

PremiUm-CNN: Propagating Uncertainty Towards Robust Convolutional Neural Networks

2022 IEEE International Conference on Acoustics, Speech and Signal Processing

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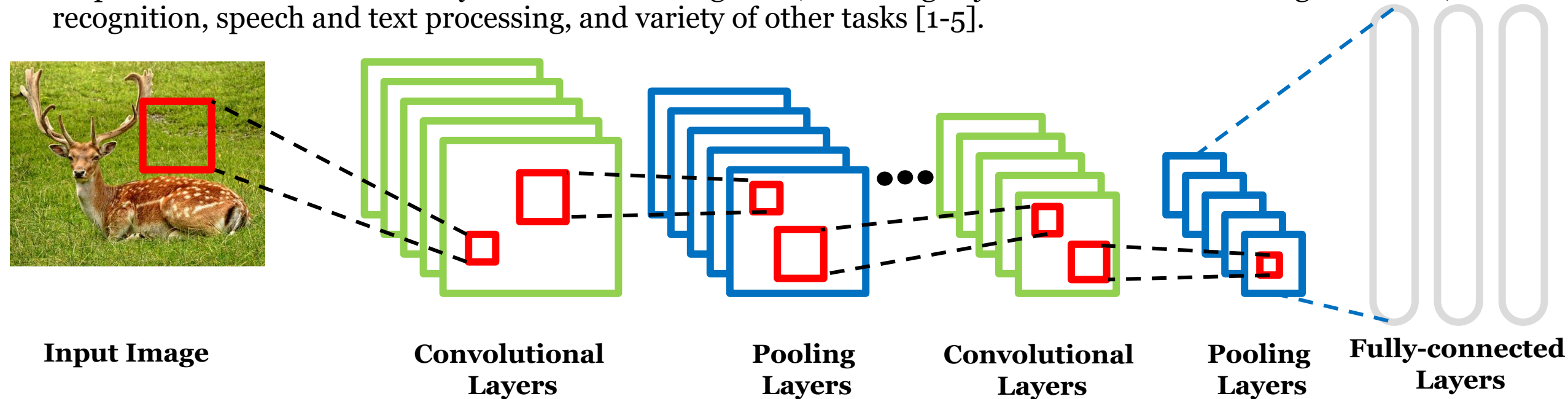
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May 9, 2022

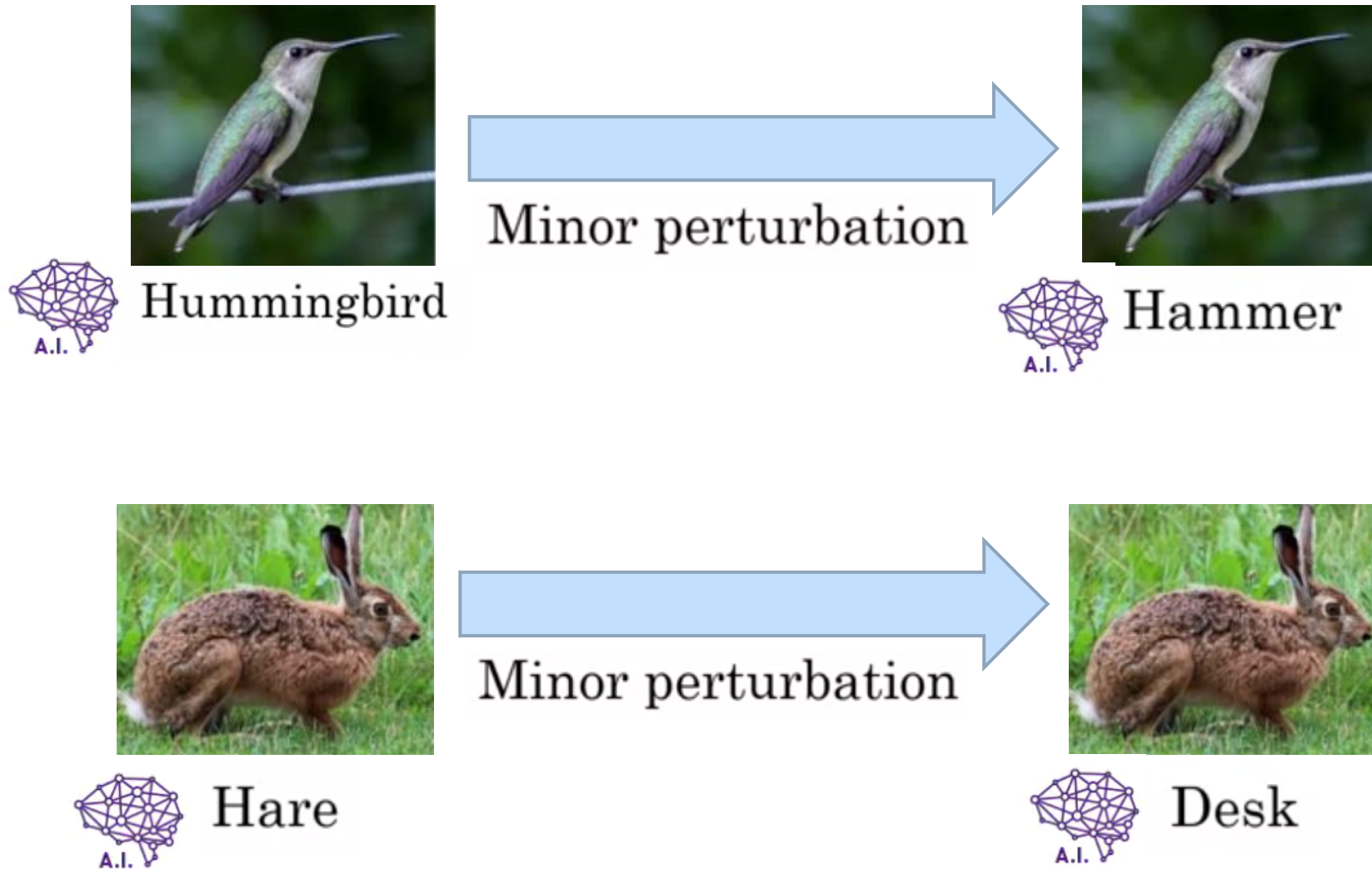
Neural Networks

Deep Neural Networks also known as *convolutional neural networks* are composed of multiple levels of nonlinear operations that aim at learning features hierarchies.

Machine learning models based on deep neural networks (DNNs) have achieved significant improvements and surpassed human-level accuracy in various learning tasks, including object identification and segmentation, face recognition, speech and text processing, and variety of other tasks [1-5].



Robustness and Trustworthiness



Limitations of Deep Neural Networks

1. Lack of Uncertainty Estimation

DNNs are unable to provide calibrated confidence or a measure of uncertainty in their predictions [6].

2. Vulnerability to Noise and Adversarial Attacks

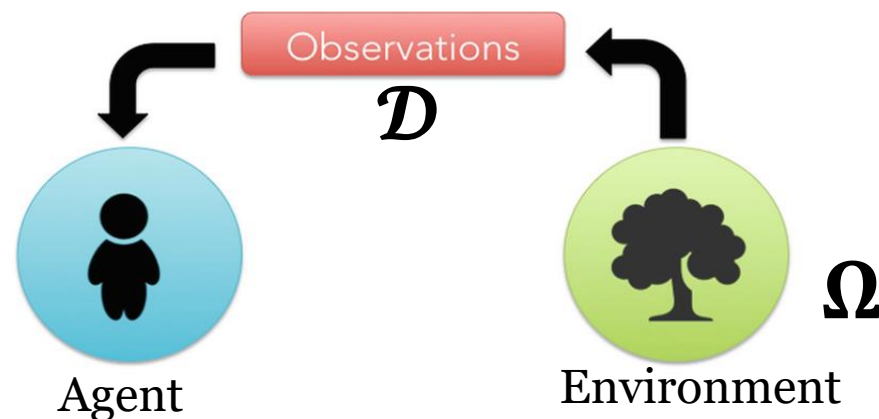
DNNs are vulnerable to noisy or perturbed inputs which might easily drive the model towards an incorrect prediction [7].

Detected as a speed sign



Quantifying the confidence of a model's prediction is crucial in applications, where decision-making and control is handed over to autonomous systems, such as autonomous control of drones and self-driving cars and healthcare diagnosis systems.

Bayesian Inference in Deep Neural Networks



Prior: $p(\Omega)$

prior knowledge about the parameters, Ω , before observing any data.

Likelihood: $p(\mathcal{D}|\Omega)$

the process by which the data is generated given a particular Ω .

Posterior: $p(\Omega|\mathcal{D}) = \frac{p(\Omega)p(\mathcal{D}|\Omega)}{\sum_{\theta} p(\Omega)p(\mathcal{D}|\Omega)}$

captures the total knowledge about Ω after observing $\mathcal{D}$.

- ❑ The posterior distribution of the parameters is used to find the predictive distribution of any new data point $\mathcal{X}^*$ by marginalizing out the model's parameters,

$$p(\mathbf{y}^*|\mathcal{X}^*, \mathcal{D}) = \int p(\mathbf{y}^*|\mathcal{X}^*, \Omega) p(\Omega|\mathcal{D}) d\Omega$$

Variational Inference (VI) Framework

- ❑ Exact Bayesian inference on the parameters of a DNN is intractable due to the functional form of a DNN that consists of multiple layers of non-linearities and the high dimensionality of the parameter space [13].
- ❑ Various approaches have been proposed to approximate the posterior distribution of the weights given the data including the well-known Variational Inference (VI) [8 – 14].
- ❑ VI methods approximate the true posterior $p(\boldsymbol{\Omega} | \mathcal{D})$ with a simpler parametrized variational distribution $q_{\phi}(\boldsymbol{\Omega})$.
- ❑ The optimal parameters of the variational posterior ϕ^* are found by minimizing the Kullback-Leibler (KL) divergence between the approximate and the true posterior,

$$\begin{aligned}\phi^* &= \operatorname{argmin} \operatorname{KL}[q_{\phi}(\boldsymbol{\Omega}) || p(\boldsymbol{\Omega} | \mathcal{D})] \\ &= \operatorname{argmin} \operatorname{KL}[q_{\phi}(\boldsymbol{\Omega}) || p(\boldsymbol{\Omega})] - E_{q_{\phi}(\boldsymbol{\Omega})}\{\log p(\mathcal{D} | \boldsymbol{\Omega})\}\end{aligned}$$

- ❑ The optimization objective is given by the evidence lower bound (ELBO) $\mathcal{L}(\phi; \mathcal{D})$

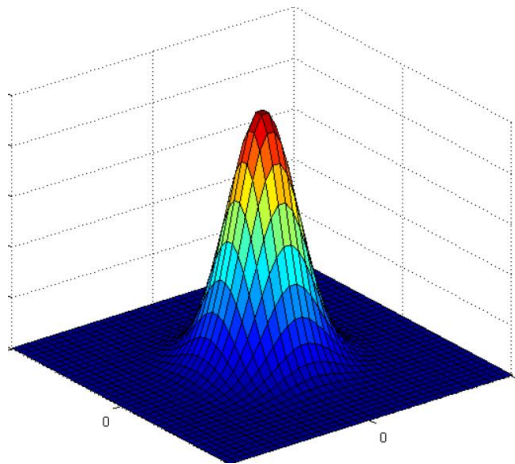
$$\mathcal{L}(\phi; \mathcal{D}) = E_{q_{\phi}(\boldsymbol{\Omega})}\{\log p(\mathcal{D} | \boldsymbol{\Omega})\} - \operatorname{KL}[q_{\phi}(\boldsymbol{\Omega}) || p(\boldsymbol{\Omega})]$$

Log-Likelihood

Regularization

The Challenge in Density Propagation

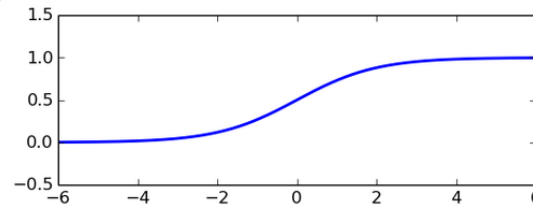
- The challenge remains in propagating the variational distribution $q_{\phi}(\mathbf{\Omega})$ over the parameters of a DNN through stacked layers of non-linearities.



Multivariate Gaussian Distribution

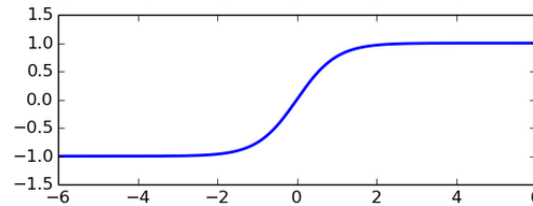


Nonlinear Activation Functions



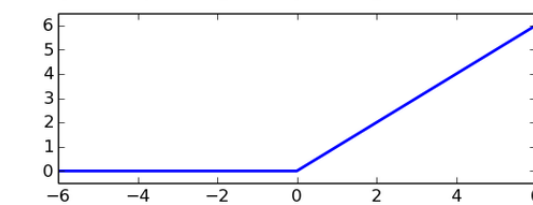
Sigmoid

$$\phi(z) = \frac{1}{1 + e^{-z}}$$



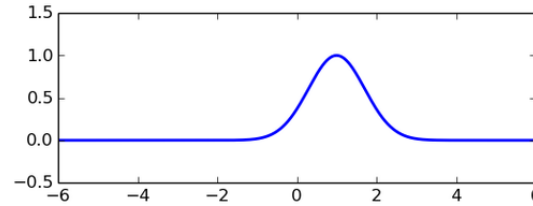
Hyperbolic Tangent

$$\phi(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$



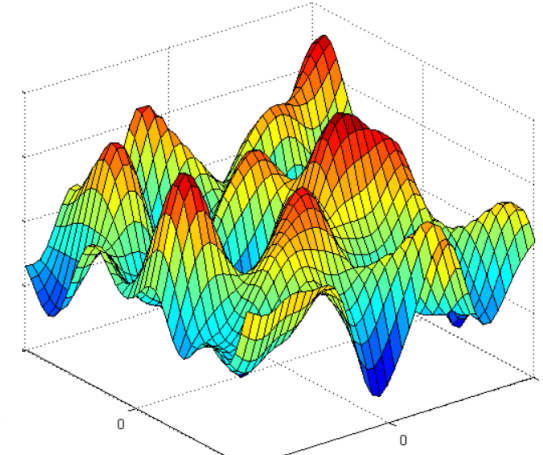
Rectified Linear

$$\phi(z) = \begin{cases} 0 & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases}$$



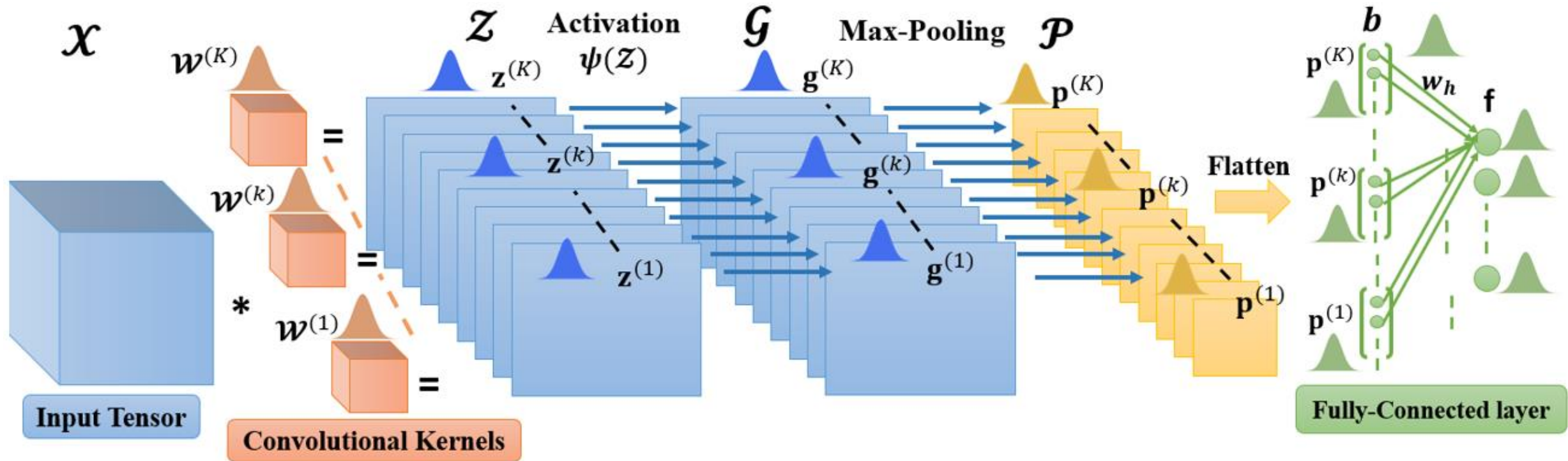
Radial Basis Function

$$\phi(z, c) = e^{-(\epsilon \|z - c\|)^2}$$



Unknown Distribution

Variational Density Propagation – Convolutional Neural Network



We consider a convolutional neural network with:

- ☐ One convolutional layer
- ☐ Nonlinearity (e.g. ReLU activation),
- ☐ Max-pooling layer,
- ☐ One fully connected.

Extended Variational Density Propagation (*exVDP*)

Propagation of Mean and Covariance

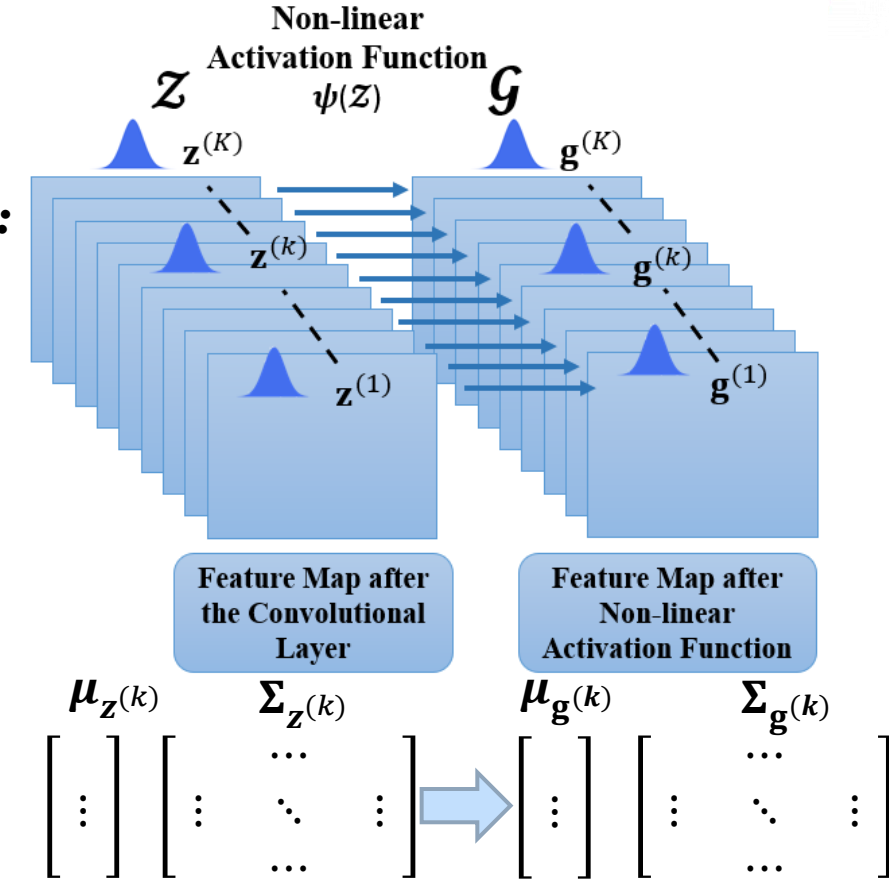
Non-linear activation layer – first-order Taylor approximation:

$$\psi(z_i) = \psi(\mu_{z_i}) + (z_i - \mu_{z_i}) \frac{d\psi(\mu_{z_i})}{dz_i} + \frac{1}{2!} (z_i - \mu_{z_i})^2 \frac{d^2\psi(\mu_{z_i})}{dz_i^2} + \dots$$

$$\mu_{g_i} = E(g_i) \approx \psi(\mu_{z_i})$$

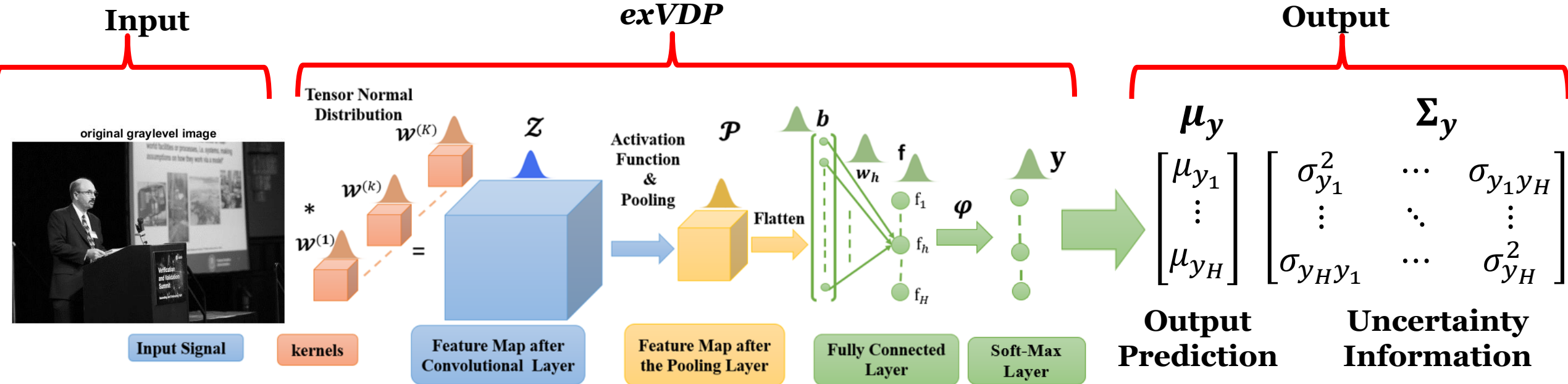
$$\Sigma_{\mathbf{g}^{(k)}} = \begin{cases} \sigma_{g_i}^2 = \text{Var}(g_i) \approx \sigma_{z_i}^2 \left(\frac{d\psi(\mu_{z_i})}{dz_i} \right)^2, & \text{if } i = j \\ \sigma_{g_i g_j} = \text{Cov}(g_i, g_j) \approx \sigma_{z_i z_j} \left(\frac{d\psi(\mu_{z_i})}{dz_i} \right) \left(\frac{d\psi(\mu_{z_j})}{dz_j} \right), & \text{if } i \neq j \end{cases}$$

g_i is the i^{th} element of the feature map, ψ is element-wise activation function.
We remove the superscript k for simplicity.



Extended Variational Density Propagation (*exVDP*)

Propagation of Mean and Covariance



Soft-Max Layer:

$$\mu_y \approx \varphi(\mu_f), \quad \Sigma_y \approx J_\varphi \Sigma_f J_\varphi^T$$

$$J_\varphi(\mu_f) = \text{diag}(\mu_y) - \mu_y \mu_y^T$$

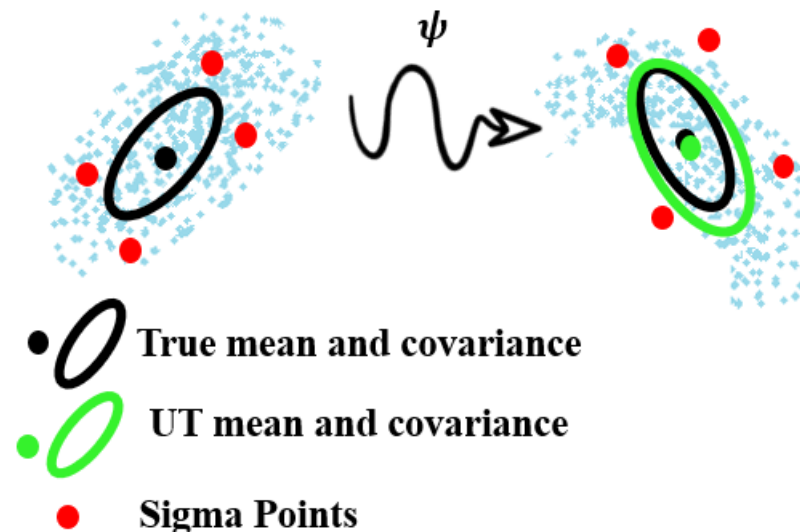
where φ is the Soft-max function and J_φ is the Jacobian matrix of φ with respect to f evaluated at μ_f .

Unscented Variational Density Propagation (*unVDP*)- Propagation of Sigma Points

Unscented Transformation:

- ❑ The linearization, performed in the exVDP propagation may result in accumulation of errors especially in deep neural networks with a large number of stacked non-linear activations.
- ❑ The unscented transformation (UT) can provide estimates of the mean and covariance after non-linear transformation which are correct at least up to the third order [15].
- ❑ In the UT framework, the probability density function (pdf) is specified using a set of carefully chosen samples, called sigma points.

Non-Linear Function



Evidence Lower Bound (ELBO) Objective Function

$$\mathcal{L}(\phi; \mathbf{y} | \mathcal{X}) = E_{q_{\phi}(\boldsymbol{\Omega})} \{ \log p(\mathbf{y} | \mathcal{X}, \boldsymbol{\Omega}) \} - \text{KL}[q_{\phi}(\boldsymbol{\Omega}) || p(\boldsymbol{\Omega})]$$

Backpropagation

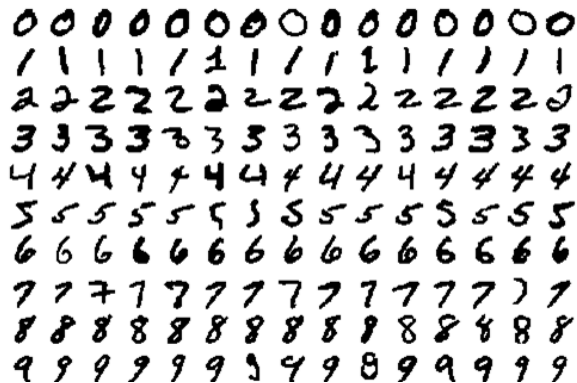
- ❑ In the forward pass, we propagated the mean and covariance matrix of the variational distribution $q_{\phi}(\boldsymbol{\Omega})$ across the network layers and calculated the objective function $\mathcal{L}(\phi; \mathbf{y} | \mathcal{X})$.
- ❑ In the back-propagation pass, we compute the gradient of the objective function $\nabla \mathcal{L}(\phi; \mathbf{y} | \mathcal{X})$ w.r.t the variational parameters ϕ and update ϕ using the gradient descent update rule.

Simulation Results and Discussion

Image Classification on MNIST and CIFAR-10

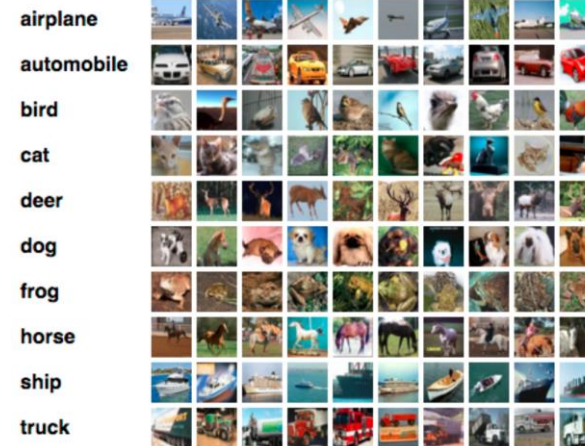
- We present test accuracy of *unVDP*, *exVDP* compared with Bayes-by-Backprop (BBB), and a deterministic CNN for the MNIST and with Bayes-CNN, and Dropout CNN for CIFAR-10 with varying levels of adversarial and Gaussian noise added to the test set.

MNIST Dataset



Gaussian noise level	unVDP	exVDP	BBB	CNN
Zero (No noise)	97.9%	97.8%	97.8%	97.7%
Low	95.1%	94.1%	86.4%	79.6%
Medium	86.7%	84.6%	76.7%	70.5%
High	74.8%	73.4%	63.8%	55.9%
Adversarial noise level				
Low	97.5%	96.6%	91.5%	58.7%
Medium	84.9%	84.4%	45.9%	14.7%
High	66.1%	51.6%	16.5%	14.5%

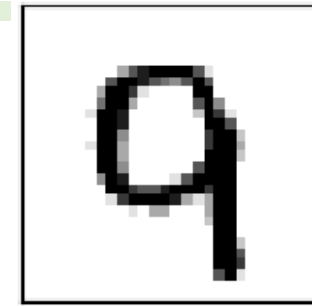
CIFAR-10 Dataset



Gaussian noise level	<i>unVDP</i>	<i>exVDP</i>	Bayes-CNN	Dropout CNN
Zero (No noise)	92.5%	91.8%	92.1%	91.0%
Low	92.3%	91.4%	87.0%	89.0%
Medium	91.9%	90.9%	86.8%	87.2%
High	90.1%	89.1%	85.2%	86.0%
Adversarial noise level				
Low	88.2%	88.1%	76.2%	77.0%
Medium	85.4%	82.3%	69.1%	53.0%
High	76.5%	67.7%	42.2%	33.0%

Self-Awareness and Robustness

Analysis of the Output Covariance Matrix



True: 9, Pred: 9

Prediction of
Deterministic CNN

**Output Mean and Covariance Matrix of exVDP for Noise-free Input
(Correctly Classified Input)**

Output Covariance Matrix

Output
Prediction

	0	1	2	3	4	5	6	7	8	9		0	
0	1.3E-12	-1E-20	6.7E-16	6.9E-15	3.4E-13	3.2E-14	2.9E-18	-7E-15	1.7E-16	8.3E-13		1.2E-08	0
1	-1E-20	5.3E-24	-5E-22	3.1E-21	4.6E-19	2.4E-20	-1E-25	-2E-19	1.1E-22	3.6E-19		2.4E-14	1
2	6.7E-16	-5E-22	3E-16	1.4E-16	-6E-15	-5E-16	2.9E-20	4.6E-16	6.8E-19	9.1E-15		1.8E-10	2
3	6.9E-15	3.1E-21	1.4E-16	1.7E-14	-7E-14	1.8E-15	2.8E-20	2.2E-14	3.1E-18	9.2E-14		1.3E-09	3
4	3.4E-13	4.6E-19	-6E-15	-7E-14	1.4E-10	8.4E-13	2.7E-17	-2E-13	2.5E-15	7.6E-12		1.2E-07	4
5	3.2E-14	2.4E-20	-5E-16	1.8E-15	8.4E-13	7.6E-13	1.8E-18	-5E-14	1.2E-16	4.8E-13		8.9E-09	5
6	2.9E-18	-1E-25	2.9E-20	2.8E-20	2.7E-17	1.8E-18	2.2E-21	-5E-18	9.5E-21	2.2E-17		5E-13	6
7	-7E-15	-2E-19	4.6E-16	2.2E-14	-2E-13	-5E-14	-5E-18	5.8E-12	-2E-16	1.9E-13		2.5E-08	7
8	1.7E-16	1.1E-22	6.8E-19	3.1E-18	2.5E-15	1.2E-16	9.5E-21	-2E-16	5.9E-18	1.8E-15		2.5E-11	8
9	8.3E-13	3.6E-19	9.1E-15	9.2E-14	7.6E-12	4.8E-13	2.2E-17	1.9E-13	1.8E-15	1.3E-10		1	9

8E-10	0
5E-13	1
6E-09	2
8E-06	3
5E-07	4
1E-08	5
1E-10	6
5E-07	7
2E-08	8
1	9

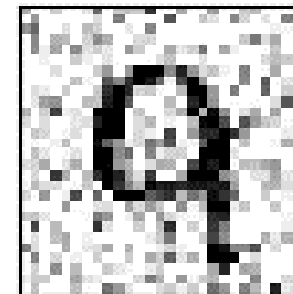
Ground Truth

Network Prediction

If the yellow block is not shown, then the network prediction and the ground truth are the same.

Self-Awareness and Robustness

Gaussian Noise



True: 9, Pred: 9

Prediction of
Deterministic
CNN

Output Mean and Covariance Matrix of exVDP for Input Corrupted with Low level of Gaussian Noise (Correctly Classified Input)

Output Covariance Matrix

Output
Prediction

	0	1	2	3	4	5	6	7	8	9		0	
0	0.0133	8E-07	0.0002	2E-05	0.0003	2E-05	3E-05	0.0001	0.00017	0.0029		0.005	0
1	8E-07	7E-08	1E-07	4E-08	5E-07	5E-08	6E-08	3E-07	2.99E-07	5E-06		1E-05	1
2	0.0002	1E-07	0.0155	1E-05	0.0003	9E-07	2E-05	4E-05	0.000109	0.0013		0.0056	2
3	2E-05	4E-08	1E-05	8E-05	6E-06	2E-06	1E-06	9E-06	7.25E-06	0.0002		0.0004	3
4	0.0003	5E-07	0.0003	6E-06	0.1216	-2E-05	2E-05	0.0001	0.000373	0.0022		0.0153	4
5	2E-05	5E-08	9E-07	2E-06	-2E-05	1E-04	8E-07	1E-05	8.07E-06	0.0003		0.0004	5
6	3E-05	6E-08	2E-05	1E-06	2E-05	8E-07	0.0002	4E-06	1.33E-05	0.0001		0.0005	6
7	0.0001	3E-07	4E-05	9E-06	0.0001	1E-05	4E-06	0.004	6.16E-05	0.0016		0.0028	7
8	0.0002	3E-07	0.0001	7E-06	0.0004	8E-06	1E-05	6E-05	0.0034	0.0018		0.0026	8
9	0.0029	5E-06	0.0013	0.0002	0.0022	0.0003	0.0001	0.0016	0.001753	0.5083		0.9674	9

0.0009	0
6E-06	1
0.0019	2
0.0007	3
0.0234	4
0.0121	5
0.0006	6
0.0038	7
0.0037	8
0.9529	9

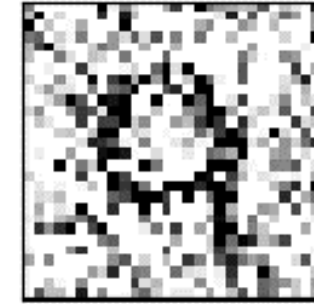
Ground Truth

Network Prediction

If the yellow block is not shown, then the network prediction and the ground truth are the same.

Self-Awareness and Robustness

Gaussian Noise



True: 9, Pred: 9

Prediction of
Deterministic
CNN

Output Mean and Covariance Matrix of exVDP for Input Corrupted with High level Gaussian Noise (Correctly Classified Input)

Output Covariance Matrix

Output
Prediction

1.1E-11	0
3.9E-16	1
0.00083	2
3.1E-08	3
0.02638	4
0.00825	5
3.2E-18	6
8.5E-06	7
3.8E-06	8
0.96454	9

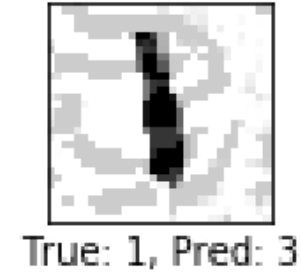
	0	1	2	3	4	5	6	7	8	9		0	
0	0.72614	7.3E-06	0.02063	0.00011	0.00301	0.00041	5.4E-05	0.02911	0.00164	0.10533		0.03217	0
1	7.3E-06	1.4E-06	5.3E-06	4.6E-08	4.9E-07	4.9E-07	2.9E-08	1.4E-05	1.2E-06	4.7E-05		4.3E-05	1
2	0.02063	5.3E-06	6.30839	0.00028	0.00323	-2E-05	0.0001	0.04422	0.00198	0.1513		0.10437	2
3	0.00011	4.6E-08	0.00028	0.00012	2.7E-06	6E-06	3.2E-07	0.00017	5.1E-06	0.00115		0.00042	3
4	0.00301	4.9E-07	0.00323	2.7E-06	0.05826	-0.0001	9.8E-06	0.00286	0.00048	0.01931		0.00889	4
5	0.00041	4.9E-07	-2E-05	6E-06	-0.0001	0.00451	1.1E-06	0.00222	1.7E-05	0.00518		0.00248	5
6	5.4E-05	2.9E-08	0.0001	3.2E-07	9.8E-06	1.1E-06	1.2E-05	7E-05	5.2E-06	0.00024		0.00013	6
7	0.02911	1.4E-05	0.04422	0.00017	0.00286	0.00222	7E-05	10.2073	0.00447	0.2822		0.1372	7
8	0.00164	1.2E-06	0.00198	5.1E-06	0.00048	1.7E-05	5.2E-06	0.00447	0.00649	0.01209		0.00301	8
9	0.10533	4.7E-05	0.1513	0.00115	0.01931	0.00518	0.00024	0.2822	0.01209	29.1693		0.71129	9

Ground Truth
Network Prediction

If the yellow block is not shown, then the network prediction and the ground truth are the same.

Self-Awareness and Robustness Adversarial Noise

Example: Adversarial Noise (the targeted attack class is digit “3”)



Prediction of
Deterministic
CNN

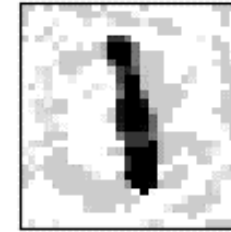
2E-13	0
0.0238	1
8E-08	2
0.9762	3
7E-10	4
5E-08	5
5E-10	6
1E-09	7
8E-06	8
2E-13	9

Output Covariance Matrix

Output Prediction

	0	1	2	3	4	5	6	7	8	9			
0	2.8E-12	2E-07	1.1E-09	1.4E-07	2.3E-10	8E-11	4.2E-11	1.1E-09	1.8E-09	2.1E-11		2E-07	0
1	2E-07	1.39853	0.00093	0.11747	0.0003	8.4E-05	4.7E-05	0.0006	0.00154	2E-05		0.1529	1
2	1.1E-09	0.00093	7.9E-05	0.00079	1.3E-06	3.5E-07	2.9E-07	7.7E-07	6.6E-06	1.1E-07		0.0011	2
3	1.4E-07	0.11747	0.00079	1.09673	0.00017	6.9E-05	3.8E-05	0.00068	0.00088	1.4E-05		0.8427	3
4	2.3E-10	0.0003	1.3E-06	0.00017	4.4E-06	1.1E-07	1.1E-07	1.3E-06	2.2E-06	2.9E-08		0.0002	4
5	8E-11	8.4E-05	3.5E-07	6.9E-05	1.1E-07	5.7E-07	1.8E-08	1.1E-07	7.6E-07	8.7E-09		9E-05	5
6	4.2E-11	4.7E-05	2.9E-07	3.8E-05	1.1E-07	1.8E-08	1E-07	1.8E-07	3.7E-07	4.5E-09		3E-05	6
7	1.1E-09	0.0006	7.7E-07	0.00068	1.3E-06	1.1E-07	1.8E-07	4.4E-05	6.9E-06	1E-07		0.0011	7
8	1.8E-09	0.00154	6.6E-06	0.00088	2.2E-06	7.6E-07	3.7E-07	6.9E-06	0.00018	2E-07		0.0018	8
9	2.1E-11	2E-05	1.1E-07	1.4E-05	2.9E-08	8.7E-09	4.5E-09	1E-07	2E-07	1.7E-08		2E-05	9

exVDP

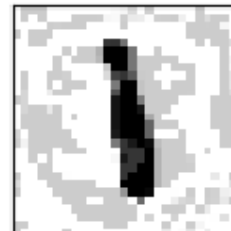


Output Covariance Matrix

Output Prediction

	0	1	2	3	4	5	6	7	8	9		0	
0	4.35E-07	-0.00033	2.68E-07	0.000318	2.91E-06	2.88E-07	1.17E-06	7.16E-07	1.02E-05	6.49E-09		4.1E-05	0
1	-0.00033	19.50457	-0.00061	-19.4682	-0.00653	-0.00066	-0.00265	-0.0016	-0.02399	-1.5E-05		0.59416	1
2	2.68E-07	-0.00061	1.42E-06	0.000578	5.29E-06	5.18E-07	2.12E-06	1.29E-06	1.85E-05	1.18E-08		7.5E-05	2
3	0.000318	-19.4682	0.000578	19.43496	0.006104	0.000625	0.002506	0.001518	0.021562	1.44E-05		0.40145	3
4	2.91E-06	-0.00653	5.29E-06	0.006104	0.000171	5.64E-06	2.33E-05	1.39E-05	0.000202	1.29E-07		0.00082	4
5	2.88E-07	-0.00066	5.18E-07	0.000625	5.64E-06	1.62E-06	2.27E-06	1.37E-06	1.99E-05	1.27E-08		8E-05	5
6	1.17E-06	-0.00265	2.12E-06	0.002506	2.33E-05	2.27E-06	2.72E-05	5.58E-06	8.1E-05	5.14E-08		0.00033	6
7	7.16E-07	-0.0016	1.29E-06	0.001518	1.39E-05	1.37E-06	5.58E-06	9.99E-06	4.86E-05	3.12E-08		0.0002	7
8	1.02E-05	-0.02399	1.85E-05	0.021562	0.000202	1.99E-05	8.1E-05	4.86E-05	0.002048	4.51E-07		0.00285	8
9	6.49E-09	-1.5E-05	1.18E-08	1.44E-05	1.29E-07	1.27E-08	5.14E-08	3.12E-08	4.51E-07	8.38E-10		1.8E-06	9

unVDP

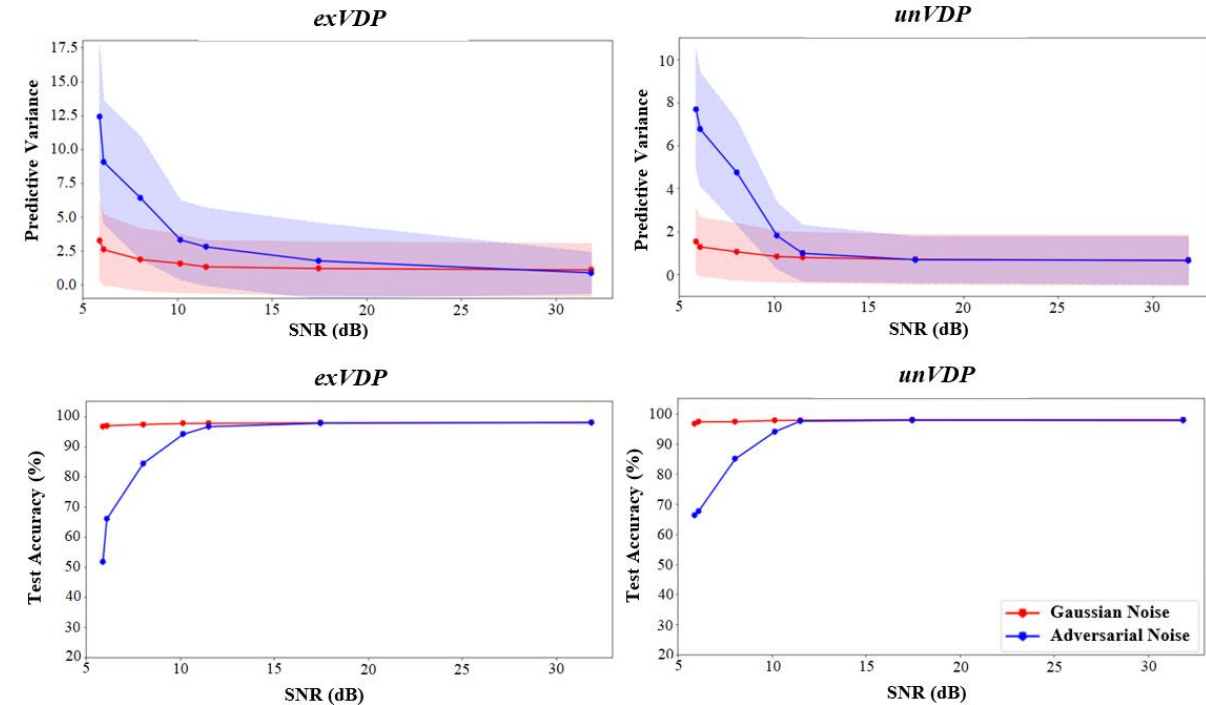
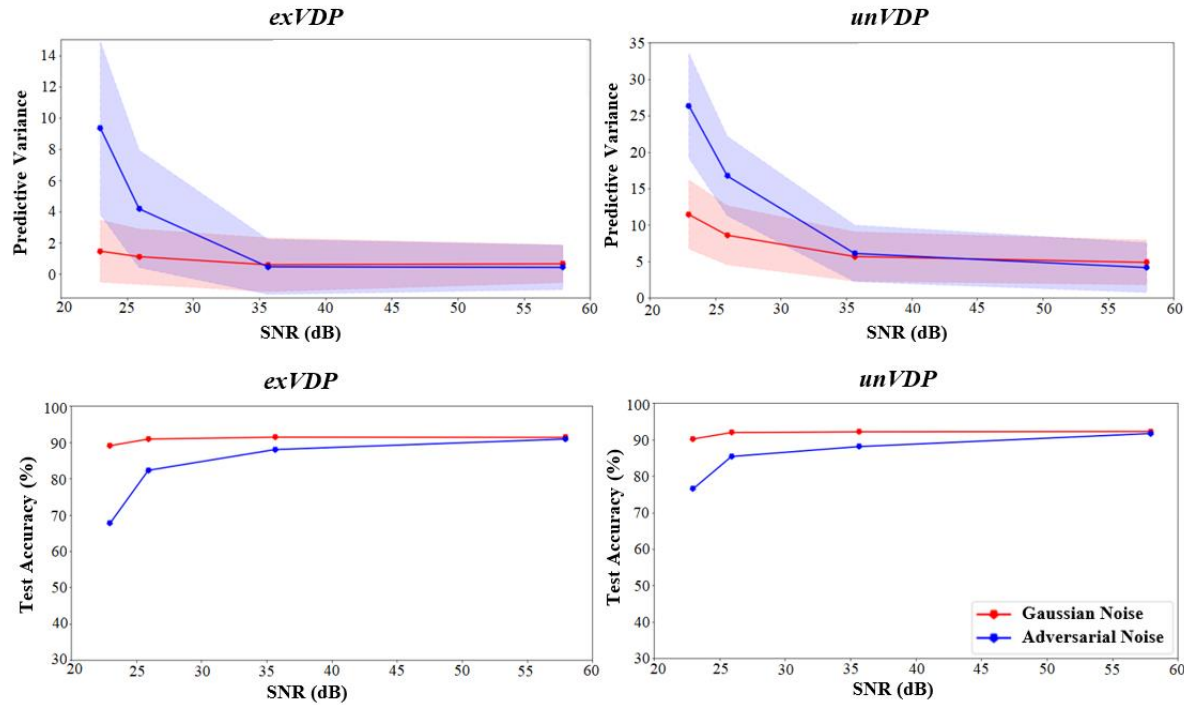


Ground Truth
Network Prediction

Self-Awareness and Robustness Analysis of the Output Variance

CIFAR-10 Dataset

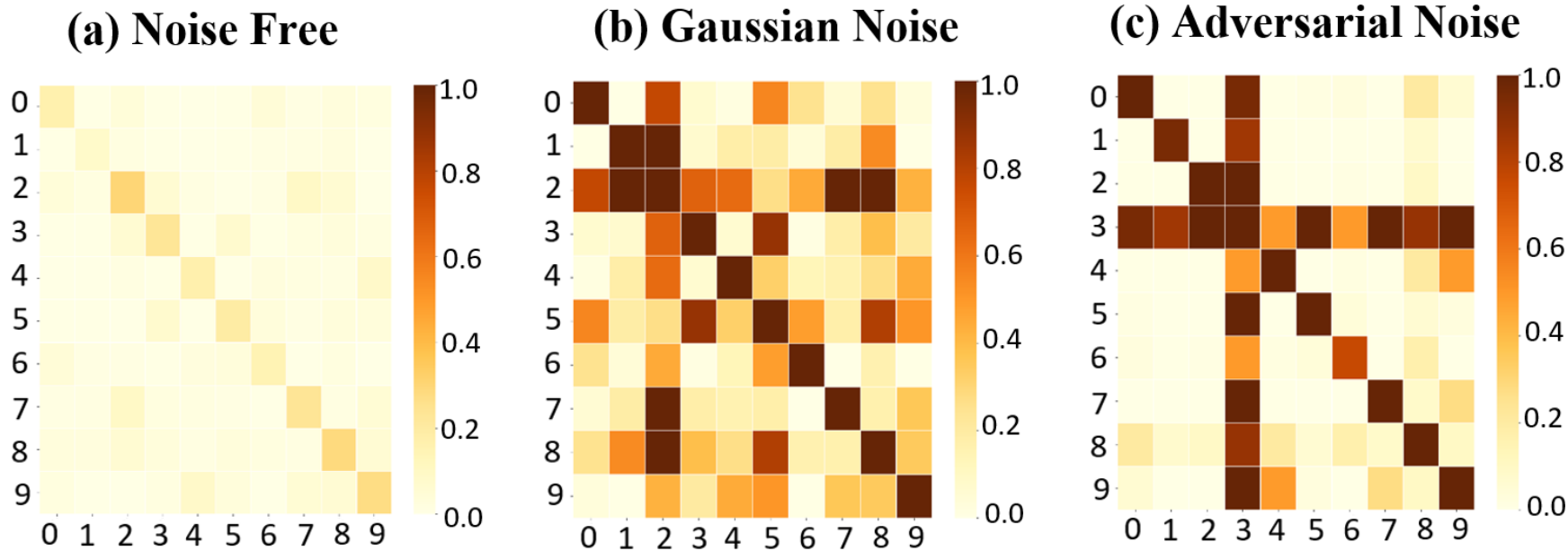
MNIST Dataset



Self-Awareness and Robustness

Analysis of the Output Covariance Matrix

- ❑ The heat-maps represent the average output covariance matrices of the *exVDP* model on MNIST dataset for three cases: (a) noise-free, (b) Gaussian noise, and (c) adversarial noise.
- ❑ The average test accuracies for the three cases were 97.8%, 84.6%, and 84.4%, respectively.
- ❑ Each pixel of the heat-map is a normalized average of absolute value of the covariance for all 10,000 test examples.
- ❑ The targeted adversarial examples were generated to fool the model into predicting digit “3” [16].

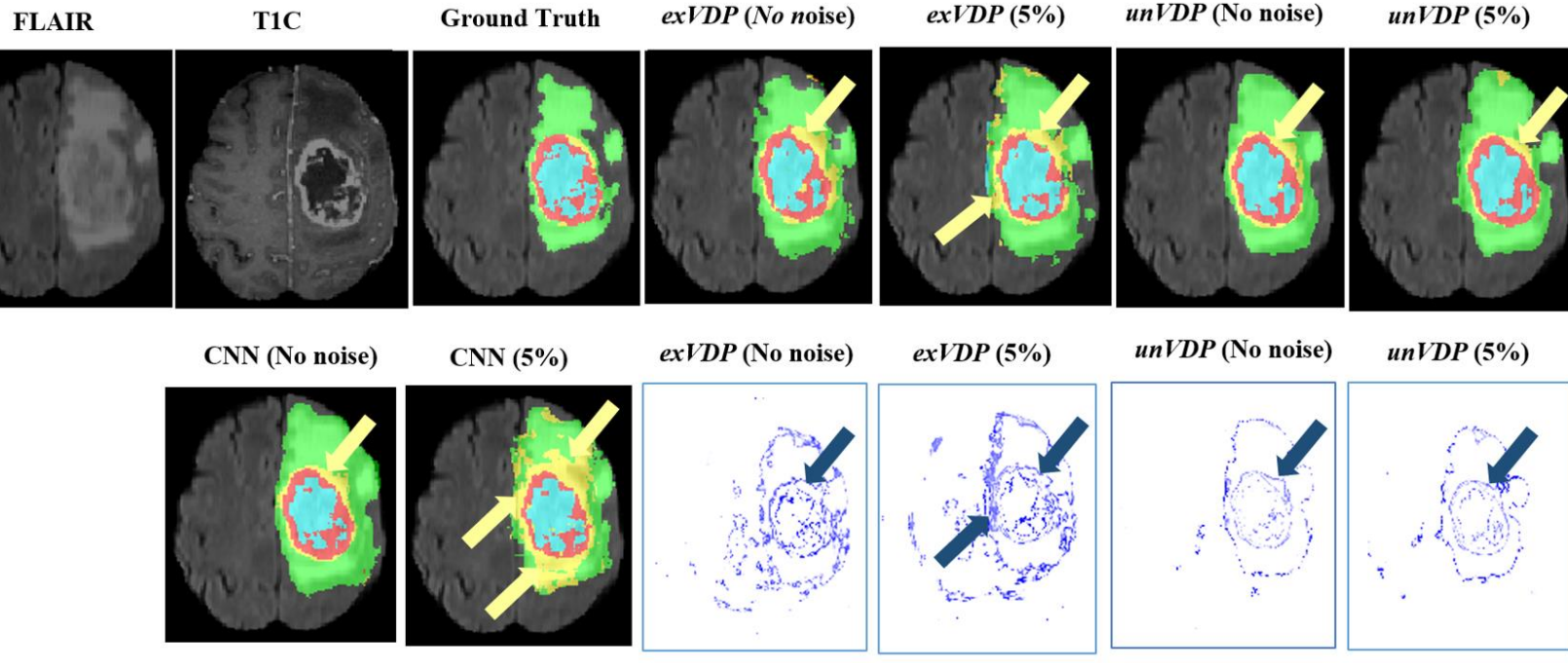


Application to Brain Tumor Segmentation in MRI Images

- We evaluate the performance of proposed *exVDP* and *unVDP* models on High Grade Glioma (HGG) brain tumor segmentation task using Brain Tumor Segmentation Challenge (BraTS) 2015 dataset [17].
- The uncertainty map will allow physicians to quickly review the segmentation results and, if needed, make corrections of tumor boundaries in the regions where the uncertainty is high.
- We evaluated the models before and after adding Gaussian noise or targeted adversarial attack (targeted class is class 3, i.e., “non-enhancing tumor”).

Method	Tumor Regions	Noise level		
		Zero (No noise)	Adversarial 5%	Gaussian 5%
unVDP	Complete	85.3%	81.7%	83.0%
	Core	81.9%	78.7%	80.7%
	Enhancing	83.7%	75.4%	81.7%
exVDP	Complete	80.8%	77.4%	80.6%
	Core	74.6%	72.6%	74.5%
	Enhancing	74.0%	69.8%	73.9%
CNN	Complete	78.0%	43.4%	66.9%
	Core	65.0%	47.1%	51.9%
	Enhancing	75.0%	43.9%	55.7%

The evaluation of the segmentation results was done using Dice Similarity Coefficient (DSC).



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Acknowledgment

The authors would like to thank the financial support of

- ☐ NSF ECCS 1903466
- ☐ NSF CCF-1527822
- ☐ NSF DUE-1610911
- ☐ NSF CRII: RI-2153413



National Science Foundation
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- ☐ Lockheed Martin Inc.



- ☐ ACM SIGHPC/Intel Computational & Data Science Fellowship



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