Are Uncertainty Quantification Capabilities of Evidential Deep Learning a Mirage?

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Recall: Evidential Deep Learning

- Place a Dirichlet distribution on the output

$$D(\mathbf{p} \mid \boldsymbol{\alpha}) = \begin{cases} \frac{1}{B(\boldsymbol{\alpha})} \prod_{i=1}^{K} p_i^{\alpha_i - 1} & \text{for } \mathbf{p} \in \mathcal{S}_K, \\ 0 & \text{otherwise,} \end{cases}$$

- Minimize the MSE loss function with regularizing terms.

$$\mathcal{L}(\Theta) = \sum_{i=1}^{N} \mathcal{L}_i(\Theta) + \lambda_t \sum_{i=1}^{N} \mathrm{KL}\left[D(\mathbf{p}_i \mid \tilde{\boldsymbol{\alpha}}_i) \parallel D\left(\mathbf{p}_i \mid \langle 1, \ldots, 1 \rangle\right)\right]$$

$$\mathcal{L}_i(\Theta) = \int \|\mathbf{y}_i - \mathbf{p}_i\|_2^2 \frac{1}{B(\boldsymbol{\alpha}_i)} \prod_{j=1}^{K} p_{ij}^{\alpha_{ij}-1} \, \mathrm{d}\mathbf{p}_i$$

~~Introduction~~ Conclusion

- Uncertainty learned by most of the EDL methods has **no** statistical meaning.
- Problems with EDL arise from ignoring the **model uncertainty** for computational effiency.
- The authors suggest that EDL methods can be better interpreted as energy-based out-of-distribution (OOD) detection algorithms.

Recent work has reported EDL limitations

- Bengs et al. (NeurIPS 2022): non-vanishing distributional uncertainty
- Bengs et al. (ICML 2023): a possibility of non-existence of proper scoring rules for meta distributions
- Jürgens et al. (ICML 2024): a gap between learned uncertainty and an ideal meta distribution
- What is proposed by the authors in this paper (NeurIPS 2024)?

Introduction

This paper:

- Unifies various objective functions (loss function to minimize) of a wide class of EDL methods.
- Provides empirical evidence to point out the fundamental limitations of the learned uncertainties by EDL.
- Presents several findings showing that existing EDL methods are essentially OOD detectors.

Problem Setting

- Aim to learn $p(y \mid x)$, given data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}$ drawn from underlying $p(x, y)$ over $\mathcal{X} \times \mathcal{Y}$.
  - $\mathcal{Y} = [C] := \{1, 2, ..., C\}$ for classification, $\mathcal{Y} \in \mathbb{R}$ for regression.
  - Here we mainly discuss classification settings.
- With a trained parametric classifier $p(y|x, \psi)$, the predictive posterior distribution is given by:

$$p(y \mid x, \mathcal{D}) := \int p(y \mid x, \psi) p(\psi \mid \mathcal{D}) \, \mathrm{d}\psi$$

$p(y \mid x, \psi)$ captures *aleatoric uncertainty*, while $p(\psi \mid \mathcal{D})$ describes *epistemic uncertainty*.

Problem Setting

For EDL approach:

- Decompose $p(y \mid x, \psi) = \int p(\boldsymbol{\pi} \mid x, \psi) p(y \mid \boldsymbol{\pi}) \, \mathrm{d}\boldsymbol{\pi}$, where $\pi \in \Delta^{C-1}$ is a probability vector.
  - $p(\boldsymbol{\pi} \mid x, \psi)$ is a *meta distribution* over predictions at x. $p(y \mid \boldsymbol{\pi}) = \pi_y$ is a fixed likelihood model.
  - Usually $p(\boldsymbol{\pi} \mid x, \psi)$ is a conjugate prior (in the same probability distributions family) of $p(y \mid \boldsymbol{\pi})$, but sometimes not.
- The full decomposition:

$$p(y \mid x, \mathcal{D}) = \iint \underbrace{p(y \mid \boldsymbol{\pi})}_{\text{aleatoric}} \underbrace{p(\boldsymbol{\pi} \mid x, \psi)}_{\textit{distributional}} \underbrace{p(\psi \mid \mathcal{D})}_{\text{model}} \, \mathrm{d}\psi \, \mathrm{d}\boldsymbol{\pi}$$

Problem Setting

Consider marginalizing out ψ:

$$p(y \mid x, \mathcal{D}) = \iint p(y \mid \boldsymbol{\pi}) p(\boldsymbol{\pi} \mid x, \mathcal{D}) \mathrm{d}\boldsymbol{\pi}$$

EDL assumes the best single model ψ^* learned with data $\mathcal{D}$, without any randomness in $p(\psi \mid \mathcal{D})$:

$$p(\psi \mid \mathcal{D}) = \delta(\psi - \psi^*) \Longrightarrow p(\boldsymbol{\pi} \mid x, \mathcal{D}) \approx p(\boldsymbol{\pi} \mid x, \psi^*)$$

This simplification allows its computational efficiency but leads to fake distributional uncertainty.

For the following formulas, we use $p_\psi(\boldsymbol{\pi} \mid x)$ instead of $p(\boldsymbol{\pi} \mid x, \psi)$ since a single model ψ is assumed in this context.

EDL Taxonomy

Criterion 1. Parametric Form of Meta Distribution

The parametric form of $\alpha_\psi(x)$ in Dirichlet distribution $p_\psi(\boldsymbol{\pi} \mid x) = \mathrm{Dir}(\boldsymbol{\pi}; \boldsymbol{\alpha}_\psi(x))$:

- Direct parametrization: parameterize $\boldsymbol{\alpha}_\psi(x))$ by a direct output of a neural network. But it can arbitrary values on the OOD data points.
- Density parametrization: $\boldsymbol{\alpha}_\psi(x) \leftarrow \boldsymbol{\alpha}_0 + \boldsymbol{N}_\psi(x)$, where for $y \in [C]$, $(\boldsymbol{N}_\psi(x))_y := N_y p_{\psi_2}(f_{\psi_1}(x) \mid y)$. $f_{\psi_1}(x)$ is a feature extractor, and $p_{\psi_2}(z \mid y)$ is a tractable density model such as normalizing flows.

EDL Taxonomy

Criterion 2. Objective Function Function to minimize for representative EDL methods:

- Prior Networks (FPriorNet/RPriorNet): Given $\nu \gg 1$, $\boldsymbol{\alpha}_0 = \mathbf{1}_C$ and $\boldsymbol{e}_y$ as the one-hot true label, minimize

$$\mathbb{E}_{p(x,y)}\left[D\left(\mathrm{Dir}(\boldsymbol{\pi};\boldsymbol{\alpha}_0+\nu\boldsymbol{e}_y), p_\psi(\boldsymbol{\pi}\mid x)\right)\right]+\gamma_{\text{ood}}\mathbb{E}_{p_{\text{ood}}(x)}\left[D\left(\mathrm{Dir}(\boldsymbol{\pi};\boldsymbol{\alpha}_0), p_\psi(\boldsymbol{\pi}\mid x)\right)\right]$$

  Here $D(p,q) = D(p \parallel q)$ in FPriorNet, and $D(p,q) = D(q \parallel p)$ in RPriorNet.

- EDL: minimize the MSE loss with a reverse KL regularizer

$$\ell_{\text{MSE}}(\psi;x,y) := \mathbb{E}_{p_\psi(\boldsymbol{\pi}|x)}\left[\|\boldsymbol{\pi}-\boldsymbol{e}_y\|^2\right]+\lambda D\left(p_\psi(\boldsymbol{\pi}\mid x) \parallel \mathrm{Dir}(\boldsymbol{\pi};\boldsymbol{\alpha}_0)\right).$$

EDL Taxonomy

- Belief Matching: minimize VI loss justified by variational inference framework

$$\ell_{\mathrm{VI}}(\psi; x, y) := \mathbb{E}_{p_\psi(\boldsymbol{\pi}|x)}\left[\log \frac{1}{\pi_y}\right] + \lambda D\left(p_\psi(\boldsymbol{\pi} \mid x) \,\|\, \mathrm{Dir}(\boldsymbol{\pi}; \boldsymbol{\alpha}_0)\right).$$

- Posterior Networks (PostNet and NatPN): minimize the uncertainty-aware cross entropy (UCE) loss

$$\ell_{\mathrm{UCE}}(\psi; x, y) := \mathbb{E}_{p_\psi(\boldsymbol{\pi}|x)}\left[\log \frac{1}{\pi_y}\right] - \lambda h\left(p_\psi(\boldsymbol{\pi} \mid x)\right).$$

Unifying EDL Objectives for Classification

Define the *tempered likelihood*: for $\nu > 0$, define

$$p^{(\nu)}(\boldsymbol{\pi} \mid y) := \frac{p^{(\nu)}(\boldsymbol{\pi}, y)}{\int p^{(\nu)}(\boldsymbol{\pi}, y)\, \mathrm{d}\boldsymbol{\pi}}, \quad \text{where} \quad p^{(\nu)}(\boldsymbol{\pi}, y) := \frac{p(\boldsymbol{\pi}) p^{\nu}(y \mid \boldsymbol{\pi})}{\int p(\boldsymbol{\pi}) \sum_y p^{\nu}(y \mid \boldsymbol{\pi})\, \mathrm{d}\boldsymbol{\pi}}.$$

- The prior distribution $p(\boldsymbol{\pi}) = \mathrm{Dir}(\boldsymbol{\pi}; \boldsymbol{\alpha}_0)$ with $\alpha_0 = \mathbf{1}_C$.
- The likelihood model of Prior/Post Net and BM is categorical: $p(y \mid \boldsymbol{\pi}) = \pi_y$. It is easy to check $p^{(\nu)}(\boldsymbol{\pi} \mid y) = \mathrm{Dir}(\boldsymbol{\pi}; \boldsymbol{\alpha}_0 + \nu \boldsymbol{e}_y)$.
- The likelihood model of EDL is Gaussian: $p(y \mid \boldsymbol{\pi}) = \mathcal{N}(\boldsymbol{e}_y; \boldsymbol{\pi}, \sigma^2 \boldsymbol{I}_C)$, which does not admit a closed form expression for $p^{(\nu)}(\boldsymbol{\pi} \mid y)$.

Unifying EDL Objectives for Classification

Introduce a *unified objective function*:

$$\mathcal{L}(\psi) := \mathbb{E}_{p(x,y)}\left[D\left(p^{(\nu)}(\boldsymbol{\pi} \mid y), p_\psi(\boldsymbol{\pi} \mid x)\right)\right] + \gamma_{\text{ood}}\mathbb{E}_{p_{\text{ood}}(x)}\left[D\left(p(\boldsymbol{\pi}), p_\psi(\boldsymbol{\pi} \mid x)\right)\right]$$

for some divergence function $D(\cdot,\cdot)$, a tempering parameter $\nu > 0$, and an OOD regularization parameter $\gamma_{\text{ood}} \geq 0$ with a distribution p_{ood} for OOD samples.

The paper proves that under certain settings, the unified objective function is equivalent to different EDL objective functions.

"Optimal" Meta Distribution

Here we focus on the reverse-KL type EDL methods.

Theorem

For any prior $p(\boldsymbol{\pi})$ and likelihood $p(y \mid \boldsymbol{\pi})$, we have

$$\min_{\psi} \mathbb{E}_{p(x,y)} \left[D\left(p_\psi(\boldsymbol{\pi} \mid x) \parallel p_\nu(\boldsymbol{\pi} \mid y) \right) \right] \equiv \min_{\psi} \mathbb{E}_{p(x)} \left[D\left(p_\psi(\boldsymbol{\pi} \mid x) \parallel p^\star(\boldsymbol{\pi} \mid x) \right) \right]$$

where $p^\star(\boldsymbol{\pi} \mid x) := \dfrac{p(\boldsymbol{\pi}) \exp\left(\nu \mathbb{E}_{p(y|x)}[\log p(y|\boldsymbol{\pi})]\right)}{\int p(\boldsymbol{\pi}) \exp\left(\nu \mathbb{E}_{p(y|x)}[\log p(y|\boldsymbol{\pi})]\right) \mathrm{d}\boldsymbol{\pi}}$.

When the model meta distribution $p_\psi(\boldsymbol{\pi} \mid x)$ is trained with the reverse-KL objective, it is forced to fit a **fixed** target meta distribution $p^\star(\boldsymbol{\pi} \mid x)$.

Example: Categorical Likelihood

Consider $p(\boldsymbol{\pi}) = \mathrm{Dir}(\boldsymbol{\pi}; \boldsymbol{\alpha}_0)$ and $p(y \mid \boldsymbol{\pi}) = \pi_y$, we have $p^\star(\boldsymbol{\pi} \mid x) = \mathrm{Dir}\left(\boldsymbol{\pi}; \boldsymbol{\alpha}_0 + \nu\boldsymbol{\eta}(x)\right)$, where $\boldsymbol{\eta}(x) := \mathbb{E}_{p(y|x)}[\boldsymbol{e}_y] = [p(1 \mid x), \ldots, p(C \mid x)]$ denotes the true label distribution.

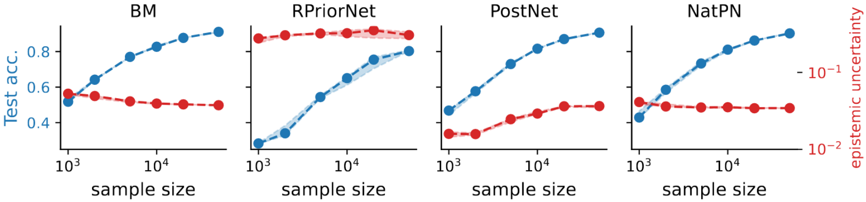
Theorem implies that

$$\min_{\psi} \mathbb{E}_{p(x,y)} \left[D\left(p_\psi(\boldsymbol{\pi} \mid x) \parallel p_\nu(\boldsymbol{\pi} \mid y) \right) \right] \equiv \min_{\psi} \mathbb{E}_{p(x)} \left[D\left(\mathrm{Dir}(\boldsymbol{\pi}; \boldsymbol{\alpha}_\psi(x)) \parallel \mathrm{Dir}(\boldsymbol{\pi}; \boldsymbol{\alpha}_0 + \nu\boldsymbol{\eta}(x)) \right) \right].$$

This shows that $\boldsymbol{\alpha}_\psi(x)$ is forced to match $\boldsymbol{\alpha}_0 + \nu\boldsymbol{\eta}(x)$ as *fixed* target.

EDL Methods Learn False Epistemic Uncertainty

Based on the theorem, even with infinite data, the learned "distributional uncertainty" would remain constant for ID data.

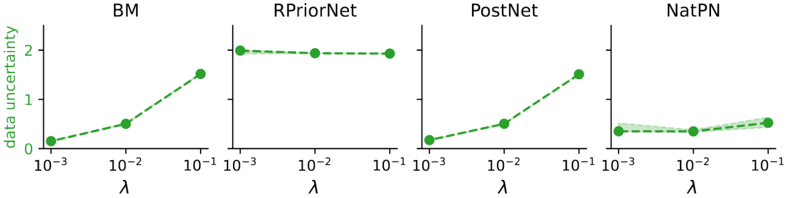


(a) Epistemic Uncertainty: CIFAR10

Figure: Epistemic uncertainty does not vanish with an increasing number of observed samples.

EDL Methods Learn False Aleatoric Uncertainty

EDL methods quantify aleatoric uncertainty as $\mathbb{E}_{p_\psi(\boldsymbol{\pi}|x)}\left[H\left(p(y \mid \boldsymbol{\pi})\right)\right]$. In classification example, the optimal meta distribution is $p_{\psi^\star} = \mathrm{Dir}(\boldsymbol{\pi}; \alpha_0 + \nu\boldsymbol{\eta}(x))$, suggesting that the aleatoric uncertainty would depend on the hyper-parameter $\lambda = \nu^{-1}$, which should be a fixed constant from the underlying label distribution $p(y \mid x)$.



(b) Aleatoric Uncertainty: CIFAR10

Figure: EDL methods learn model-dependent aleatoric uncertainty that depends on hyper-parameter λ.

EDL Methods Are EBM-Based OOD Detector

For EDL methods with Dirichlet prior and categorical model, the induced model predictive distribution is $p_\psi(y \mid x) = \mathbb{E}_{p_\psi(\boldsymbol{\pi}|x)}[p(y \mid \boldsymbol{\pi})] = \frac{\alpha_{\psi,y}(x)}{\mathbf{1}_C^\top \boldsymbol{\alpha}_\psi(x)}$.

In the OOD detection literature, there exists an energy-based model(EBM) based algorithm. Consider a standard classifier with exponentiated logits $\beta_\phi(x)$, whose prediction is given as $p_\phi(y \mid x) := \frac{\beta_{\phi,y}(x)}{\mathbf{1}_C^\top \boldsymbol{\beta}_\phi(x)}$.

The algorithm relates the denominator to a free energy $E_\phi(x) := -\log \mathbf{1}_C^\top \boldsymbol{\beta}_\phi(x)$. The model is trained to minimize

$$-\mathbb{E}_{p(x,y)}[\log p_\psi(y \mid x)] + \tau \left\{ \mathbb{E}_{p(x)}\left[\max(0, E_\phi(x) - m_{\text{id}})^2\right] + \mathbb{E}_{p_{\text{o.o.d}}(x)}\left[\max(0, m_{\text{ood}} - E_\phi(x))^2\right] \right\}$$

This reveals that this EBM-based OOD framework has an almost identical learning mechanism to the EDL methods.

EDL Methods Prefer Smaller λ

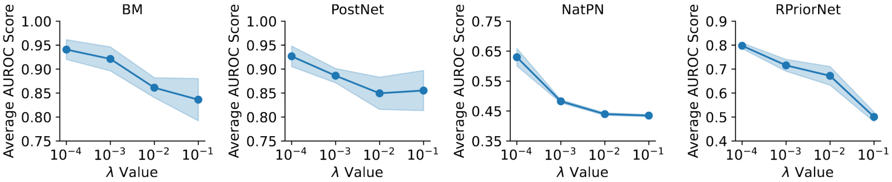


Figure: OOD Detection Performance v.s. λ on CIFAR10

The EDL model is encouraged to fit its output to a large target, so that the summation of the output is large for ID data, and small for OOD data.

Recommendations

It is worth reading, but as a **review** paper. Need to first read some papers about different EDL methods and limitations of them.