# Towards Maximizing the Representation Gap between In-Domain & Out-of-Distribution Examples

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NEURAL INFORMATION PROCESSING SYSTEMS

## 1. Introduction

- Deep learning based models produce wrong predictions without any warning
- This raises questions about their reliability for sensitive real-world applications
- Determining source of uncertainty can allow manual intervention in an informed way, enhancing the reliability of DNN based models

## 2. Types of Predictive Uncertainty

**Model or Epistemic uncertainty**

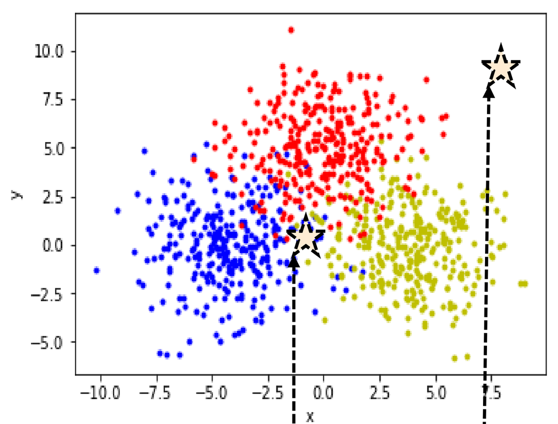
- Uncertainty in estimating network parameters
- Reducible with enough training data

**Data or Aleatoric uncertainty**

- Arises due to the natural complexities of the underlying distribution, such as class overlap, label noise, homoscedastic and heteroscedastic noise

**Distributional uncertainty**

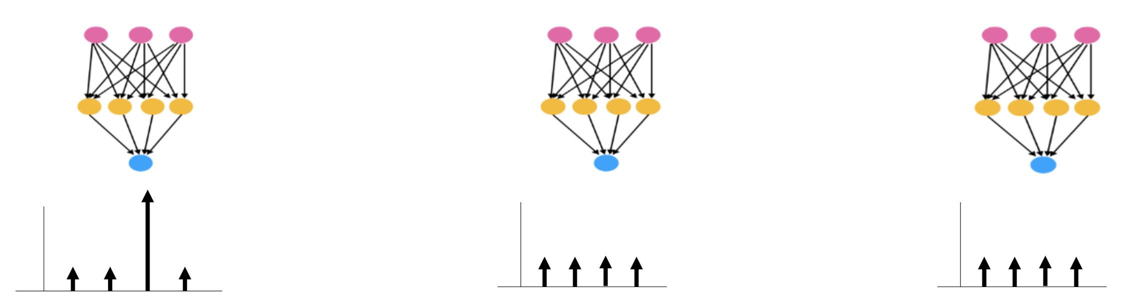
- Distributional mismatch between the training and test examples during inference
- Test data is out-of-distribution (OOD)



In-domain example with Data uncertainty

OOD example leading to distributional uncertainty

## 3. Existing Approaches: Non-Bayesian

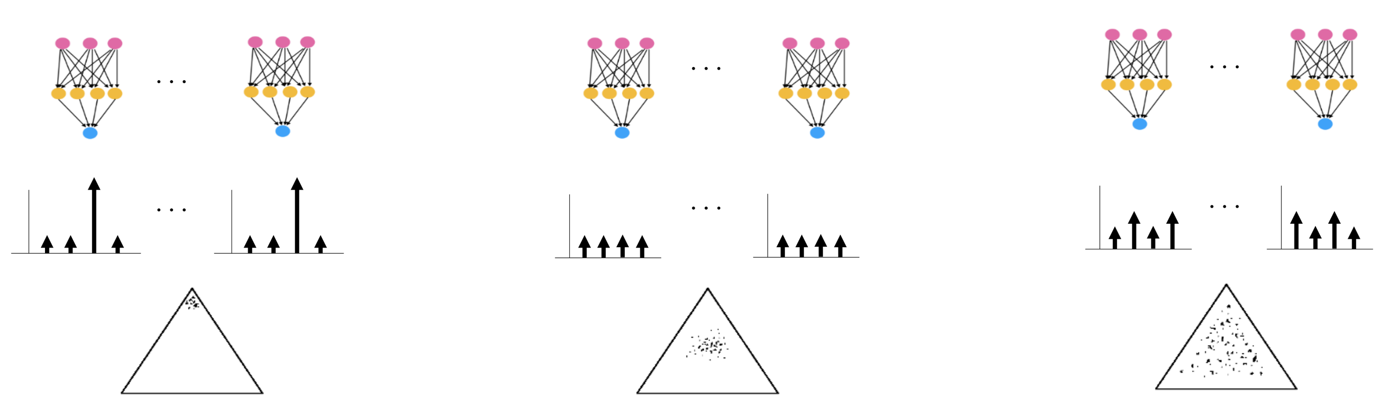


**In-Domain confident** **In-Domain Miss** **OOD**

Limitation:

- In the presence of high data uncertainty among multiple classes, existing OOD detectors produce similar representation for both in-domain and OOD examples.
- Compromise their performance for OOD detection

## 4. Existing Approaches: Bayesian



**In-Domain Confident.** At one corner of the simplex.

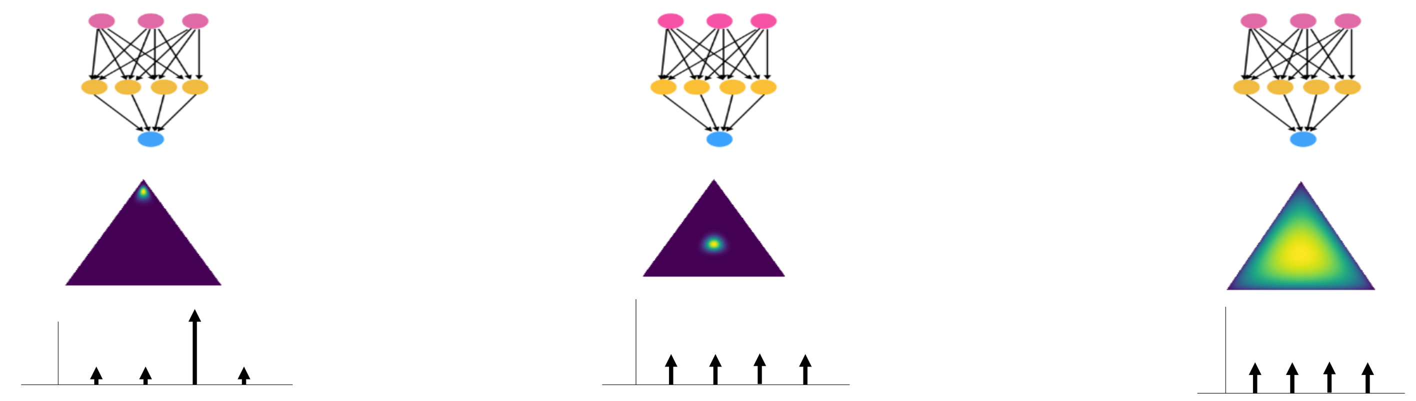
**In-Domain Miss:** Middle of the simplex.

**OOD** Scattered over simplex.

Limitation:

- Computationally expensive to produce the ensemble
- Difficult to control this desired behavior

## 5. Existing Dirichlet Prior Network (DPN)



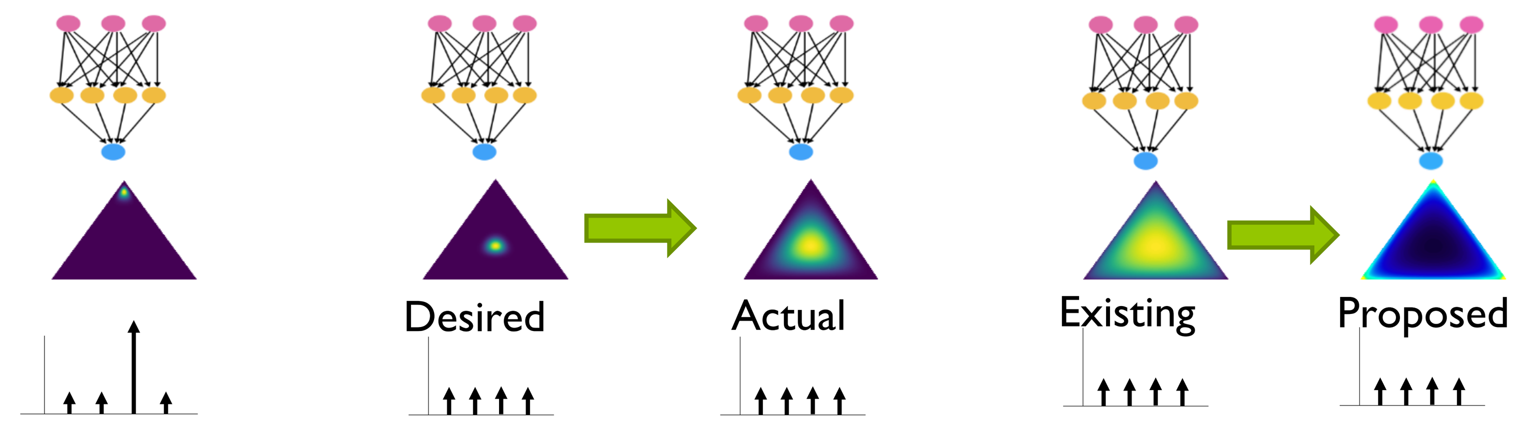
In-Domain Confident
Sharp dist. at a corner
⇒Unimodal categorical.

In-Domain Miss
Sharp dist. in middle
⇒ Multi-modal categorical

OOD
Flat Dirichlet
⇒ Uniform categorical

Emulating the behavior of Bayesian (ensemble) approaches [Malinin & Gales, 2018; 2019]
Parameterize a prior Dirichlet distribution to the categorical over a simplex

## 6. Proposed Representation for OOD




In-Domain Confident    In-Domain Miss    OOD

- Maximize representation gap by producing sharp multi-modal Dirichlet for OODs.
- We show that existing RKL loss cannot produce this representation.
- We propose a novel loss function for DPN to address this limitation.

## 7. Dirichlet Distribution

Parameterized using the concentration parameters, $\boldsymbol{\alpha} = \{\alpha_1, \cdots, \alpha_K\}$

$$Dir(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma\alpha_0}{\prod_{c=1}^{K}\Gamma\alpha_c}\prod_{c=1}^{K}\mu_c^{\alpha_c - 1}, \qquad where\ \alpha_c > 0\ \forall\ c$$

$\alpha_0 = \sum \alpha_c$ denotes the precision of the Dirichlet distribution.

- Larger $\alpha_0$ with at least one $\alpha_c > 0$ produces a sharp unimodal Dirichlet
- $\alpha_c < 1\ \forall\ c$ produces sharp multi-modal Dirichlet

(100, 100, 100)    (10, 10, 10)    (1, 1, 1)    (0.1, 0.1, 0.1)

Visualization of Dirichlet distributions for different concentration parameters

## 8. A standard DNN with soft-max is a DPN

- Concentration parameters of the Dirichlet is exponential of logits: $\alpha_c = \exp(z_c(\boldsymbol{x}^*))$
- *Categorical posterior, obtained from soft-max, is the mean of the Dirichet distribution*

$$p\left(\frac{y = \omega_c}{\boldsymbol{x}^*}\right) = \frac{\alpha_c}{\alpha_0} = \frac{\exp(z_c(\boldsymbol{x}^*))}{\sum_c \exp(z_c(\boldsymbol{x}^*))}$$

- **Limitation:** Cannot control the individual $\alpha_c$ to produce desired Dirichlet distributions.

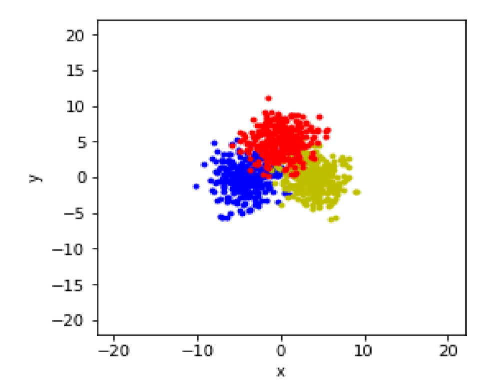
## 9. Proposed Loss Function

Proposed a novel regularizer to control the concentration parameters, $\alpha_c$
Train using both in-domain and OOD training examples in multi-task fashion

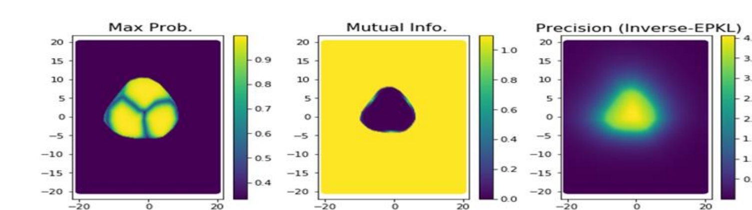
- In-domain: $\mathbb{E}_{p_{in}(x,y)}\left[-\log p(y|x,\boldsymbol{\theta}) - \frac{\lambda_{in}}{K}\sum sigmoid(z_c(x))\right]$ where $\lambda_{in} > 0$
- OOD: $\mathbb{E}_{p_{in}(x,y)}\left[\mathcal{H}_{ce}(\mathcal{U}; p(y|x,\boldsymbol{\theta})) - \frac{\lambda_{in}}{K}\sum sigmoid(z_c(x))\right]$ where $\lambda_{out} < \lambda_{in}$

$\lambda_{out} > 0$    $\lambda_{out} < 0$ (Proposed)

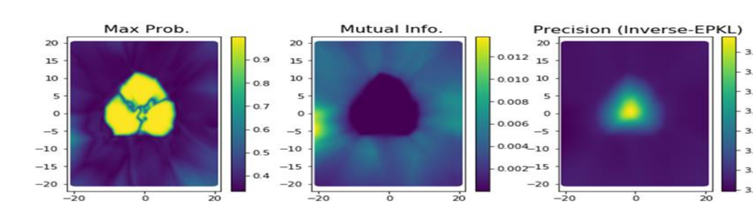
## 10. Results on Synthetic Dataset



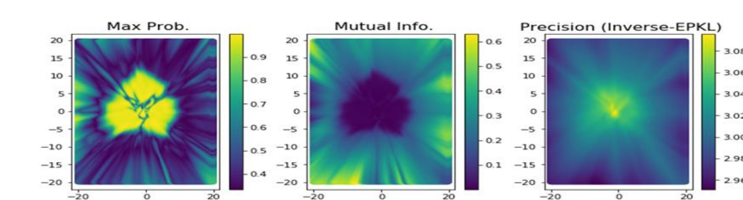
In-Domain Training Data




DPN$^{-}$ using $\lambda_{in} > 0$ & $\lambda_{out} < 0$ (Proposed)




DPN$^{+}$ using $\lambda_{in} > \lambda_{out} > 0$




DPN$_{\text{rev}}$ using RKL [Malinin & Gales, 2019]

## 11. Results on Benchmark Datasets

| | OOD | Tiny [29] | | | | STL-10 [32] | | | | LSUN [33] | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Max.P | MI | $\alpha_0$ | D.Ent | Max.P | MI | $\alpha_0$ | D.Ent | Max.P | MI | $\alpha_0$ | D.Ent |
| C10 | Baseline | 88.9±0.0 | - | - | - | 75.9±0.0 | - | - | - | 90.3±0.0 | - | - | - |
| | MCDP | 88.7±0.1 | 88.1±0.1 | - | - | 76.2±0.0 | 76.0±0.0 | - | - | 90.6±0.0 | 90.2±0.0 | - | - |
| | DE | 88.9±NA | 87.8±NA | - | - | 76.0±NA | 75.6±NA | - | - | 90.3±NA | 89.7±NA | - | - |
| | OE | 98.2±0.1 | - | - | - | 81.4±1.2 | - | - | - | 98.4±0.3 | - | - | - |
| | DPN$_{rev}$ | 97.5±0.5 | 97.8±0.4 | 97.8±0.4 | 97.7±0.4 | 81.6±1.7 | 82.2±1.7 | 82.2±1.6 | 81.9±1.7 | 98.5±0.4 | 98.7±0.3 | 98.7±0.3 | 98.7±0.3 |
| | DPN$^{+}$ | 98.0±0.2 | 98.0±0.2 | 98.0±0.2 | 98.0±0.2 | 81.6±1.4 | 81.8±1.2 | 81.8±1.2 | 81.8±1.2 | 98.2±0.3 | 98.3±0.4 | 98.3±0.4 | 98.3±0.4 |
| | DPN$^{-}$ | **99.0**±0.1 | **99.0**±0.1 | 97.7±0.1 | 6.0±0.3 | 84.7±0.4 | **85.3**±0.5 | 84.9±0.5 | 34.6±0.4 | 99.2±0.1 | **99.3**±0.0 | 98.1±0.1 | 5.0±0.2 |
| | OOD | Tiny [29] | | | | STL-10 [32] | | | | LSUN [33] | | | |
| | | Max.P | MI | $\alpha_0$ | D.Ent | Max.P | MI | $\alpha_0$ | D.Ent | Max.P | MI | $\alpha_0$ | D.Ent |
| C100 | Baseline | 68.8±0.2 | - | - | - | 69.6±0.0 | - | - | - | 72.5±0.0 | - | - | - |
| | MCDP | 69.7±0.3 | 70.6±0.3 | - | - | 70.7±0.1 | 71.6±0.2 | - | - | 74.5±0.1 | 75.9±0.2 | - | - |
| | DE | 68.9±NA | 69.6±NA | - | - | 69.6±NA | 70.2±NA | - | - | 72.6±NA | 73.4±NA | - | - |
| | OE | 89.5±1.0 | - | - | - | 91.2±0.7 | - | - | - | 92.2±0.9 | - | - | - |
| | DPN$_{rev}$ | 81.2±0.2 | 83.8±0.1 | 83.8±0.1 | 83.5±0.1 | 87.2±0.1 | 89.3±0.1 | 89.3±0.1 | 89.0±0.1 | 86.7±0.0 | 89.3±0.1 | 89.3±0.1 | 88.9±0.1 |
| | DPN$^{+}$ | 85.9±0.3 | 92.2±0.1 | 92.2±0.1 | 92.3±0.1 | 89.1±0.2 | 95.0±0.0 | 95.0±0.0 | 94.8±0.0 | 90.3±0.3 | 95.0±0.1 | 95.0±0.1 | 95.0±0.1 |
| | DPN$^{-}$ | 89.2±0.1 | **94.5**±0.1 | **94.5**±0.1 | 38.1±0.5 | 92.8±0.1 | **96.8**±0.1 | **96.8**±0.1 | 25.4±0.4 | 92.8±0.1 | **96.5**±0.1 | **96.5**±0.1 | 31.5±0.4 |
| | OOD | CIFAR-10 [28] | | | | CIFAR-100 [28] | | | | Textures [34] | | | |
| | | Max.P | MI | $\alpha_0$ | D.Ent | Max.P | MI | $\alpha_0$ | D.Ent | Max.P | MI | $\alpha_0$ | D.Ent |
| TIM | Baseline | 76.9±0.2 | - | - | - | 73.6±0.2 | - | - | - | 70.9±0.2 | - | - | - |
| | MCDP | 77.4±0.1 | 77.5±0.2 | - | - | 74.0±0.2 | 73.6±0.2 | - | - | 70.3±0.2 | 63.6±0.2 | - | - |
| | DE | 76.9±NA | 77.7±NA | - | - | 73.7±NA | 75.3±NA | - | - | 71.1±NA | 76.2±NA | - | - |
| | OE | 91.3±0.4 | - | - | - | 89.5±0.5 | - | - | - | 95.8±0.3 | - | - | - |
| | DPN$_{rev}$ | 85.4±0.7 | 82.8±1.4 | 81.9±1.6 | 85.6±0.9 | 84.2±0.8 | 82.5±1.4 | 81.7±1.6 | 85.0±0.9 | 90.9±0.3 | 91.2±0.6 | 90.6±0.6 | 92.6±0.3 |
| | DPN$^{+}$ | 99.2±0.0 | 99.7±0.0 | 99.7±0.0 | 99.6±0.0 | 98.8±0.0 | 99.5±0.0 | 99.5±0.0 | 99.4±0.0 | 96.5±0.1 | 98.4±0.0 | 98.4±0.0 | 98.2±0.0 |
| | DPN$^{-}$ | 99.7±0.0 | **99.9**±0.0 | **99.9**±0.0 | 3.5±0.1 | 98.7±0.1 | **99.6**±0.0 | **99.6**±0.0 | 7.5±0.2 | 95.8±0.1 | **98.7**±0.1 | **98.7**±0.1 | 19.3±0.4 |

AUROC scores for OOD detection (Higher scores are better)

Please refer to our paper for additional details and more experimental results:

ArXiv Paper Link    GitHub Code Link