# Deep Deterministic Uncertainty: A New Simple Baseline

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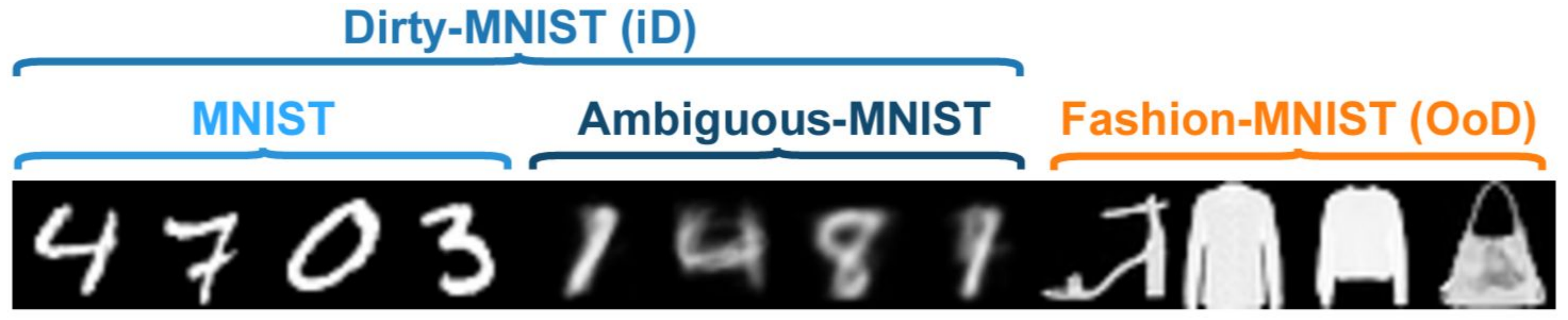
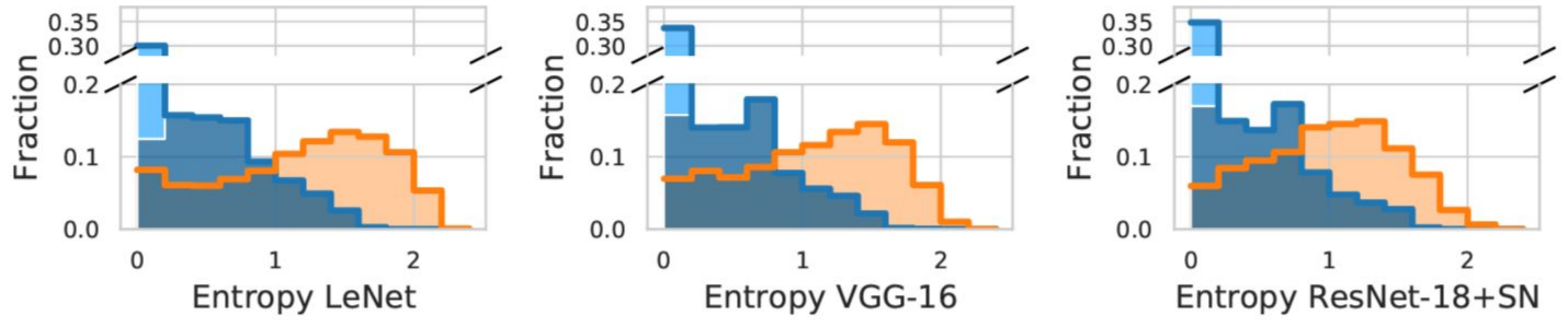
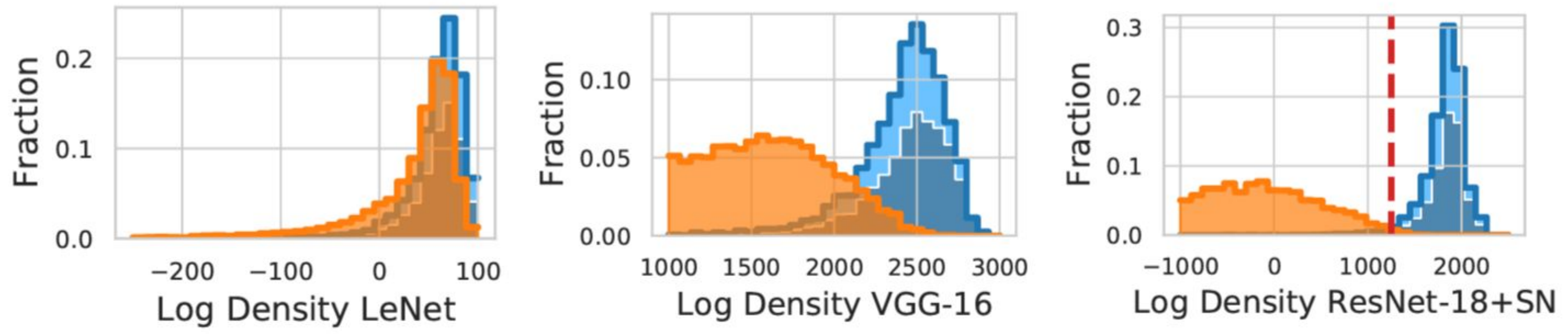



(a) Dirty-MNIST (iD) and Fashion-MNIST (OoD)




(b) Softmax entropy




(c) Feature-space density

## Motivation: Capture & Disentangle Uncertainty

- **Epistemic Uncertainty:** uncertainty due to *lack of data* and reducible with exposure to more data. E.g., **Fashion-MNIST**.
- **Aleatoric Uncertainty:** uncertainty due to inherently *noisy observations or ambiguity* in data, generally not reducible through exposure to more data. E.g., **Ambiguous MNIST** above.
- Popular methods like **deep-ensembles** can capture these uncertainties. But they are computationally intensive.
- Single forward pass methods like **DUQ** and **SNGP** either don't scale to large number of classes, have difficult to tune hyper-parameters or are not specifically modelled to disentangle epistemic and aleatoric uncertainty.

## DDU: A Simple Solution

**Sensitive & Smooth Feature Space:** To prevent features from points distant on the image space to be mapped close to each other in the feature space (i.e., *feature collapse*), we encourage ***bi-Lipschitzness*** in the feature extractor.

$$K_1||x_1 - x_2||_I \leq ||f_\theta(x_1) - f_\theta(x_2)||_F \leq K_2||x_1 - x_2||_I$$

We achieve this through ***Residual Connections + Spectral Normalization***.

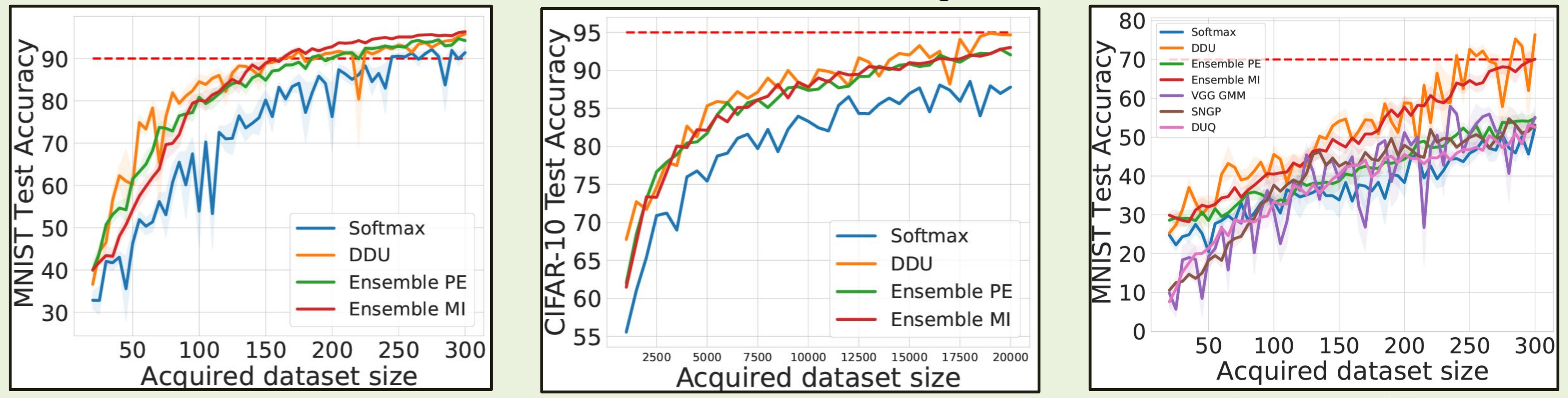
- **Feature Space Density $p(z = f_\theta(x))$ (Epistemic):** With a constrained feature space, a density estimator as simple as ***Gaussian Discriminant Analysis (GDA)*** modeled on the feature space can estimate epistemic uncertainty.
- **Softmax Entropy $H[Y|x,\theta]$ (Aleatoric):** For points having low epistemic uncertainty (iD), entropy of the softmax distribution can capture aleatoric uncertainty (ambiguity in data).

```python
# instantiate models
model = create_sensitive_smooth_model()
gda = create_gda()

# train
training_samples, training_labels = load_training_set()
model.fit(training_samples, training_labels)

training_features = model.features(training_samples)
gda.fit(training_features, training_labels)

# test
test_feature = model.features(test_sample)
epistemic_uncertainty = -gda.log_density(test_feature)

is_ood = epistemic_uncertainty <= ood_threshold
if not is_ood:
 prediction = model.softmax_layer(test_feature)
 aleatoric_uncertainty = entropy(prediction)
 return 0, aleatoric_uncertainty

return epistemic_uncertainty, np.log(num_classes)
```

## OoD Detection (ImageNet vs ImageNet-O)

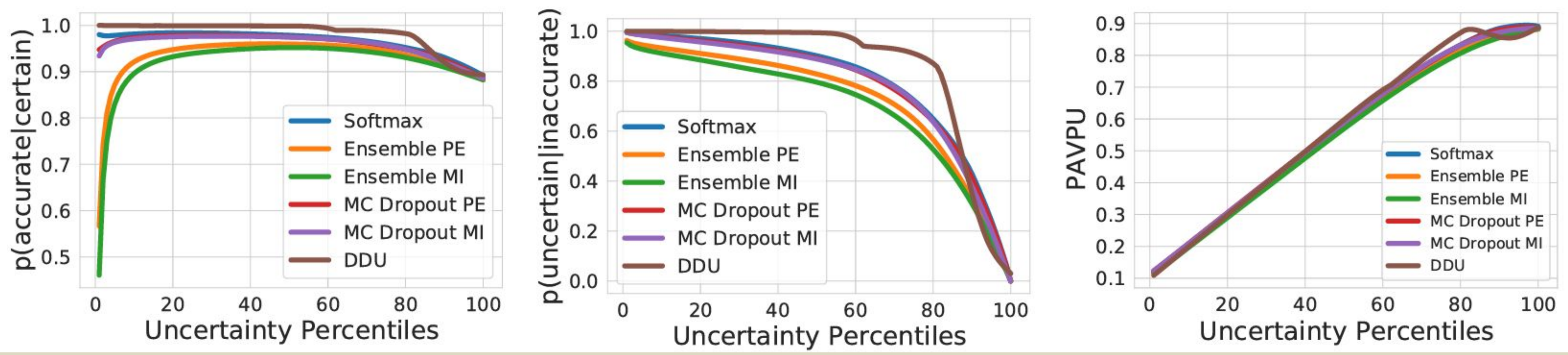
| Model | Accuracy (↑) Deterministic | Accuracy (↑) 3-Ensemble | ECE (↓) Deterministic | ECE (↓) 3-Ensemble | AUROC (↑) Softmax Entropy | AUROC (↑) Energy-based Model | AUROC (↑) DDU | AUROC (↑) 3-Ensemble PE | AUROC (↑) 3-Ensemble MI |
|---|---|---|---|---|---|---|---|---|---|
| ResNet-50 | $74.8 \pm 0.05$ | 76.01 | $2.08 \pm 0.11$ | 2.07 | $51.42 \pm 0.61$ | $55.76 \pm 0.81$ | $\mathbf{71.29 \pm 0.08}$ | 60.3 | 62.43 |
| Wide-ResNet-50-2 | $76.75 \pm 0.11$ | 77.58 | $1.18 \pm 0.07$ | 1.22 | $52.71 \pm 0.23$ | $57.13 \pm 0.4$ | $\mathbf{73.12 \pm 0.19}$ | 60.45 | 64.81 |
| VGG-16 | $72.48 \pm 0.02$ | 73.54 | $2.62 \pm 0.11$ | 2.59 | $50.67 \pm 0.22$ | $52.04 \pm 0.23$ | $54.32 \pm 0.14$ | 58.74 | **60.56** |

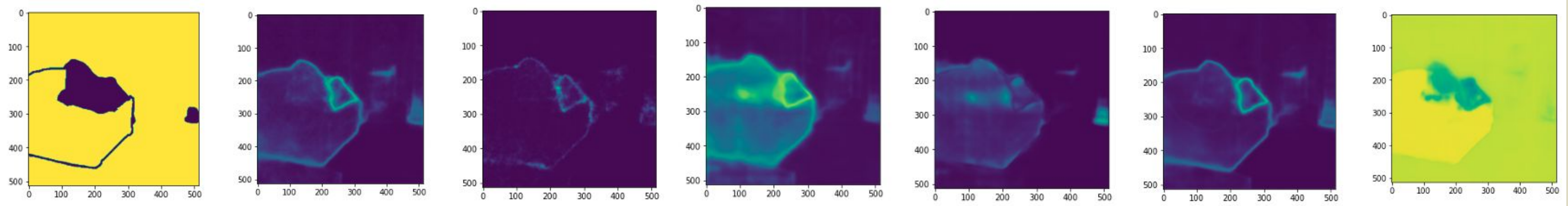
## Active Learning




MNIST CIFAR-10 Dirty-MNIST

## Semantic Segmentation (Pascal VOC)



(a) Accuracy (b) MCD PE (c) MCD MI (d) En PE (e) En MI (f) Entropy (g) Density

| Baseline | Softmax | MC Dropout | Deep Ensemble | DDU |
|---|---|---|---|---|
| **mIoU** | 78.53 | 78.61 | 78.47 | 78.53 |
| **Runtime (ms)** | $275.48 \pm 1.91$ | $1576.75 \pm 1.56$ | $875.87 \pm 0.79$ | $\mathbf{263.83 \pm 2.79}$ |