Evidential Uncertainty Quantification: A Variance-Based Perspective

Ruxiao Duan[1], Brian Caffo[2,3], Harrison X. Bai[4], Haris I. Sair[3,4], and Craig Jones[3,4,5]
[1]Department of Applied Mathematics and Statistics, [2]Department of Biostatistics,
[3]Malone Center for Engineering in Healthcare, [4]Department of Radiology and Radiological Science, [5]Department of Computer Science
Whiting School of Engineering, School of Public Health, School of Medicine | Johns Hopkins University

Evidential Deep Learning

- **Evidential deep learning (EDL)**
  - a non-Bayesian approach to estimate aleatoric uncertainty (AU) and epistemic uncertainty (EU) by modeling the evidential prior of target distribution
- **Entropy-based classification EDL**
  - quantifies total uncertainty as predictive entropy
  - decomposes uncertainty by information theory
- **Variance-based classification EDL (ours)**
  - quantifies total uncertainty as predictive variance
  - decomposes uncertainty by law of total covariance

Variance-Based Evidential Deep Learning

- **Classification problem notations**
  - C: number of classes
  - $\boldsymbol{y}$: target one-hot label vector
  - $\mathbf{p}$: class probability vector
  - $\boldsymbol{\alpha}$: prior distribution parameters (model prediction)
- **Fundamental probability distribution assumptions**

$$\mathbf{y} \sim \mathrm{Multinomial}(1, \mathbf{p})$$
$$\mathbf{p} \sim \mathrm{Dirichlet}(\boldsymbol{\alpha})$$

- **Covariance matrix decomposition**

$$\mathrm{Cov}[\mathbf{y}] := \mathbb{E}\left[(\mathbf{y} - \mathbb{E}[\mathbf{y}])(\mathbf{y} - \mathbb{E}[\mathbf{y}])^{\mathrm{T}}\right] = \mathrm{Diag}(\bar{\mathbf{p}}) - \bar{\mathbf{p}}\bar{\mathbf{p}}^{\mathrm{T}}$$

$$\mathrm{Cov}[\mathbf{y}]^{\mathrm{alea}} := \mathbb{E}\left[\mathrm{Cov}[\mathbf{y}|\mathbf{p}]\right] = \frac{\alpha_0}{\alpha_0 + 1}\left(\mathrm{Diag}(\bar{\mathbf{p}}) - \bar{\mathbf{p}}\bar{\mathbf{p}}^{\mathrm{T}}\right)$$

$$\mathrm{Cov}[\mathbf{y}]^{\mathrm{epis}} := \mathrm{Cov}\left[\mathbb{E}[\mathbf{y}|\mathbf{p}]\right] = \frac{1}{\alpha_0 + 1}\left(\mathrm{Diag}(\bar{\mathbf{p}}) - \bar{\mathbf{p}}\bar{\mathbf{p}}^{\mathrm{T}}\right)$$

$$\alpha_0 := \sum_{i=1}^{C} \alpha_i \qquad \bar{\mathbf{p}} := \mathbb{E}[\mathbf{p}] = \frac{\boldsymbol{\alpha}}{\alpha_0}$$

- **Class-level evidential uncertainties**

$$\mathrm{U}_i^{\mathrm{alea}} := \mathrm{Cov}[\mathbf{y}]_{i,i}^{\mathrm{alea}} = \frac{\alpha_0}{\alpha_0 + 1}\bar{\mathrm{p}}_i(1 - \bar{\mathrm{p}}_i)$$

$$\mathrm{U}_i^{\mathrm{epis}} := \mathrm{Cov}[\mathbf{y}]_{i,i}^{\mathrm{epis}} = \frac{1}{\alpha_0 + 1}\bar{\mathrm{p}}_i(1 - \bar{\mathrm{p}}_i)$$

- **Sample-level evidential uncertainties**

$$\mathrm{U}^{\mathrm{alea}} := \sum_{i=1}^{C} \mathrm{U}_i^{\mathrm{alea}} = \frac{\alpha_0}{\alpha_0 + 1}\left(1 - \sum_{i=1}^{C} \bar{\mathrm{p}}_i^2\right)$$

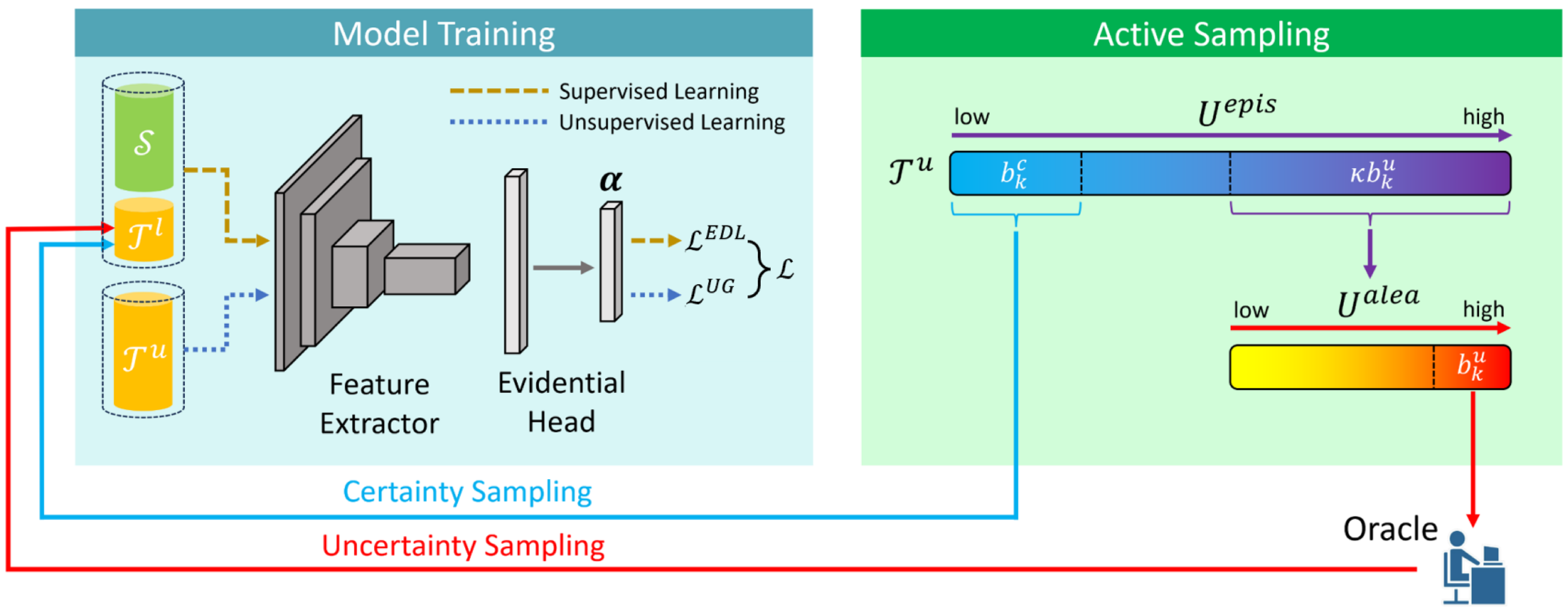
$$\mathrm{U}^{\mathrm{epis}} := \sum_{i=1}^{C} \mathrm{U}_i^{\mathrm{epis}} = \frac{1}{\alpha_0 + 1}\left(1 - \sum_{i=1}^{C} \bar{\mathrm{p}}_i^2\right)$$

- **Class correlation matrix**

$$\mathrm{Corr}[\mathbf{y}] := \frac{\mathrm{Cov}[\mathbf{y}]}{\sigma(\mathbf{y})\sigma(\mathbf{y})^{\mathrm{T}}}$$

$$\sigma(\mathbf{y}) := \sqrt{\mathrm{diag}(\mathrm{Cov}[\mathbf{y}])}$$

Active Domain Adaptation



EDL-based active domain adaptation (ADA) framework DUC with concurrent certainty and uncertainty sampling

- **Domain gap reduction**: model trained by uncertainties of unlabeled target dataset
- **Uncertainty sampling**: two-round sampling strategy based on evidential uncertainties
- **Certainty sampling**: certain samples identified by EU for semi-supervised learning

Experiment Results and Analysis

- **Sample-level uncertainty quantification**

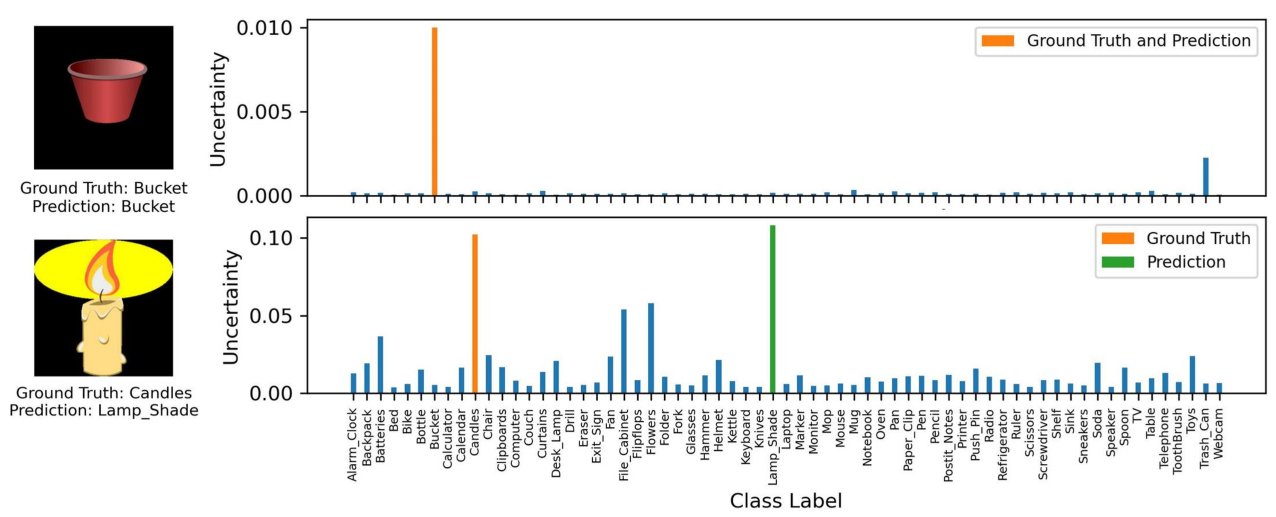
U	Office-Home		Visda-2017	
	w/o CS	w/ CS	w/o CS	w/ CS
Entropy	78.1	79.3	89.3	89.3
Variance	78.2	79.5	89.4	89.5

ADA accuracy (%) *CS: certainty sampling

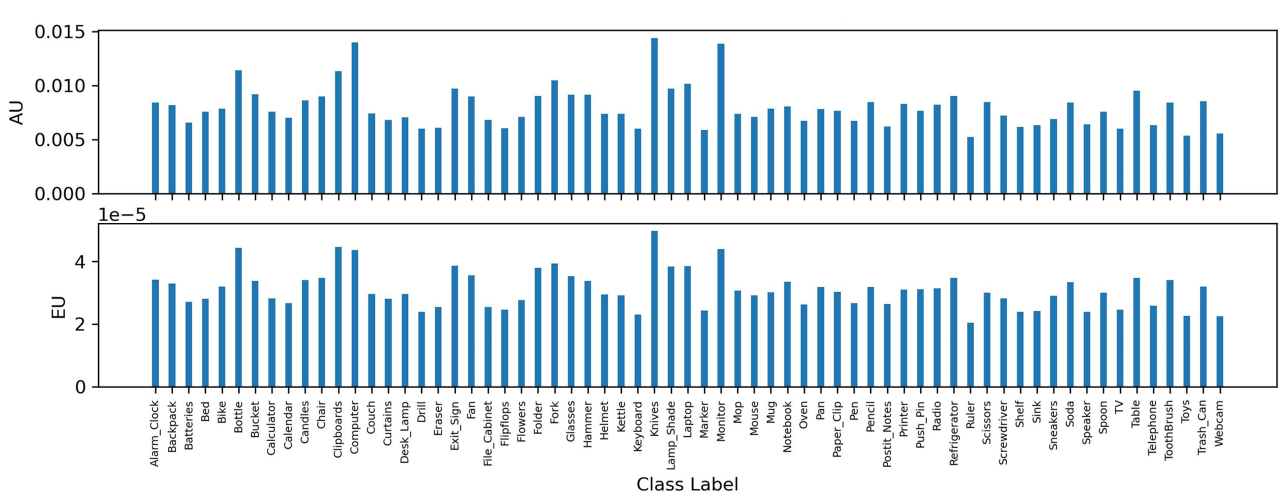
U	Office-Home		Visda-2017	
	AU	EU	AU	EU
Entropy	83.0	81.7	75.6	73.8
Variance	83.3	82.0	75.3	73.8

Misclassification detection AUC (%)

- **Class-level uncertainty quantification**

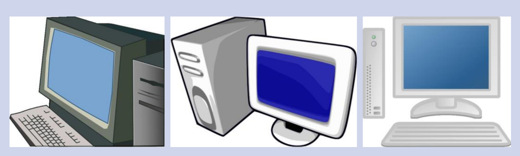
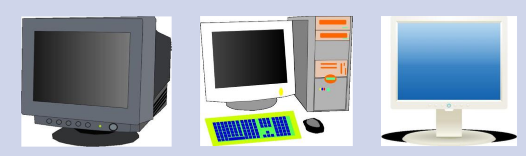
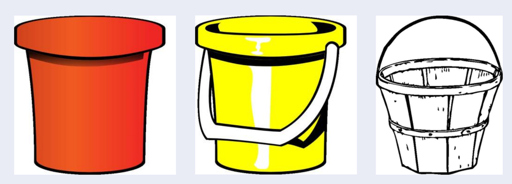
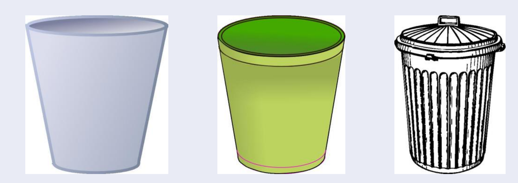
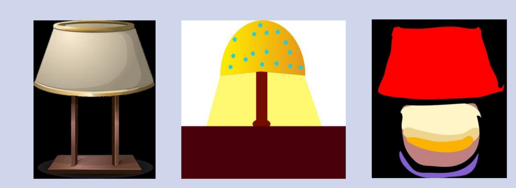


Class-level uncertainties of two Office-Home images



Class uncertainties of Office-Home Clipart

- **Between-class correlation quantification**

Class Pair		Corr
Computer 	Monitor 	-0.364
Bucket 	Trash Can 	-0.239
Desk Lamp 	Lamp Shade 	-0.226

Three most correlated class pairs in Office-Home Clipart

- **Compared with entropy-based EDL, the variance-based approach**
  - achieves equivalent performance on sample-level uncertainty quantification
  - provides class-level evidential uncertainties
  - provides between-class correlations