Learning and Probabilistic Inference with Constraints and its Applications

Zhe Zeng

Advisor: Prof. Guy Van den Broeck
Overview

• **Goal**: To enable machine learning models to perform learning and probabilistic inference under constraints
Bayesian Deep Learning [arithmetic constraints]

• **Goal**: Marginalization over the weight space
  • to aggregate models with low loss

Loss Surface  Predictions and Uncertainty

\[
p(y \mid x) = \int p(y \mid x, w) p(w \mid D) \, dw
\]

\[
E_{p(y \mid x)}[y] = \int y \, p(y \mid x) \, dy
\]

under constraints from ReLU:
\[
x \cdot w \geq 0
\]

• **Solution**: efficiently and effectively by **Weighted Model Integration**

Z. Zeng, G. Van den Broeck. Collapsed Inference for Bayesian Deep Learning, Beyond Bayes, ICML Workshop, 2022
Gradient Estimator for k-Subset [discrete constraints]

• **Goal:** Modeling a distribution of \( k \)-subsets of elements \( p_\theta(z \mid \sum_i z_i = k) \)

**Example.** Learn to Explain 🍺

<table>
<thead>
<tr>
<th>Key Words (( k = 10 ))</th>
<th>Taste Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>a lite bodied beer with a pleasant taste. was like a reddish color. a little like wood and caramel with a hop finish. has a sort of fruity flavor like grapes or cherry that is sort of buried in there. mouth feel was lite, sort of bubbly. not hard to down, though a bit harder then one would expect given the taste.</td>
<td>0.7</td>
</tr>
</tbody>
</table>

• **Solution:**
SIMPLE that computes exact samples and exact derivatives

Weakly Supervised Learning [discrete constraints]

- **Goal:** To train classifiers under weak supervisions

<table>
<thead>
<tr>
<th>classical</th>
<th>learning from label proportions</th>
<th>multiple instance learning</th>
<th>learning from positive and unlabeled data</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x$</td>
<td>$y$</td>
<td>${x_i}_{i=1}^k$</td>
<td>$\hat{y} = \sum y_i/k$</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td></td>
<td>1/3</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td></td>
<td>3/5</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Solution:** To use *probability* of these *constraints on label counts* being satisfied as training objectives

Ongoing and Future Work

• To build machine learning models
  • that can deal with complicated constraints
  • and deliver accurate and efficient inference

• Applications to various fields
  • computational chemistry: metal-organic frameworks
  • more ……
• Thank you for your time!

• Q & A

• Email: zhezeng@cs.ucla.edu