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Beyond First-Order Uncertainty Estimation with Evidential Models for Open-World Recognition

Charles Corbière 1 2  Marc Lafon 1  Nicolas Thome 1  Matthieu Cord 2 3  Patrick Pérez 2

Abstract

In this paper, we tackle the challenge of jointly quantifying in-distribution and out-of-distribution (OOD) uncertainties. We introduce KLoS, a KL-divergence measure defined on the class-probability simplex. By leveraging the second-order uncertainty representation provided by evidential models, KLoS captures more than existing first-order uncertainty measures such as predictive entropy. We design an auxiliary neural network, KLoSNet, to learn a refined measure directly aligned with the evidential training objective. Experiments show that KLoSNet acts as a class-wise density estimator and outperforms current uncertainty measures in the realistic context where no OOD data is available during training. We also report comparisons in the presence of OOD training samples, which shed a new light on the impact of the vicinity of this data with OOD test data.

1. Introduction

Obtaining reliable predictive uncertainty estimates is crucial to safely deploy models in open-world conditions (Bendale & Boult, 2015). Notable progress has been made with the renewal of Bayesian neural networks (MacKay, 1992) and ensembling (Lakshminarayanan et al., 2017). These techniques describe an implicit probability density over the predictive categorical distribution obtained from sampling. A recent class of models, coined evidential (Sensoy et al., 2018; Malinin & Gales, 2019; Joo et al., 2020), proposes instead to explicitly learn the concentration parameters of a Dirichlet distribution over output probabilities. They have been shown to improve generalisation (Joo et al., 2020) and OOD detection (Nandy et al., 2020). Based on the subjective logic framework (Josang, 2016), evidential models capture different sources of uncertainty. First-order uncertainty relates to the expectation of the Dirichlet distribution and is caused by conflicting evidence, e.g., class confusion. Second-order uncertainty expresses the lack of evidence in a prediction (Shi et al., 2020), which is characterized by the spread of the Dirichlet distribution. For instance, huskies share lots of features with wolves although being a breed of dog, which leads to a large 1st-order uncertainty due to class confusion in Fig. 1a. In presence of a drawing of a husky, Fig. 1b, a similar class confusion is expected, but a lower amount of evidence due to the distribution shift. Surprisingly, previous works do not leverage the distribution over probabilities on the simplex to derive such a joint measure of the two sources of uncertainty. Some methods focus on OOD detection by characterizing only the distribution spread, e.g., using mutual information (Malinin & Gales, 2019). Approaches targeting total uncertainty actually reduce probability distributions on the simplex to their expected value and compute first-order uncertainty measures, e.g., predictive entropy (Sensoy et al., 2018). However, these measures are invariant to the spread of the distribution (Fig. 1), whereas uncertainty caused by class confusion and lack of evidence should be cumulative, a property naturally fulfilled by the predictive variance in Bayesian regression (Murphy, 2012). In addition, some methods for evidential models use auxiliary data during training to enforce higher

Figure 1. Limitations of 1st-order uncertainty measures. (a) In-distribution image with conflicting evidence. (b) OOD image with same class confusion is supposed to have larger total uncertainty, which is correctly reflected by its KLoS score.
distribution spread on OOD inputs. But when deprived access to OOD training data, the low-dispersion behavior is not guaranteed for all OOD examples (Charpentier et al., 2020; Sensoy et al., 2020) and 2nd-order uncertainty measures struggle to discriminate from in-distribution examples.

**Contributions.** We introduce KLoS, a KL-divergence measure on the simplex based on the Dirichlet distribution. KLoS provides richer estimates than standard first-order measures by considering both 1st-order and 2nd-order uncertainties. Noting that KLoS naturally reflects the training objective used in evidential models, we propose to learn an auxiliary model, KLoSNet, to regress the values of this objective for training samples and to improve uncertainty estimation. Experiments on simultaneous detection of misclassifications and OOD samples show the benefits of KLoSNet thanks to its class-wise density estimator behaviour, a crucial property in the absence of OOD training data. We also shed a new light on the impact of the type of OOD training samples for existing measures.

2. Capturing 1st- and 2nd-Order Uncertainties

2.1. Background: Evidential Neural Networks

Let us consider a training dataset $D$ composed of $N$ i.i.d. samples $(x, y)$ drawn from an unknown joint distribution $p(x, y)$. We denote $\pi = (\pi_1, \cdots, \pi_C)$ the random variable over categorical probabilities, where $\sum_{c=1}^{C} \pi_c = 1$, and which lives on the $(C-1)$-dimensional simplex $\Delta^{C-1}$. Bayesian models and ensemble approaches approximate the posterior predictive distribution $p(y \mid \pi, x)$ by marginalizing over a network’s parameters $\theta$ via Monte-Carlo sampling or explicit ensembling. But this comes at the cost of multiple forward passes. Evidential Neural Networks (ENN) propose instead to model explicitly the posterior distribution over categorical probabilities by a Dirichlet distribution,

$$q_\theta(\pi \mid x) = \text{Dir}(\pi \mid \alpha) = \frac{\Gamma(\alpha_0)}{\prod_{c=1}^{C} \Gamma(\alpha_c)} \prod_{c=1}^{C} \pi_c^{\alpha_c - 1},$$  

(1)

where whose concentration parameters $\alpha = \exp f(x, \theta)$ are output by a network $f$ with parameters $\theta$; $\Gamma$ is the Gamma function and $\alpha_0 = \sum_{c=1}^{C} \alpha_c$. Precision $\alpha_0$ controls the sharpness of the density with more mass concentrating around the mean as $\alpha_0$ grows. By conjugate property, the predictive distribution for a new point $x^*$ is

$$P(y = c \mid x^*, D) \approx \mathbb{E}_{q_\theta(\pi \mid x^*)}[\pi_c] = \frac{\exp f_c(x^*, \theta)}{\sum_{c=1}^{C} \exp f_c(x^*, \theta)},$$

which is the output of a network with softmax activation.

ENN training is formulated as a variational approximation to minimize the KL divergence between the distribution $q_\theta(\pi \mid x)$ and the true posterior $p(\pi \mid x, y)$. Following Joo et al. (2020), we use the non-informative uniform prior $p(\pi \mid x) = \text{Dir}(\pi \mid 1)$. The evidential training objective thus reads:

$$\mathcal{L}_{\text{var}}(\theta; D) = \frac{1}{N} \sum_{(x, y) \in D} \left( \psi(\alpha_y) - \psi(\alpha_0) \right) + \lambda \text{KL}(\text{Dir}(\pi \mid \alpha) \parallel \text{Dir}(\pi \mid 1)), \quad (2)$$

where $\psi$ is the digamma function and with hyperparameter $\lambda > 0$. In particular, minimizing this loss enforces training sample’s precision $\alpha_0$ to remain close to $C + 1/\lambda$.

2.2. A KL-Divergence Measure on the Simplex

By explicitly learning a distribution of the categorical probabilities $\pi$, evidential models can distinguish first-order from second-order uncertainty on the simplex. Inputs with large first-order uncertainty due to class confusion will have a distribution closer to the simplex center. Conversely, inputs with large second-order uncertainty are expected to present flat distributions, reflecting the lack of evidence of the model on these points. To encompass both types of uncertainty, an efficient measure needs to encapsulate both the sharpness of the distribution and its location on the simplex.

We introduce a novel measure, named KLoS for “KL on Simplex”, that computes the KL divergence between the model’s output and a sharp Dirichlet distribution with concentrations $\gamma_0 \hat{y}$ focused on the predicted class $\hat{y}$:

$$\text{KLoS}(x) \triangleq \text{KL}(\text{Dir}(\pi \mid \alpha) \parallel \text{Dir}(\pi \mid \gamma_0 \hat{y})), \quad (3)$$

where $\alpha = \exp f(x, \theta)$ are model’s output and $\gamma_0 = (1, \cdots, 1, \tau, 1, \cdots, 1)$ are the uniform concentration parameters except for the predicted class with $\tau = 1/\lambda + 1$.

The lower KLoS is, the more certain the prediction is. Correct predictions will have Dirichlet distributions closer to the posterior distribution and will thus be associated with a low uncertainty measure (Fig. 2a). Samples with high class confusion will present concentration parameters closer to the simplex’s center than the target Dirichlet objective, resulting in a higher KLoS measure (Fig. 2b). KLoS also penalizes samples having a different precision $\alpha_0$ than the precision $\alpha_0^* = \tau^* + C - 1$ of the target $\gamma_0$. For instance, samples with lacking evidence, i.e., having smaller precision than $\alpha_0^*$ (Fig. 2c), receive a larger KLoS score. Since in-distribution samples are enforced to have precision close to $\alpha_0^*$ during
training, KLoS will be effective to detect various types of OOD samples whose precision is far from $\alpha_0$, and acts as a class-wise density estimator (see also Section 3.1). In contrast, second-order uncertainty measures, such as the mutual information, assume that OOD samples have smaller $\alpha_0$, a property difficult to fulfill for models trained only with in-distribution samples (see Section 3.3).

2.3. Improving First-Order Uncertainty Representation with Confidence Learning

When the model misclassifies an example, i.e., the predicted class $\hat{y}$ differs from the ground truth $y$, KLoS measures the distance between the ENN’s output and the wrongly estimated posterior $p(\pi|x, \hat{y})$. Measuring instead the distance to the true posterior distribution $p(\pi|x, y)$ (green region in Fig. 3) would more likely yield a greater value, reflecting the fact that the classifier made an error. Thus, a better measure for misclassification detection would be:

$$KLoS^*(x, y) \triangleq KL\left(\text{Dir}(\pi|x) \parallel \text{Dir}(\pi|\gamma_y)\right),$$

where $\gamma_y$ corresponds to the uniform concentrations except for the true class $y$ with $\tau = 1/\lambda + 1$.

Connecting KLoS$^*$ with evidential training objective. Choosing such value for $\tau$ results in KLoS$^*$ matching the objective function in Eq. (2). This means that KLoS$^*$ is explicitly minimized during training for in-distribution samples and reflects the fact that the model is confident about its prediction if its score is close to zero.

Obviously, the true class of an output is not available when estimating confidence on test samples. We propose to learn KLoS$^*$ by introducing an auxiliary confidence neural network, termed KLoSNet, with parameters $\omega$, which outputs a confidence prediction $C(x, \omega)$. KLoSNet consists of a small decoder, composed of several dense layers attached to the penultimate layer of the original classification network. During training, we seek $\omega$ such that $C(x, \omega)$ is close to KLoS$^*$ $(x, y)$, by minimizing

$$L_{\text{KLoSNet}}(\omega; D) = \frac{1}{N} \sum_{(x, y) \in D} \left| C(x, \omega) - KLoS^*(x, y) \right|^2.$$  

At test time, we now directly use KLoSNet’s scalar output $C(x, \omega)$ as our uncertainty estimate.

3. Experiments

We evaluate our approach against various baselines: 1st-order uncertainty metrics (Maximum Class probability (MCP) and predictive entropy (Entropy)), 2nd-order metrics (mutual information (Mut. Inf.), differential entropy (Diff. Ent.) and expected pairwise KL-divergence (EPKL)), post-training methods for OOD detection (ODIN (Liang et al., 2018) and Mahalanobis (Lee et al., 2018)) and for misclassification detection (ConfidNet (Corbière et al., 2019)). Uncertainty measures are derived from the same evidential model trained with $\lambda = 10^{-2}$. We rely on the learned classifier to train our auxiliary confidence model KLoSNet, using the same training set. Except in Section 3.3, we consider setups where no OOD data is available for training. All training details are available in Appendix A.

3.1. Synthetic Experiment

We analyse the behavior of the KLoS measure and the limitations of existing first- and second-order uncertainty metrics on a 2D synthetic dataset composed of three Gaussian-distributed classes with equidistant means and identical isotropic variance (Fig. 4). OOD samples are drawn from a ring around the in-distribution dataset and are only used for evaluation. Fig. 4b shows that Entropy correctly assigns large uncertainty along decision boundaries, which is convenient to detect misclassifications, but yields low uncertainty for points far from the distribution. Surprisingly, Mut. Inf. (Fig. 4c) decreases when moving away from the training data. This behavior is due to the linear nature of the toy dataset where models assign higher concentration parameters far from decision boundaries, hence smaller spread on the simplex, as also noted by Charpentier et al. (2020). Additionally, Mut. Inf. does not reflect the uncertainty caused by class confusion along decision boundaries. In contrast, KLoS allows discriminating both misclassifications and OOD samples from correct predictions as uncertainty increases far from in-distribution samples for each class (Fig. 4d). By measuring a distance between the model’s output and a class-wise target distribution, we can observe that KLoS acts as a density estimator for each class.

3.2. Comparative Experiments

When jointly detecting in-distribution misclassifications and OOD samples, correct predictions are considered as positive samples while misclassified inputs and OOD examples constitute negative samples. Following standard practices (Hendrycks & Gimpel, 2017), we use the area under the ROC curve (AUROC) to evaluate threshold-independent
Table 1. Comparative experiments on CIFAR-10. Misclassification (Mis.), OD and simultaneous (Mis+OOD) detection results (mean % AUROC and std. over 5 runs). Bold type indicates significantly best performance ($p < 0.05$) according to paired t-test.

<table>
<thead>
<tr>
<th>Method</th>
<th>LSUN</th>
<th>TinyImageNet</th>
<th>STL-10</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mis.</td>
<td>OOD</td>
<td>Mis+OOD</td>
</tr>
<tr>
<td>MCP (Hendrycks &amp; Gimpel, 2017)</td>
<td>87.6 ± 1.6</td>
<td>79.7 ± 1.1</td>
<td>84.9 ± 1.1</td>
</tr>
<tr>
<td>Entropy (Sensory et al., 2018)</td>
<td>83.5 ± 2.4</td>
<td>83.8 ± 0.3</td>
<td>87.9 ± 0.2</td>
</tr>
<tr>
<td>ConfIdNet (Corbière et al., 2019)</td>
<td>90.2 ± 0.8</td>
<td>82.1 ± 1.5</td>
<td>87.6 ± 1.1</td>
</tr>
<tr>
<td>Mut. Inf. (Malinin &amp; Gales, 2019)</td>
<td>84.1 ± 1.5</td>
<td>84.6 ± 0.6</td>
<td>85.1 ± 1.0</td>
</tr>
<tr>
<td>Diff. Ent. (Malinin &amp; Gales, 2018)</td>
<td>86.8 ± 1.0</td>
<td>85.6 ± 0.5</td>
<td>87.2 ± 0.7</td>
</tr>
<tr>
<td>EPKL (Malinin, 2019)</td>
<td>83.9 ± 1.5</td>
<td>84.5 ± 0.7</td>
<td>85.1 ± 1.0</td>
</tr>
<tr>
<td>ODIN (Liang et al., 2018)</td>
<td>86.0 ± 2.0</td>
<td>79.5 ± 1.2</td>
<td>83.8 ± 1.5</td>
</tr>
<tr>
<td>Mahalanobis (Lee et al., 2018)</td>
<td>91.2 ± 0.3</td>
<td>88.9 ± 0.2</td>
<td>91.3 ± 0.1</td>
</tr>
<tr>
<td>KLoSNet (Ours)</td>
<td>92.5 ± 0.6</td>
<td>87.6 ± 0.9</td>
<td>91.7 ± 0.9</td>
</tr>
</tbody>
</table>

4. Discussion

We propose KLoSNet, an auxiliary model to estimate the uncertainty of a classifier for both in-domain and out-of-domain inputs. Experiments demonstrate its effectiveness on simultaneous detection of misclassifications and of OOD samples, and reveal its class-wise density estimation behavior. Far from being the panacea, using training OOD samples depends critically on the choice of these samples for existing uncertainty measures. Conversely, KLoS is more robust to this choice and can alleviate their use altogether.
A. Experimental Setup

In this section, we provide comprehensive details about the datasets, the implementation and the hyperparameters of the experiments shown in Section 3.
Synthetic Data. The training dataset (Fig. 4a) consists of 1,000 samples \((x, y)\) from a distribution \(p(x, y)\) over \(\mathbb{R}^2 \times \{1, 2, 3\}\) defined as:

\[
p(x = x, y = y) = \frac{1}{3} N(x = x| \mu_y, \sigma^2 I_{2 \times 2}),
\]

where \(\mu_1 = (0, \sqrt{3}/2), \mu_2 = (-1, -\sqrt{3}/2), \mu_3 = (1, -\sqrt{3}/2)\) and \(\sigma = 4\). The marginal distribution of \(x\) is a Gaussian mixture with three equally weighted components having equidistant centers and equal spherical covariance matrices.

The test dataset consists of 1,000 other samples from this distribution. Finally, we construct an out-of-distribution (OOD) dataset following Malinin & Gaines (2019), by sampling 100 points in \(\mathbb{R}^2\) such that they form a ‘ring’ with large noise around the training points. Some OOD samples will be close to the in-distribution while others will be very far (see Fig. 3 of the paper). The number of OOD samples has been carefully chosen so that it amounts approximately to the number of test points misclassified by the classifier. Classification is performed by a simple logistic regression.

A set of five models is trained for 200 epochs using the evidential training objective (Eq. 7 of the paper) with regularization parameter \(\lambda = 5\times 10^{-4}\) and Adam optimizer with learning rate 0.02. Uncertainty metrics – MCP, Entropy, Mut. Inf., Malahanobis and KLoS – are computed from these models.

Image Classification Datasets. Experiments are conducted using CIFAR-10 and CIFAR-100 datasets (Krizhevsky, 2009). They consist in \(32 \times 32\) natural images featuring 10 object classes for CIFAR-10 and 100 classes for CIFAR-100. Both datasets are composed with 50,000 training samples and 10,000 test samples. We further randomly split the training set to create a validation set of 10,000 images.

OOD datasets are TinyImageNet\(^1\) – a subset of ImageNet (10,000 test images with 200 classes) –, LSUN (Yu et al., 2015) – a scene classification dataset (10,000 test images of 10 scenes) – and STL-10 – a dataset similar to CIFAR-10 but with different classes. We downsamples each image of TinyImageNet, LSUN and STL-10 to size \(32 \times 32\).

Training Details. We implemented in PyTorch (Paszke et al., 2019) a VGG-16 architecture (Simonyan & Zisserman, 2015) in line with the previous works of (Malinin & Gaines, 2019; Charpentier et al., 2020; Nandy et al., 2020), with fully-connected layers reduced to 512 units. In both experiments, the models are trained for 200 epochs with a batch size of 128 images, using a stochastic gradient descent with Nesterov momentum of 0.9 and weight decay 5e-4. The learning rate is initialized at 0.1 and reduced by a factor of 10 at 50% and 75% of the training progress. Images are randomly horizontally flipped and shifted by ±4 pixels as a form of data augmentation.

<table>
<thead>
<tr>
<th>CIFAR-10</th>
<th>CIFAR-100</th>
</tr>
</thead>
<tbody>
<tr>
<td>Train</td>
<td>99.0 ±0.1</td>
</tr>
<tr>
<td>Val</td>
<td>93.6 ±0.1</td>
</tr>
<tr>
<td>Test</td>
<td>93.0 ±0.3</td>
</tr>
</tbody>
</table>

Table 2. Mean accuracies (%) and std. over five runs.

KLōSNet. We start from the pre-trained evidential model described above. As detailed in Section 2.3, KLōSNet consists of a small decoder attached to the penultimate layer of the main network. In CIFAR experiments, this corresponds to VGG16’s fc1 layer of size 512. This auxiliary neural network is composed of five fully-connected layers of size 400, except for the last layer obviously. KLōSNet decoder’s weights \(\omega\) are trained for 100 epochs with \(\ell_2\) loss (Eq. 11 in the main paper) and with Adam optimizer with learning rate 1e-4. As KLōS\(^*\) ranges from zero to large positive values (>1000), one may encounter some issues when training KLōSNet. Consequently, we apply a sigmoid function, \(\sigma(x) = \frac{1}{1 + e^{-x}}\), after computing the KL-divergence between NN’s output and \(\gamma_y\). To prevent over-fitting, training is stopped when validation AUC metric for misclassification detection starts decreasing. Then, a second training step is performed by initializing new encoder \(E'\) such that \(\theta_{E'} = \theta_E\) and by optimizing weights \((\theta_{E'}, \omega)\) for 30 epochs with Adam optimizer with learning rate 1e-6. We stop training once again based on validation AUC metric.

B. Additional Results

B.1. Results on CIFAR-100 and with ResNet-18

In Table 3, we extend our comparative experiments on simultaneous detection to CIFAR-100 dataset and to mod-
Table 3. Comparative experiments on CIFAR-10 and CIFAR-100 with ResNet-18 architectures. Misclassification (Mis.), out-of-distribution (OOD) and simultaneous (Mis+OOD) detection results (mean ± AUROC and std. over 5 runs). Bold type indicates significantly best performance (p < 0.05) according to paired t-test.

<table>
<thead>
<tr>
<th>Method</th>
<th>LSUN</th>
<th>CIFAR-10</th>
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<tbody>
<tr>
<td></td>
<td>OOD</td>
<td>Mis+OOD</td>
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<tr>
<td>MCP</td>
<td>84.8 ± 3.9</td>
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<tr>
<td>Entropy</td>
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<td>79.6 ± 4.1</td>
<td>82.8 ± 0.9</td>
</tr>
<tr>
<td>ContrastDist</td>
<td>90.7 ± 4.1</td>
<td>84.9 ± 4.1</td>
<td>81.9 ± 1.6</td>
</tr>
<tr>
<td>Mult. Inf.</td>
<td>80.6 ± 4.6</td>
<td>77.0 ± 4.2</td>
<td>79.4 ± 1.4</td>
</tr>
<tr>
<td>Diff. Ent.</td>
<td>82.7 ± 4.0</td>
<td>78.5 ± 4.1</td>
<td>81.1 ± 0.8</td>
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<tr>
<td>EPKL</td>
<td>80.2 ± 4.0</td>
<td>76.8 ± 4.1</td>
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</tr>
<tr>
<td>Mahalanobis</td>
<td>91.2 ± 4.0</td>
<td>90.7 ± 4.0</td>
<td>91.8 ± 0.2</td>
</tr>
<tr>
<td>KLoSNet (Ours)</td>
<td>95.9 ± 4.0</td>
<td>93.1 ± 4.1</td>
<td>94.4 ± 0.4</td>
</tr>
</tbody>
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Table 4. Impact of confidence learning. Comparison of detection performances between KLoS and KLoSNet for CIFAR-10 and CIFAR-100 experiments with VGG-16 architecture.

<table>
<thead>
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</table>

B.2. Impact of Confidence Learning

To evaluate the effect of the uncertainty measure KLoS and of the auxiliary confidence network KLoSNet, we report a detailed ablation study in Table 4. We can notice that KLoSNet improves misclassification over KLoS but also OOD detection in every benchmark. We intuit that learning to improve misclassification detection also helps to spot some OOD inputs that share similar characteristics.

B.3. Impact of Adversarial Perturbations

In the original papers, ODIN and Mahalanobis preprocess inputs by adding small inverse adversarial perturbations to reinforce networks in their prediction; this has also the observed benefit to make in-distribution and out-of-distribution samples more separable. The tuning of the adversarial noise’s magnitude depends on the evaluated OOD data. In Figure 7a, we plot the AUC of each detection task with different values of perturbation magnitude $\varepsilon$ with ODIN, Mahalanobis and our criterion KLoS, using SVHN as OOD dataset. Even though there exists a particular noise value for improved OOD detection (Fig. 7a, middle), increasing noise magnitude deteriorates performances in misclassification detection (Fig. 7a, left) for each method. Best results on the simultaneous detection task (Fig. 7a, right) correspond to $\varepsilon = 0$, as done in previous experiments.
on any method (ODIN, Mahalanobis and KLoS) when using inverse adversarial perturbations for OOD detection with LSUN, TinyImageNet and STL-10 datasets. Similar results are observed in (Liang et al., 2018) (Appendix B, Fig. 8) when using WideResNet architectures. Regarding Mahalanobis (Lee et al., 2018), the authors only provided ablation for SVHN dataset.

C. Link between KLoS* and Evidential Training Objective

Let us remind the definition of KLoS as a KL divergence between the model’s output and a sharp Dirichlet distribution with concentrations $\gamma_y$ focused on the predicted class $\hat{y}$:

$$\text{KLoS}^*(x, y) \triangleq \text{KL} \left( \text{Dir}(\pi|\alpha) \ || \ \text{Dir}(\pi|\gamma_y) \right), \quad (7)$$

where $\alpha = \exp f(x, \theta)$ is model’s output and $\gamma_y = (1, \ldots, 1, \tau, 1, \ldots, 1)$ are the uniform concentration parameters except for the true class with $\tau = 1/\lambda + 1$.

The KL-divergence between two Dirichlet distributions can be obtained in closed form and KLoS* can be calculated as:

$$\text{KLoS}^*(x, y) = \text{KL} \left( \text{Dir}(\pi|\alpha) \ || \ \text{Dir}(\pi|\gamma_y) \right) \quad (8)$$

$$= \log \Gamma(\alpha_0) - \log \Gamma(C - 1 + 1/\lambda)$$

$$+ \log \Gamma(1 + 1/\lambda) - \sum_{c=1}^{C} \log \Gamma(\alpha_c)$$

$$+ \sum_{c \neq y} (\alpha_c - 1) (\psi(\alpha_c) - \psi(\alpha_0))$$

$$+ (\alpha_y - (1 + 1/\lambda)) (\psi(\alpha_y) - \psi(\alpha_0)).$$

(9)

On the other hand, the KL-divergence between the model’s output and a uniform Dirichlet distribution $\text{Dir}(\pi|1)$ reads:

$$\text{KL} \left( \text{Dir}(\pi|\alpha(x, \theta)) \ || \ \text{Dir}(\pi|1) \right)$$

$$= \log \Gamma(\alpha_0) - \log \Gamma(C) - \sum_{c=1}^{C} \log \Gamma(\alpha_c)$$

$$+ \sum_{c=1}^{C} (\alpha_c - 1) (\psi(\alpha_c) - \psi(\alpha_0)).$$

(10)

Hence, KLoS* can be written as:

$$\text{KLoS}^*(x, y) = \frac{1}{\lambda} (\psi(\alpha_y) - \psi(\alpha_0))$$

$$+ \text{KL} \left( \text{Dir}(\pi|\alpha(x, \theta)) \ || \ \text{Dir}(\pi|1) \right)$$

$$+ \left( \log \Gamma(1 + 1/\lambda) - \log \Gamma(C - 1 + 1/\lambda) \right.$$

$$- \log \Gamma(C) \right). \quad (11)$$

Let us decompose $\mathcal{L}_{\text{var}}(\theta; D) = \frac{1}{N} \sum_{(x, y) \in D} l_{\text{var}}(x, y, \theta)$. We retrieve that $\text{KLoS}^*(x) \propto l_{\text{var}}(x, y, \theta) + r$ where $r =$