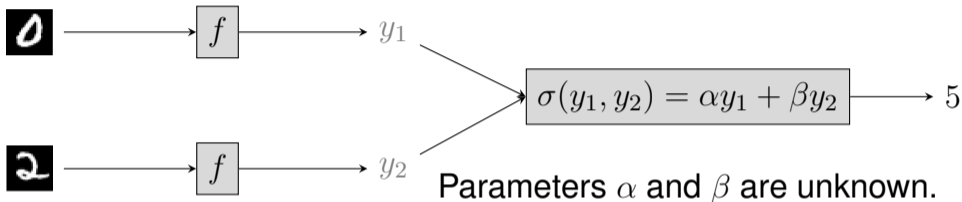
Challenges: σ may not be 1-1



Challenges

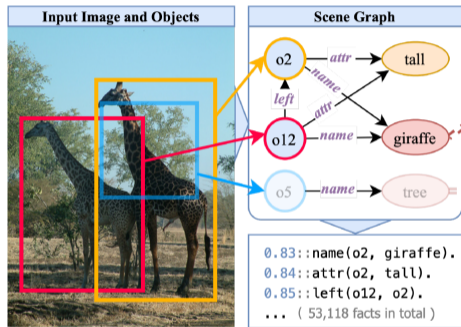
- σ may not be 1-1.
- σ may be unknown.

Challenges: σ may be unknown



- Learning under unknown weighted sums allows us to simultaneously perform *theory induction* due to the relationship between integer linear programming and Boolean satisfiability [32].

Visual QA (SIGMOD 2023)



$Q(O) \leftarrow \text{NAME}(\textit{herbivore}, O)$
 $\text{NAME}(N, O) \wedge \text{NAME}(N', O) \rightarrow \text{ISA}(N', N)$
 $\rightarrow \text{ISA}(\textit{giraffe}, \textit{herbivore})$
 $\rightarrow \text{ISA}(\textit{deer}, \textit{herbivore})$

Table: Recall@5 on VQAR [13].

Testset	LXMERT [34]	RVC [11]	TG-Guided VQA
C5	64.05%	74.62%	87.01%
C6	56.51%	72.04%	85.45%

Efthymia Tsamoura, Jaehun Lee, and Jacopo Urbani. Probabilistic Reasoning as Scale: Trigger Graphs to the Rescue. In SIGMOD, 2023.

On the power of σ

Our formulation is general enough to represent different languages, e.g.,

- non-linear functions.
- Systems of Boolean equations.
- Datalog.

Our formulation can express logical theories via backward reasoning [15].

Efthymia Tsamoura and Loizos Michael **Neural-Symbolic Integration: a Compositional Perspective**. In AAI, pages 5051-5060, 2021.

Benefits of our learning setting

The unique benefit over end-to-end neural models [41] is that it offers the ability to reuse the latent models— particularly useful in NLP [25, 27].

Objective

- Develop **necessary** and **sufficient** conditions that ensure classifier *learnability*– will formally introduced the notion later.
- When σ is known, this condition is called *M-unambiguity*.

Neurosymbolic losses

- Losses based on weighted model counting [4, 45].
- Losses based on fuzzy logic semantics [31, 39].
- Learning based on expectation maximization [19, 29].
- Learning via differentiation through argmax [25, 27].

We will not cover this topic in this talk.

Kaifu Wang, **Efthymia Tsamoura**, and Dan Roth. **On learning latent models with multi-instance weak supervision**. In NeurIPS, 2023.

Kaifu Wang, **Efthymia Tsamoura**, and Dan Roth. **On characterizing and mitigating imbalances in multi-instance weak supervision**. CoRR, abs/2407.10000, 2024.

Notation

Supervised learning

x (given)

y (given)

-

-

\mathcal{D}

$[f](x)$

$\ell^{01}(y, y') := 1\{y \neq y'\}$

$\mathcal{R}^{01}(f) :=$

$E_{(X, Y) \sim \mathcal{D}}[\ell^{01}([f](X), Y)]$

MI-PLL

$\mathbf{x} = x_1, \dots, x_M$ (given)

$\mathbf{y} = y_1, \dots, y_M$ (unknown)

$s = \sigma(\mathbf{y})$ (given)

σ (given)

\mathcal{D}_p

$[f](x)$

$\ell_\sigma^{01}(\mathbf{y}, s) := 1\{\sigma(\mathbf{y}) \neq s\}$

$\mathcal{R}_p^{01}(f; \sigma) :=$

$E_{(\mathbf{X}, S) \sim \mathcal{D}_p}[\ell_\sigma^{01}([f](\mathbf{X}), S)]$

Meaning

input(s)

gold label(s)

partial label

transition function

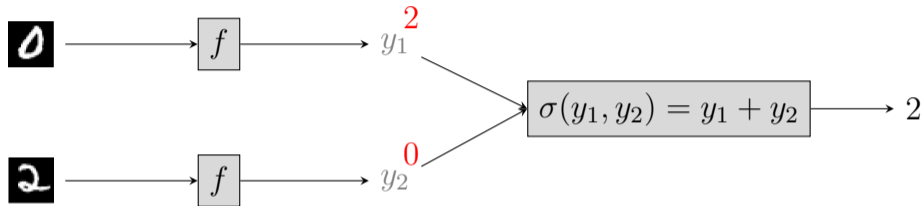
training distribution (drawing M independent samples from \mathcal{D})

prediction

zero-one (partial) loss

zero-one (partial) risk

Notation: 2SUM



- $\sigma(y_1, y_2) = y_1 + y_2$.
- $\ell_\sigma^{01}(y_1 = \mathbf{2}, y_2 = \mathbf{0}, s = \mathbf{2}) = \mathbf{0}$.
- $\ell_\sigma^{01}(y_1 = \mathbf{2}, y_2 = \mathbf{1}, s = \mathbf{2}) = \mathbf{1}$.
- The partial risk $\mathcal{R}_p^{01}(f; \sigma)$ is the probability of predicting the wrong sum.

PAC-style learnability

An MI-PLL problem instance is *learnable*, if there exists an algorithm \mathcal{A} , that takes as **input** partial samples and **outputs** a classifier $\mathcal{A}(\mathcal{T}_P) \in \mathcal{F}$, such that

- for any data distribution and
- any $\delta, \epsilon \in (0, 1)$

there is an integer $m_{\epsilon, \delta}$, such that $m_P \geq m_{\epsilon, \delta}$, where m_P is the size of partial samples, implies $\mathcal{R}^{01}(\mathcal{A}(\mathcal{T}_P)) \leq \epsilon$ with probability at least $1 - \delta$.

PAC-style learnability: informal definition

An MI-PLL problem instance is *learnable*, if for any user-defined $\delta, \epsilon \in (0, 1)$, it is **highly likely** (with probability at least $1 - \delta$), that the learned classifier does **few mistakes** ($\mathcal{R}^{01}(\mathcal{A}(\mathcal{T}_P)) \leq \epsilon$), via using a **large enough number of training samples** ($m_P \geq m_{\epsilon, \delta}$).

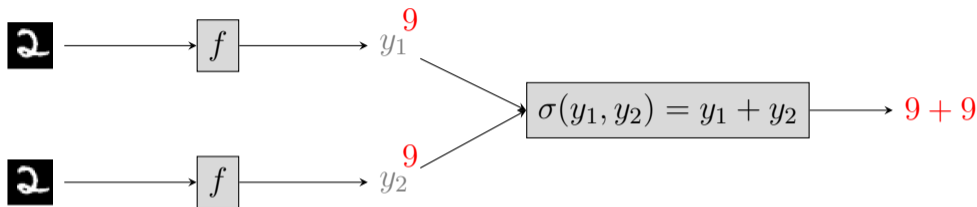
Learnability: intuition

- To prove learnability of an MI-PLL problem instance, we must bound $\mathcal{R}^{01}(f)$ (zero-one risk) with $\mathcal{R}_p^{01}(f; \sigma)$ (zero-one **partial** risk), under *any* training distribution.

Learnability: intuition

- In other words, **mistakes** under the partial training samples, should be informative of the **classification errors** made by f , under *any* training distribution.

Learning under the spike distribution: intuition



- Suppose the mass is concentrated in a single element $\mathbf{2}$ (gold label is $\mathbf{2}$).
- Suppose f misclassifies $\mathbf{2}$ as $\mathbf{9}$.
- Then, the gold labels are $(\mathbf{2}, \mathbf{2})$, but the classifier outputs $(\mathbf{9}, \mathbf{9})$.
- If $\mathbf{2} + \mathbf{2} = \mathbf{9} + \mathbf{9}$, then $\mathcal{R}_p^{01}(f; \sigma) = \mathbf{0}$, while $\mathcal{R}^{01}(f) \neq \mathbf{0}$.
- Hence, classifier errors are **concealed**.

A sufficient and necessary learnability condition

Definition (*M*-unambiguity)

Transition σ is *M-unambiguous* if for any two label vectors $\mathbf{y} = (y, \dots, y)$ and $\mathbf{y}' = (y', \dots, y')$, such that $\mathbf{y} \neq \mathbf{y}'$, we have $\sigma(\mathbf{y}) \neq \sigma(\mathbf{y}')$.

Let's map the definition to our example.

- Suppose the mass is concentrated in a single element **2** (gold label is **2**).
- Suppose f misclassifies **2** as **9**.
- Then, the gold labels are **(2, 2)**, but the classifier outputs **(9, 9)**.
- If **2 + 2 = 9 + 9**, then $\mathcal{R}_p^{01}(f; \sigma) = 0$, while $\mathcal{R}^{01}(f) \neq 0$.
- Hence, classifier errors are **concealed**.

M -unambiguity: example

Example (Sum of two digits)

Transition $\sigma^*(y_1, y_2) \rightarrow y_1 + y_2$ **is** M -unambiguous, since for any two different integers y and y' , we have:

$$y + y \neq y' + y'$$

M -unambiguity: example

Example (Product of two digits)

Transition $\sigma^*(y_1, y_2) \rightarrow y_1 \times y_2$ **is** M -unambiguous, since for any two different integers y and y' , we have:

$$y \times y \neq y' \times y'$$

M -unambiguity: counter example

Example (XOR)

Transition $\sigma^*(y_1, y_2) \rightarrow y_1 \oplus y_2$ **is not** M -unambiguous, since we have:

$$0 \oplus 0 = 1 \oplus 1$$

Is M -unambiguity a good condition?

Definition (M -unambiguity)

Transition σ is M -unambiguous if for any two label vectors $\mathbf{y} = (y, \dots, y)$ and $\mathbf{y}' = (y', \dots, y')$, such that $\mathbf{y} \neq \mathbf{y}'$, we have $\sigma(\mathbf{y}) \neq \sigma(\mathbf{y}')$.

- M -unambiguity: invertibility only under inputs of the same class.
- Looser conditions can be obtained when the input data distribution is not a spike.

Key result

Theorem. If σ is M -unambiguous, then $\mathcal{R}^{01}(f) \leq \mathcal{O}(\mathcal{R}_P^{01}(f; \sigma)^{1/M})$.

Learnability under M -unambiguity

Theorem

Suppose \mathcal{F} is realizable under $\ell_{\mathbb{P}}^{01}$ and $[\mathcal{F}]$ has a finite Natarajan dimension $d_{[\mathcal{F}]}$. Then for any $\epsilon, \delta \in (0, 1)$, there exists a universal constant $C_0 > 0$, such that with probability at least $1 - \delta$, the empirical partial risk minimizer with $\widehat{\mathcal{R}}_{\mathbb{P}}^{01}(f; \sigma; \mathcal{T}_{\mathbb{P}}) = 0$ has a classification risk $\mathcal{R}^{01}(f) < \epsilon$, if

$$m_{\mathbb{P}} \geq C_0 \frac{c^{2M-2}}{\epsilon^M} \left(d_{[\mathcal{F}]} \log(6cM d_{[\mathcal{F}]}) \log \left(\frac{|\mathcal{Y}|^{2M-2}}{\epsilon^M} \right) + \log \left(\frac{1}{\delta} \right) \right)$$

Number of samples to ensure with probability $\geq 1 - \delta$ that f does few mistakes ($\mathcal{R}^{01}(\mathcal{A}(\mathcal{T}_{\mathbb{P}})) \leq \epsilon$)

Summary of results

- Better convergence rates via forcing additional conditions.
- Learnability under **multiple classifiers**.
- Learnability under **non-deterministic** σ .
- Learnability under **unknown** σ .
- Rademacher error bounds under logic-based losses [45] based on weighted model counting [4, 45].
- Error bounds under approximations [13].

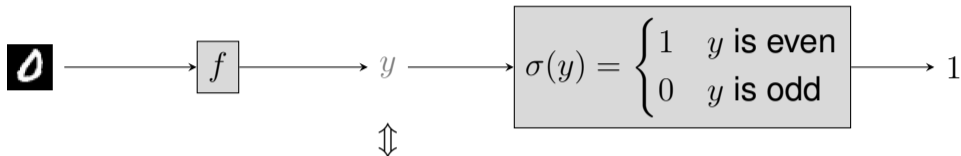
Kaifu Wang, **Efthymia Tsamoura**, and Dan Roth. **On learning latent models with multi-instance weak supervision**. In NeurIPS, 2023.

MI-PLL vs other ML problems

Relevant problems in ML

- **Partial label learning (PLL)** [2, 8, 14, 22, 30, 44, 46, 48].
- Learning via transition matrices [6, 7, 40, 50].

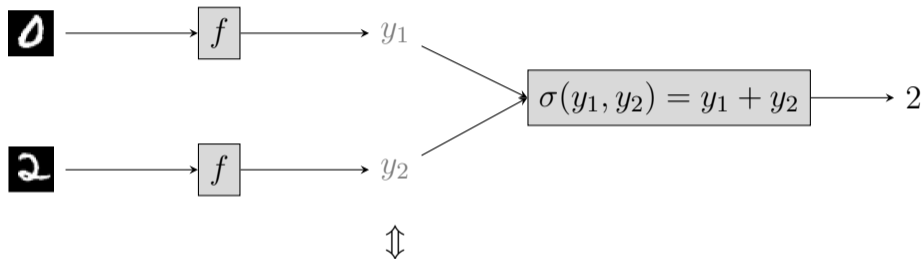
Example: PLL



(0 , $\{0, 2, 4, 6, 8\}$) ← PLL training example

↑
Mutually exclusive candidate labels

Relationship of our problem to PLL



$((0, 2), \{(0, 2), (2, 0), (1, 1)\})$

← MI-PLL training example

↑
Mutually exclusive candidate label vectors

Key differences with PLL

- Multiple vs single input.
- Deterministic vs stochastic σ .
- Prior learnability results ([2, 8, 21]) rely on assumptions that are violated in our setting, i.e., that $\gamma < 1$, where

$$\gamma := \sup_{\underbrace{\mathcal{D}(x, y) > 0}_{\text{density}}, y' \neq y} \overbrace{\mathbb{P}_{(x, y) \sim \mathcal{D}}(\underbrace{y'}_{\text{noisy label}} \in \sigma(\underbrace{y}_{\text{gold label}}))}_{\text{probability noisy } y' \text{ co-occurs with } y}$$

Key differences with PLL

- Multiple vs single input.
- Deterministic vs stochastic σ .
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$$\gamma := \sup_{\underbrace{\mathcal{D}(x, y) > 0}_{\text{density}}, y' \neq y} \mathbb{P}_{(x, y) \sim \mathcal{D}} \left(\underbrace{y'}_{\text{noisy label}} \in \sigma \left(\underbrace{y}_{\text{gold label}} \right) \right)$$

probability noisy y' co-occurs with y

- M -unambiguity reduces to small ambiguity for single inputs ($M = 1$).
- Shown learnability under non-deterministic σ (proper extension of small ambiguity).

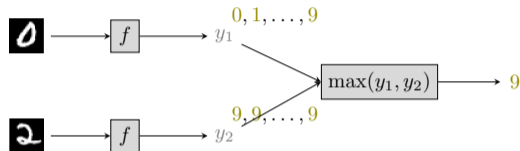
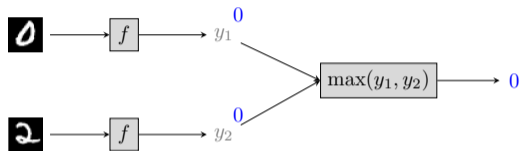
Learning imbalances in MI-PLL

Kaifu Wang, **Efthymia Tsamoura**, and Dan Roth. **On characterizing and mitigating imbalances in multi-instance weak supervision**. CoRR, abs/2407.10000, 2024.

Learning imbalances: what are they?

- Major differences in the errors occurring when classifying instances of different classes (aka *class-specific risks*).

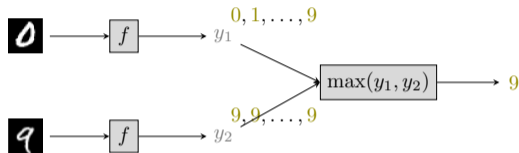
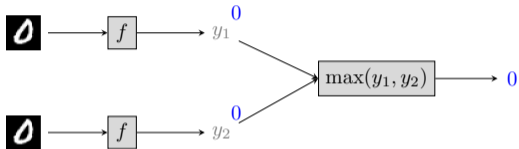
Learning imbalances: 2MAX



Question: Which class is easier to learn if the number of $(\mathbf{0}, \mathbf{0}), 0$ samples equals the number of $(\mathbf{0}, \mathbf{9}), 9$ samples.

Answer: Intuitively, class 0, as learning 0 reduces to *supervised learning*.

Learning imbalances: 2MAX



Question: Which class is easier to learn if *the number of 0's equals that of 9's*.

Answer: We have **more** samples of the form $((0, 9), 9)$ than of the form $((0, 0), 0)$.
Hence, class 9 might be easier to learn?

Learning imbalances: 2MAX

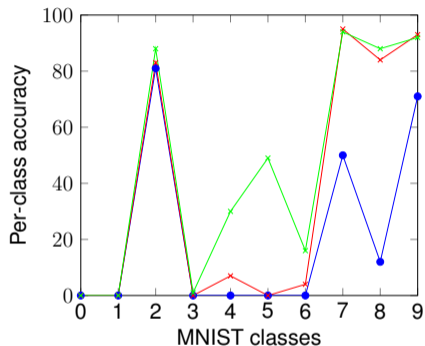


Figure: Accuracy of the MNIST classifier. Blue, red and green curves show accuracy at 20, 40 and 100 epochs. Learning converges in 100 epochs.

Learning imbalances in traditional machine learning

- Core ML problem [1, 3, 5, 16, 24, 26, 35, 36], as real data is imbalanced.
- ML techniques cannot characterize imbalances in our setting:
 - Work for long-tail data only– we also have imbalances due to σ .

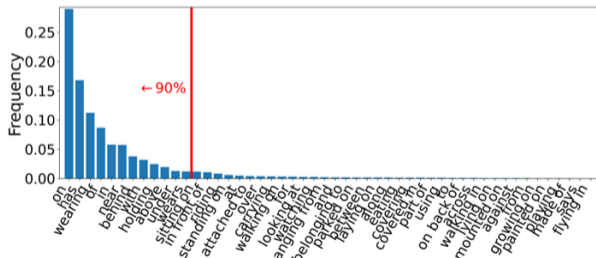
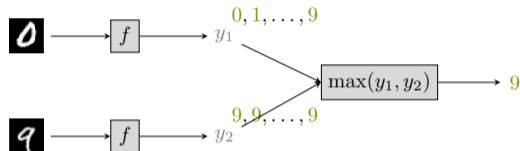
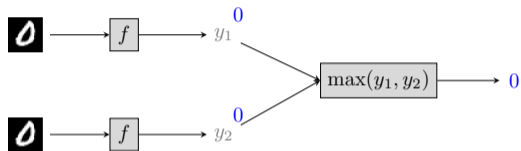


Figure: Distribution of classes in Visual Genome [17].

Learning imbalances: 2MAX



ML characterizations would naively say: **it is equally difficult to learn classes 0 and 9** if the instance distributions are uniform.

Learning imbalances: theoretical characterization

- We bounded the class-specific risk $R_j(f)$ via function:

Transition, e.g., max Class

$$\Phi_{\sigma, j}(R_P(f; \sigma))$$

Probability of wrong overall output,
e.g., wrong maximum

- This bound is computed by solving a quadratic program.

Extends our previous results!

- Bound $\Phi_{\sigma, j}(R_P(f; \sigma))$ does not rely on M -unambiguity.
- Tighter bounds than what we discussed already.

Learning imbalances: theoretical characterization

- We bounded the class-specific risk $R_j(f)$ via function:

Transition, e.g., max Class

$$\Phi_{\sigma, j} (R_P(f; \sigma))$$

Probability of wrong overall output,
e.g., wrong maximum

- We can derive a computable bound for $R_j(f)$ using a dataset of partial sample and tools, such as VC-dimension and the Rademacher complexity.

Learning imbalances: theoretical characterization

Theorem

Let $d_{[\mathcal{F}]}$ be the Natarajan dimension of $[\mathcal{F}]$, $c = |\mathcal{Y}|$, and $m_{\mathcal{P}}$ be the number of partial samples. Given a confidence level $\delta \in (0, 1)$, we have that $R_j(f) \leq \Phi_{\sigma,j}(\tilde{R}_{\mathcal{P}}(f; \sigma, \mathcal{T}_{\mathcal{P}}, \delta))$ with probability $1 - \delta$ for any label $j \in [c]$, where

$$\tilde{R}_{\mathcal{P}}(f; \sigma, \mathcal{T}_{\mathcal{P}}, \delta) = \hat{R}_{\mathcal{P}}(f; \sigma, \mathcal{T}_{\mathcal{P}}) + \sqrt{\frac{2 \log(em_{\mathcal{P}}/2d_{[\mathcal{F}]} \log(6Mc^2d_{[\mathcal{F}]} / e))}{m_{\mathcal{P}}/2d_{[\mathcal{F}]} \log(6Mc^2d_{[\mathcal{F}]} / e)}} + \sqrt{\frac{\log(1/\delta)}{2m_{\mathcal{P}}}}$$

Generalization bound

Empirical partial risk

Learning imbalances: 2MAX

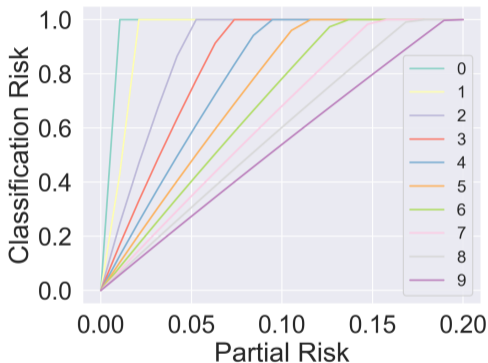
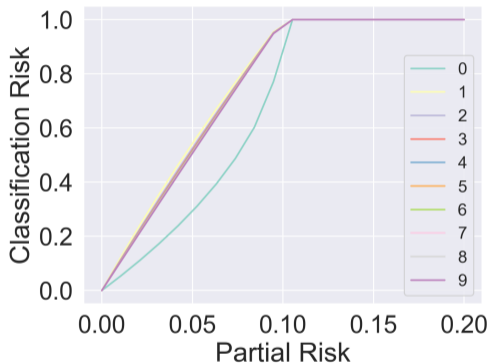


Figure: Class-specific upper bounds. (left) Partial labels are uniform. (right) Hidden labels are uniform.

Learning imbalances: testing-time mitigation

Classifier's predictions P

$$\begin{matrix} & y = 0 & \cdots & y = 9 \\ \begin{matrix} 2 \\ \vdots \\ 0 \\ \vdots \\ 9 \end{matrix} & \begin{pmatrix} 0.1 & \cdots & 0.05 \\ \vdots & & \vdots \\ 0.7 & \cdots & 0.01 \\ \vdots & & \vdots \\ 0.01 & \cdots & 0.8 \end{pmatrix} & \begin{matrix} \\ \\ \text{Predictions for the } i\text{-th} \\ \\ \text{test sample} \end{matrix} \end{matrix}$$

Rationale.

Given a (gold) hidden label distribution \hat{r} , correct the predictions P to P' , so that P' adheres to \hat{r} .

Learning imbalances: testing-time mitigation

Classifier's predictions P

$$\begin{matrix} & y = 0 & \cdots & y = 9 \\ \begin{matrix} \mathbf{2} \\ \vdots \\ \mathbf{0} \\ \vdots \\ \mathbf{9} \end{matrix} & \begin{pmatrix} 0.1 & \cdots & 0.05 \\ \vdots & & \vdots \\ 0.7 & \cdots & 0.01 \\ \vdots & & \vdots \\ 0.01 & \cdots & 0.8 \end{pmatrix} & \begin{matrix} \text{Predictions for the } i\text{-th} \\ \text{test sample} \end{matrix} \end{matrix}$$

Rationale.

Given a (gold) hidden label distribution \hat{r} , correct the predictions P to P' , so that P' adheres to \hat{r} .

Challenges.

- The developed technique should be lightweight.
- P' should be close *enough* to P .
- P' should not strictly abide to \hat{r} (to tolerate noise).

Learning imbalances: testing-time mitigation

Rationale. Given a (gold) hidden label distribution \hat{r} , correct the predictions P to P' , so that P' adheres to \hat{r} .

Challenges:

- The developed technique should be lightweight.
- P' should be close *enough* to P .
- P' should not strictly abide to \hat{r} (to tolerate noise).

$$\min_{\substack{P' \in \mathbb{R}_+^{n \times c}, \\ P' \mathbf{1}_c = \mathbf{1}_n}} \langle -\log(P), P' \rangle + \tau KL(P' \mathbf{1}_n || n \hat{r}) \quad (1)$$

Closeness to original predictions (yellow arrow pointing to $\langle -\log(P), P' \rangle$)

Robustness to \hat{r} (blue arrow pointing to $\tau KL(P' \mathbf{1}_n || n \hat{r})$)

P' induces a valid distribution (green arrow pointing to $P' \mathbf{1}_c = \mathbf{1}_n$)

Learning imbalances: testing-time mitigation

- This formulation is a *robust semi-constrained optimal transport* (RSOT) problem instance [18].
- Approximate the optimal solution using the robust semi-Sinkhorn algorithm [18].

Closeness to original predictions

Robustness to \hat{r}

$$\min_{\mathbf{P}' \in \mathbb{R}_+^{n \times c}, \mathbf{P}' \mathbf{1}_c = \mathbf{1}_n} \langle -\log(\mathbf{P}), \mathbf{P}' \rangle + \tau KL(\mathbf{P}' \mathbf{1}_n || n \hat{r}) - \eta H(\mathbf{P}')$$

P' induces a valid distribution

Entropic regularization to find solutions in PTIME.

Learning imbalances: more results

- Statistically consistent technique to compute the hidden label ratios \hat{r} .
- Technique to mitigate learning imbalances at training-time.
- Improved the accuracy on multiple benchmarks by $> 20\%$.

Kaifu Wang, **Efthymia Tsamoura**, and Dan Roth. **On characterizing and mitigating imbalances in multi-instance weak supervision**. CoRR, abs/2407.10000, 2024.

Conclusions

Keywords (instead of conclusions)

- Applications.
- Scalability.
- Uncertainty– many proposals, what is the right semantics?
- Formal guarantees.

Efthymia Tsamoura, et al. **Probabilistic Reasoning at Scale: Trigger Graphs to the Rescue**. In SIGMOD, 2023.

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Efthymia Tsamoura, et al. **Beyond the Grounding Bottleneck: Datalog Techniques for Inference in Probabilistic Logic Programs**. In AAAI, 2020.

Michael Benedikt, Boris Motik, and Efthymia Tsamoura. **Goal-Driven Query Answering for Existential Rules With Equality**. In AAAI, 2018.

Thanks!

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Relevant problems in ML

- Partial label learning (PLL) [2, 8, 14, 22, 30, 44, 46, 48].
- **Learning via transition matrices** [6, 7, 40, 50].

Learning via transition matrices

- If the transition is **invertible**, then we can compute the **hidden data distribution** via its association with the **observed data distribution**. Hence, we construct an unbiased estimator for the **classification loss**.

$$\underbrace{o(\mathbf{x})}_{[\mathbb{P}(S=1|\mathbf{x}), \dots, \mathbb{P}(S=|\mathcal{S}||\mathbf{x})]} = \overbrace{\mathbf{T}(\mathbf{x})}^{\text{Transition matrix}} \underbrace{h(\mathbf{x})}_{[\mathbb{P}(Y=1|\mathbf{x}), \dots, \mathbb{P}(Y=|\mathcal{Y}||\mathbf{x})]}$$
$$\underbrace{h(\mathbf{x})}_{[\mathbb{P}(Y=1|\mathbf{x}), \dots, \mathbb{P}(Y=|\mathcal{Y}||\mathbf{x})]} = \overbrace{\mathbf{T}^+(\mathbf{x})}^{\text{Transition matrix left inverse}} \underbrace{o(\mathbf{x})}_{[\mathbb{P}(S=1|\mathbf{x}), \dots, \mathbb{P}(S=|\mathcal{S}||\mathbf{x})]}$$

Results

- Reduction of MI-PLL to learning via transition matrices is not straightforward: naive reductions lead to non-invertible matrices :)
- For non-naive reductions, we have:
 - M -unambiguity $\not\Rightarrow$ matrix invertibility.
 - Matrix invertibility $\not\Rightarrow$ M -unambiguity.

Kaifu Wang, **Efthymia Tsamoura**, and Dan Roth. **On learning latent models with multi-instance weak supervision**. In NeurIPS, 2023.