

# Uncertainty-Aware Training of Neural Networks for Selective Medical Image Segmentation

Yukun Ding<sup>1</sup>, Jinglan Liu<sup>1</sup>, Xiaowei Xu<sup>2</sup>, Meiping Huang<sup>2</sup>, Jian Zhuang<sup>2</sup>, Jinjun Xiong<sup>3</sup>, Yiyu Shi<sup>1</sup> <sup>1</sup> University of Notre Dame, <sup>2</sup> Guangdong General Hospital, <sup>3</sup> IBM

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- Background
- Motivation
- Method
- Results
- Limitation and Future Work

# Uncertainty of DNNs

- Why we need to consider the uncertainty?
  - Real-world problems are diverse
  - Identify and deal with potential failure properly
- The word "uncertainty" can be tricky e.g.,
  - This is a tumor, but I think there is a 30% of chance I'm wrong
  - This is a tumor, rotate the image a bit -> this is not a tumor
- What uncertainty are we consider here?
  - For each input  $x_i$  , the model outputs prediction  $\hat{y_i}$  , and the uncertainty score  $u_i$
  - The uncertainty score  $u_i$  indicates how likely the prediction is wrong
  - A popular baseline of uncertainty estimation: 1 (softmax probability)





#### **Selective Prediction**









• Selective segmentation



• The *practical target* and *training target*:





- For each input  $x_i \in X$ , model outputs prediction  $\hat{y}_i$ , and the uncertainty score  $u_i$ , the correctness score  $s_i = 1$  if the prediction  $\hat{y}_i$  is correct, otherwise  $s_i = 0$
- If we apply a threshold on the uncertainty, we divide the input data into two subset  $X_l = \{x_i | u_i \le t\}$  and  $X_h = X X_l$ , the coverage is defined as  $c = \frac{|X_l|}{|X|}$
- Consider the accuracy at coverage c

$$\psi_c = \frac{\sum_{x_i \in X_l} s_i}{|X_l|} \qquad \psi_1 = \frac{\sum_{x_i \in X} s_i}{|X|}$$

- Our practical target, accuracy at coverage c, depends on both the quality of prediction and the quality of uncertainty estimation
- We know how to optimize our neural network for prediction, but not for uncertainty



- Estimating the uncertainty is a probabilistic prediction problem
- Scoring rule:
  - A quantified summary measure for the quality of probabilistic predictions
- Proper scoring rule:
  - Denote the truth distribution as q and the predicted distribution as  $p_{\theta}$ , a scoring rule h is a proper scoring rule if  $h(p_{\theta}, q) \le h(q, q)$
- Strictly proper scoring rule:
  - Same as the proper scoring rule, but  $h(p_{\theta}, q) = h(q, q)$  if and only if  $p_{\theta} = q$
- Commonly used loss functions are strictly proper scoring rule
  - E.g., Cross Entropy, L2
  - This is why softmax probability can be a strong baseline for uncertainty estimation



For the uncertainty estimation in selective segmentation, we do not need a strictly proper scoring rule that tries to recover the actual distribution q.

- The uncertainty score u is only used to divide the data into two subset, we only want more correct predictions go to the low uncertainty subset and more wrong predictions go to the high uncertainty subset.
- Even if we consider all possible coverage, only the relative ranking of u matter and we don't care the specific value of u.
- So we try to find a better optimization target that is not a strictly proper scoring rule.



**Theorem 1** Denote  $\gamma = \frac{\sum_{x_i \in X_h} (1-s_i)}{|X_h|}$ , then we have the following properties about  $\psi_c$ ,  $\psi_1$ , and  $\gamma$  for  $c \in (0, 1]$ :

(i)  $\gamma$  is a proper scoring rule but not a strictly proper scoring rule for uncertainty estimation.

(*ii*) 
$$\psi_c = \frac{\psi_1 - (1 - \gamma)(1 - c)}{c}$$
, s.t.  $(1 - \gamma)(1 - c) \in [\psi_1 - c, \psi_1]$ .  
(*iii*)  $\frac{\partial \psi_c}{\partial \gamma} > 0$  and  $\frac{\partial \psi_c}{\partial \psi_1} > 0$  for any  $\gamma$  and  $c$ .

- Why  $\gamma$  :
  - $-\gamma$  is a proper scoring rule but not a strictly proper scoring rule
  - $\gamma$  fully determines  $\psi_c$  with  $\psi_1$
  - The partial derivative is always positive



#### **Uncertainty-Aware Training**

• How to optimize  $\gamma$ ?

$$\mathcal{L}_{uncertainty} = \sum_{u_j \in U_w, u_k \in U_c} \max(u_k - u_j + m, 0).$$

• The uncertainty-aware training loss:

$$\mathcal{L}_{u-seg} = \mathcal{L}_{segmentation} + \lambda \mathcal{L}_{uncertainty}$$

$$\psi_{c} \qquad \psi_{1} \qquad \gamma$$



### The Dice-Coverage Curve

- Reduced coverage leads to higher accuracy
- Uncertainty-aware training outperforms the baseline





### Quantitative Results

- Reduced coverage leads to higher accuracy
- Uncertainty-aware training outperforms the baseline

Dataset	AURC $(\%)$		Coverage	Dice $(\%)$		Dice@5PCTL (%)		
	Baseline	Ours	coverage	Baseline	Ours	Baseline	Ours	AURC
MM-WHS	0.936	0.810	0.95	$93.86 \pm 3.66$	$94.72{\pm}2.53$	83.18	89.19	100 99 96 96 97 98 96 98 99 99 99 90 99 94 94 94 94 94 94 94 94 95 94 94 94 94 94 95 94 94 94 95 94 94 95 94 94 95 94 94 95 94 95 94 95 95 95 95 95 95 95 95 95 95
			0.90	$96.73 \pm 2.30$	$97.35{\pm}1.54$	90.55	94.64	
			0.80	$98.98 {\pm} 0.79$	$99.21{\pm}0.61$	97.42	98.11	
			0.70	$99.64 {\pm} 0.31$	$99.72{\pm}0.31$	98.98	99.07	90 - Uncertainty-aware Fold 3 Baseline Fold 4
$\operatorname{GlaS}$	6.981	6.031	0.95	$78.62 \pm 16.87$	$80.80{\pm}16.48$	35.99	39.16	Baseline Fold 5
			0.90	$82.14 \pm 14.53$	$84.26{\pm}13.87$	49.77	52.46	– 0.70 0.75 0.80 0.85 0.90 0.95 1.00 Coverage
			0.80	$87.54 \pm 12.31$	$89.37{\pm}11.24$	66.63	67.90	-
			0.70	$91.45 \pm 10.86$	$92.92{\pm}9.55$	75.95	74.81	-



### **Qualitative Results**





## Per-Image Comparison

- The performance is improved by uncertainty-aware training
- With decreasing average coverage
  - Per-image coverage difference increases
  - Per-image Dice difference decreases







• It is not very efficient to do **pixel-wise** selective segmentation

- We are currently looking at **image-wise** selective segmentation
- Challenges: image-wise uncertainty measure; joint training

- $\gamma$  is a proven good target, but the  $\mathcal{L}_{uncertainty}$  is not
  - A better loss to optimize  $\gamma$  ? Or even directly optimize  $\psi_c$  ?



Thank You!Q&A