Uncertainty Estimation for Dense Prediction Tasks

Jing Zhang, Yuchao Dai, Deng-Ping Fan, Nick Barnes, Peyman Moghadam, Christian Walder, Mehrtash Harandi
Code and tutorial material are available

**Uncertainty estimation models**

We provide the implementation details of uncertainty estimation techniques. Including the ensemble based solutions and generative model based methods.
Uncertainty is inherent within Machine Learning

Input space

Output space

Query sample

Query sample prediction

Easy sample?  Hard sample?

Mean?  Variance?
Outline

• Motivation
• Background
• Aleatoric uncertainty and Epistemic Uncertainty
• Uncertainty Approximation
  ✓ Ensemble solutions
  ✓ Generative model solutions
  ✓ Bayesian latent variable model solutions
• Experiments
• Discussion and Conclusion
Motivation

• Distribution estimation vs Point estimation
  - Classification: prediction with confidence
  - Regression: prediction with variance

Uncertainty: a mechanism to understand model limitations
Motivation

- Camouflaged object detection
- Salient object detection
- Monocular depth estimation
Motivation

• Which one is salient?
Motivation

• Which one is salient?
Motivation

• Where is the camouflaged object

Camouflaged Object Segmentation dataset: Anabranchn Network for Camouflaged Object Segmentation, Le et al, CVIU, 2019
Motivation

- Where is the camouflaged object
Motivation – Depth estimation from RGB

• What’s the exact distance?
Motivation – Depth estimation from RGB

• What’s the exact distance?

• Visual ambiguity and thin items foreground, problems background (e.g., distance limitation of sensor, less data available)
Motivation

• Model can make mistakes sometimes
• Model should be aware when it makes mistakes

Uncertainty: a mechanism to understand model limitations
Confidence of $p(y|x)$?

Variance of prediction?
Motivation

• Camouflaged object detection
Motivation

- Salient object detection
Motivation

• Monocular depth estimation

Figure 5: NYUv2 Depth results. From left: input image, ground truth, depth regression, aleatoric uncertainty, and epistemic uncertainty.

Figure from “What uncertainties do we need in bayesian deep learning for computer vision?” by A. Kendall and Y. Gal.
Motivation

- Well-calibrated model
- Hard-negative mining
- Dynamic confidence supervision
Code and tutorial material are available
Outline

• Motivation
• Background
  • Aleatoric uncertainty and Epistemic Uncertainty
  • Uncertainty Approximation
    ✓ Ensemble solutions
    ✓ Generative model solutions
    ✓ Bayesian latent variable model solutions
• Experiments
• Discussion and Conclusion
Background

Given training dataset $D = \{x_i, y_i\}_{i=1}^N$, the goal of machine learning methods:

$$\min_\theta \mathbb{E}_{x,y}[\mathcal{L}(f(x, \theta), y)] = \int \mathcal{L}(f(x, \theta), y) dp(x, y) \approx \frac{1}{N} \sum_{i=1}^N \mathcal{L}(f(x_i, \theta), y_i), (x_i, y_i) \sim p(x, y)$$

Loss over a continuous distribution is approximated by empirical loss over a dataset.
Background

Given training dataset $D = \{x_i, y_i\}_{i=1}^{N}$, the goal of machine learning methods:

$$
\min_{\theta} \mathbb{E}_{x,y}[\mathcal{L}(f(x, \theta), y)] = \int \mathcal{L}(f(x, \theta), y) dp(x, y) \approx \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(f(x_i, \theta), y_i), (x_i, y_i) \sim p(x, y)
$$

$\mathbb{E}_{x,y}$: Expectation over input
$f(x, \theta)$: model hypothesis for $x$ given model parameters $\theta$
$\mathcal{L}$: (.,.) loss
$(x_i, y_i) \sim p(x, y)$: $(x_i, y_i)$ input/output sampled from true distribution

Ambiguity comes from $\theta$ and the representativeness of the sampled dataset $D$. 
Background

Given training dataset $D = \{x_i, y_i\}_{i=1}^N$, the predictive distribution is defined as:

$$p(y|x) = \int p(y|x, \theta)p(\theta)d\theta$$

where the likelihood of prediction is defined as:

$$p(y|x, \theta) = \mathcal{N}(f(x, \theta), \Sigma) \quad \text{(Regression)} \quad \text{Or} \quad p(y|x, \theta) = \text{Softmax}\left(\frac{f(x, \theta)}{\exp(\sigma^2)}\right) \quad \text{(Classification)}$$
Background

Given training dataset $D = \{x_i, y_i\}_{i=1}^N$, the predictive distribution is defined as:

$$p(y|x) = \int p(y|x, \theta)p(\theta)d\theta$$

where the likelihood of prediction is defined as:

- Regression: $p(y|x, \theta) = \mathcal{N}(f(x, \theta), \Sigma)$
- Classification: $p(y|x, \theta) = \text{Softmax}(\frac{f(x, \theta)}{\exp(\sigma^2)})$

Uncertainty origin: $(\epsilon / \Sigma), p(\theta)$

- Aleatoric uncertainty: (Intrinsic randomness of a phenomenon [1,2])
e.g., sensor noise, labeling noise
- Epistemic uncertainty: (Lack of knowledge of data [1,2])
Model noise

Background

Uncertainty origin: \( (\epsilon / \Sigma), p(\theta) \)

Aleatoric uncertainty: data related uncertainty
  (Intrinsic randomness of a phenomenon [1,2])

Epistemic uncertainty: model related uncertainty
  (Lack of knowledge of data [1,2])

Point estimation system vs Self-awareness of machine learning system

Decision making: Medical diagnosis, automatous driving, ...

Examples

Prediction: dog
Probability: 0.98

Prediction: dog
Probability: 0.95

Parsed an image of myself through the animal network and it's 98% confident I'm a dog.

Example and image from: [Dealing with Overconfidence in Neural Networks: Bayesian Approach – Jonathan Ramkissoon (jramkiss.github.io)](https://jramkiss.github.io)
Code and tutorial material are available

Uncertainty estimation models

We provide the implementation details of uncertainty estimation techniques. Including the ensemble based solutions and generative model based methods.
Outline

• Motivation
• Background
• Aleatoric uncertainty and Epistemic Uncertainty
  • Uncertainty Approximation
    ✓ Ensemble solutions
    ✓ Generative model solutions
    ✓ Bayesian latent variable model solutions
• Experiments
• Discussion and Conclusion
Aleatoric Uncertainty and Epistemic Uncertainty

• Aleatoric uncertainty: randomness, inherent noise
• Epistemic uncertainty: lack of knowledge, can be explained away with enough data, while aleatoric uncertainty cannot.

Aleatoric uncertainty: function of input, model it over outputs
Epistemic uncertainty: function of model, model it over network parameters
Examples

• What is aleatoric uncertainty? What is epistemic uncertainty?

Figure 1: Illustrating the difference between aleatoric and epistemic uncertainty for semantic segmentation on the CamVid dataset [8]. Aleatoric uncertainty captures noise inherent in the observations. In (d) our model exhibits increased aleatoric uncertainty on object boundaries and for objects far from the camera. Epistemic uncertainty accounts for our ignorance about which model generated our collected data. This is a notably different measure of uncertainty and in (e) our model exhibits increased epistemic uncertainty for semantically and visually challenging pixels. The bottom row shows a failure case of the segmentation model when the model fails to segment the footpath due to increased epistemic uncertainty, but not aleatoric uncertainty.

Figure from “What uncertainties do we need in bayesian deep learning for computer vision?” by A. Kendall and Y. Gal.
Aleatoric uncertainty modeling

• Image-level classification
  - Image-independent aleatoric uncertainty—homoscedastic uncertainty
  - Image-conditional aleatoric uncertainty—heteroscedastic uncertainty

• Pixel-level Classification/Regression
  - Pixel-conditional uncertainty
  - Image-level uncertainty
  - Dataset-level uncertainty

Constant vs Learned
Aleatoric Uncertainty--Regression:

For Gaussian likelihood: $p(y|x, \theta) = \mathcal{N}(f(x, \theta), \Sigma(x))$

$\Sigma(x) = \text{diag}((\sigma(x))^2)$ is the inherent label noise with the basic assumption:

$y = f(x, \theta) + n(x), n(x) \sim \mathcal{N}(0, \Sigma(x))$

Uncertainty-aware loss: $\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{1}{2(\sigma(x))^2} \mathcal{L}_2 + \frac{1}{2} \log((\sigma(x))^2) \right)$
Aleatoric Uncertainty--Regression:

For Gaussian likelihood:  
\[ p(y|x, \theta) = \mathcal{N}(f(x, \theta), \Sigma(x)) \]

\[ \mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{1}{2(\sigma(x))^2} \mathcal{L}_2 + \frac{1}{2} \log((\sigma(x))^2) \right) \]

For numerical stability, define \( s_i = \log((\sigma(x))^2) \):  
\[ \mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{1}{2} \exp(-s_i) \mathcal{L}_2 + \frac{1}{2} s_i \right) \]

Aleatoric uncertainty:  
\[ U_\alpha = (\sigma(x))^2 \]
For SoftMax likelihood where $p(y|x, \theta) = \text{Softmax} \left( \frac{f(x, \theta)}{\exp(\sigma^2)} \right)$

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{1}{\exp(\sigma^2)} \mathcal{L}_{ce} + \frac{1}{2} \sigma^2 \right)$$

For numerical stability, define $T = \exp(\sigma^2)$ (the temperature):

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{1}{T} \mathcal{L}_{ce} + \frac{1}{2} \log(T) \right) \quad U_a = (\sigma(x))^2$$
Trivial solution:

For Gaussian likelihood: \( p(y|x, \theta) = \mathcal{N}(f(x, \theta), \Sigma(x)) \)

\[
\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{1}{2\sigma^2} \mathcal{L}_2 + \frac{1}{2} \log(\sigma^2) \right)
\]

\( \sigma(x) = 1 \), constant! Image-independent!!
Trivial solution:

For SoftMax likelihood where \( p(y|x, \theta) = \text{Softmax}\left(\frac{f(x, \theta)}{\exp(\sigma^2)}\right) \)

\[
\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{1}{\exp(\sigma^2)} \mathcal{L}_{ce} + \frac{1}{2} \sigma^2 \right)
\]

\( \sigma(x) = 0 \) !! Temperature = 1!!
Avoid the Trivial solution:

• Two types of aleatoric uncertainty definition
  ➢ Multi-head
  ➢ Mean entropy within BNN

• Uncertainty consistency loss for sampling free aleatoric uncertainty estimation

\[ U_a = \mathbb{E}_{p(\theta|D)}[H(y|x, \theta)] \]

Stefan Depeweg et. al. Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning. ICML. 2018
Dual-head Entropy GT Prediction

\[ U_a = \mathbb{E}_{p(\theta|D)}[H(y|x, \theta)] \]
Epistemic Uncertainty

• Not directly estimated
• Defined as residual of predictive uncertainty and aleatoric uncertainty
• Mutual information of model prediction and model parameters within Bayesian Neural Network (BNN).

\[ U_e = U_p - U_a = H(y|x) - \mathbb{E}_p(\theta|D)[H(y|x, \theta)] = I(y, \theta|x) \]

\[ I(y, \theta|x) = H(y|x) - H(y|x, \theta) = H(y|x) - \mathbb{E}_p(\theta|D)[H(y|x, \theta)] \]

Stefan Depeweg et. al. Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning. ICML. 2018
Epistemic Uncertainty

For Gaussian likelihood with aleatoric uncertainty $\sigma^2$ from multi-head, the entropy based uncertainty is reduced to a function of variance, leading to epistemic uncertainty:

$$U_e = \mathbb{E}_{p(\theta|D)}[p(y|x, \theta)^2] - (\mathbb{E}_{p(\theta|D)}[p(y|x, \theta)])^2$$

The predictive uncertainty is then:

$$U_p = \mathbb{E}_{p(\theta|D)}[p(y|x, \theta)^2] - (\mathbb{E}_{p(\theta|D)}[p(y|x, \theta)])^2 + \mathbb{E}_{p(\theta|D)}[\sigma(x)^2]$$

2. Stefan Depeweg et. al. Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning. ICML. 2018
Epistemic Uncertainty

SoftMax likelihood for classification:

\[ U_p = H(y|x) \]

\[ U_e = U_p - U_a = H(y|x) - \mathbb{E}_{p(\theta|D)}[H(y|x, \theta)] = I(y, \theta|x) \]

\[ U_a = \sigma(x)^2 \quad U_a = \mathbb{E}_{p(\theta|D)}[H(y|x, \theta)] \]
Break
Outline

• Motivation
• Background
• Aleatoric uncertainty and Epistemic Uncertainty
• Uncertainty Approximation
  ✓ Ensemble solutions
  ✓ Generative model solutions
  ✓ Bayesian latent variable model solutions
• Experiments
• Discussion and Conclusion
Epistemic Uncertainty

• Not directly estimated
• Defined as residual of predictive uncertainty and aleatoric uncertainty
• Mutual information of model prediction and model parameters within Bayesian Neural Network (BNN).

Given predictive uncertainty  \( U_p = H(y|x) \)

Epistemic uncertainty: \( U_e = U_p - U_a = H(y|x) - \mathbb{E}_p(\theta|D)[H(y|x, \theta)] = I(y, \theta|x) \)

\[ I(y, \theta|x) = H(y|x) - H(y|x, \theta) = H(y|x) - \mathbb{E}_{p(\theta|D)}[H(y|x, \theta)] \]

Stefan Depeweg et. al. Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning. ICML. 2018
Uncertainty Approximation

- Recall that epistemic uncertainty is usually directly estimated, which is defined as residual of predictive uncertainty and aleatoric uncertainty or the mutual information of model prediction and model parameters within Bayesian Neural Network (BNN).

Given predictive uncertainty \( U_p = H(y|x) \)

Epistemic uncertainty: \( U_e = U_p - U_a = H(y|x) - \mathbb{E}_p(\theta|D)[H(y|x, \theta)] = I(y, \theta|x) \)

\[
I(y, \theta|x) = H(y|x) - H(y|x, \theta) = H(y|x) - \mathbb{E}_p(\theta|D)[H(y|x, \theta)]
\]

Stefan Depeweg et. al. Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning. ICML. 2018
Uncertainty Approximation

• Recall: \( U_e = U_p - U_a = H(y|x) - \mathbb{E}_{p(\theta|D)}[H(y|x, \theta)] = I(y, \theta|x) \)
• no close form solution for \( p(\theta|D) \)

\[ p(\theta|D) = p(\theta|x, y) = p(y|x, \theta)p(\theta)/p(y|x), \] where \( p(y|x) \) cannot be evaluated analytically, thus no close form solution for \( p(\theta|D) \).

• Approximation for Bayesian posterior inference
  • Variational inference
    Approximate \( p(\theta|D) \) with easy-controlled distribution \( q_\gamma(\theta) \), \( \gamma \): variational parameters. i.e. MC-dropout
  • Markov chain Monte Carlo (MCMC) methods
    Sampling based solution, correlated sequence of \( \theta_t \sim p(\theta|D) \). MC average is used as approximation of expectation----Generative model based solutions
Uncertainty Approximation

• Ensemble solutions

• Generative model solutions
  1. Adversarial distillation of Bayesian neural network posteriors. Kuan-Chieh Wang et. al. ICML. 2018

• Bayesian latent variable model solutions
  1. What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision? Alex Kendall, Yarin Gal. NeurIPS. 2017
  2. Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning. Stefan Depeweg et. al. ICML. 2018
Outline

• Motivation
• Background
• Aleatoric uncertainty and Epistemic Uncertainty

• Uncertainty Approximation
  ✓ Ensemble solutions
    ✓ MC-dropout
    ✓ Deep ensemble
    ✓ Snapshots ensemble
  ✓ Generative model solutions
  ✓ Bayesian latent variable model solutions

• Experiments
• Discussion and Conclusion
• MC dropout:

True predictive distribution:

$$p(y|x) = \int p(y|x, \theta)p(\theta)d\theta$$

MC average as approximation:

$$p(y|x) \approx \frac{1}{T} \sum_{t=1}^{T} p(y_t|x, \theta_t)$$

Where $\theta_t$ is sampled from the approximate posterior distribution $q_\gamma(\theta)$

Ensemble Solutions

• MC dropout:

  Implementation details: add dropout before every weighted layer during both training and testing.

  Pros: easy to implement, no additional parameters
  Cons: cannot control the dropout mask, mode collapse issue

Ensemble Solutions

• Deep ensemble

Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles.
Lakshminarayanan, Balaji et. al. NeurIPS. 2017
Ensemble Solutions

• Deep ensemble
  Implementation details: random initialization, multi-network, multi-head.

  Pros: easy to implement, usually suffer no mode collapse issue
  Cons: extra parameters leading to longer training time, fixed number of predictions, not very flexible.
Ensemble Solutions

• Snapshot ensemble

\[ x \rightarrow \underbrace{\text{\texttt{\scriptsize\textbf{\text{Snapshot ensemble}}}}}_{\text{\texttt{\scriptsize\textbf{\text{Snapshot ensemble}}}}} \rightarrow f(x, \theta_t) \]

\[ \theta_t: t \text{ indicates epoch} \]

Snapshot Ensembles: Train 1, Get M for Free. Gao Huang et. al. ICLR. 2017
Ensemble Solutions

• Snapshot ensemble
  Implementation details: save multiple snapshots for multiple predictions

  Pros: no extra parameters, easy to implement
  Cons: hard to determine the snapshots point
Examples

MD: MC-dropout, DE: deep ensemble, SE: snapshot ensemble

Ensemble based Uncertainty computation—regression

- Aleatoric uncertainty $U_a = \frac{1}{T} \sum_{t=1}^{T} H(y|x, \theta_t)$, or $U_a = \sigma(x)^2$
- Epistemic uncertainty

$$U_e = \mathbb{E}_p(\theta|D) [p(y|x, \theta)^2] - (\mathbb{E}_p(\theta|D)[p(y|x, \theta)])^2$$

or

$$U_e = H \left( \frac{1}{T} \sum_{t=1}^{T} p(y|x, \theta_t) \right) - \frac{1}{T} \sum_{t=1}^{T} H(y|x, \theta_t)$$

- Predictive uncertainty

$$U_p = U_a + U_e$$
Ensemble based Uncertainty computation--classification

• Aleatoric uncertainty

\[ U_a = \frac{1}{T} \sum_{t=1}^{T} H(y|x, \theta_t), \text{ or } U_a = \sigma(x)^2 \]

• Predictive uncertainty

\[ U_p = H\left(\frac{1}{T} \sum_{t=1}^{T} p(y|x, \theta_t)\right) \]

• Epistemic uncertainty

\[ U_e = H \left(\frac{1}{T} \sum_{t=1}^{T} p(y|x, \theta_t)\right) - \frac{1}{T} \sum_{t=1}^{T} H(y|x, \theta_t) \]
Examples

Aleatoric uncertainty: inherent noisy region
Epistemic uncertainty: hard samples
Predictive uncertainty: both

Outline

• Motivation
• Background
• Aleatoric uncertainty and Epistemic Uncertainty
• Uncertainty Approximation
  ✓ Ensemble solutions
  ✓ Generative model solutions
  ✓ Bayesian latent variable model solutions
• Experiments
• Discussion and Conclusion
Generative model solutions

• Latent variable models
• Energy-based model
Latent variable models

• A latent variable is a variable which is not directly observable and is assumed to affect the observable variables (manifest variables)

• A latent variable model is a statistical model that relates a set of observable variables to a set of latent variables (Latent Variable Models and Factor Analysis, David J. Bartholomew et. al, 2011)

• More formally, a latent variable model (LVM) is a probability distribution over two sets of variables $x$ and $z$ as  $p_\theta(x, z)$, or over three sets of variables $x$, $y$ and $z$ as $p_\theta(y|x, z)$ for the conditional version of the latent variable models with the conditional variable $x$. 

$$
\begin{align*}
  p_\phi(z|x) \\
  x & \quad z \\
  p_\theta(x|z) \\
\end{align*}
$$

$$
\begin{align*}
  p_\phi(z|x, y) \\
  x & \quad y \\
  p_\theta(y|x, z) \\
\end{align*}
$$
Latent variable model solutions

• Predictive distribution with extra latent variable $z$

$$p(y|x) = \int p_\theta(y|x,z)p(\theta)p(z)d\theta dz$$

Regression Likelihood:

$$p_\theta(y|x, z) = \mathcal{N}(f_\theta(x, z), \Sigma)$$

Classification Likelihood:

$$p_\theta(y|x, z) = \text{Softmax}(f_\theta(x, z)/\exp(\sigma^2))$$

Uncertainty origin: $(\epsilon / \Sigma), z, p(\theta)$

Aleatoric uncertainty

Epistemic uncertainty
Latent variable model solutions

• CVAE—Conditional Variational Auto-encoder
  ➢ Auto-Encoding Variational Bayes. Kingma, Diederik et. al. ICLR. 2014

• CGAN—Conditional Generative Adversarial Nets

• ABP—Alternating Back-Propagation
  ➢ Alternating Back-Propagation for Generator Network. Tian Han et. al. AAAI. 2016
Latent variable model solutions—VAE/CVAE

• VAE: unsupervised feature representation

\[ p_\phi(z|x) \quad \text{and} \quad p_\theta(x|z) \]

• CVAE: latent feature exploring

\[ p_\phi(z|x, y) \quad \text{and} \quad p_\theta(y|x, z) \]
• CVAE: conditional directed graph model

\[
\mathcal{L}(\theta, \phi; x) = \mathbb{E}_{q_{\phi}(z|x,y)} \left[ \log \left( p_{\theta}(y|x,z) \right) \right] - D_{KL}(q_{\phi}(z|x,y) \| p_{\theta}(z|x))
\]

Latent variable model solutions—GAN/CGAN

• GAN: min-max game
  • discriminator seeks to maximize the probability assigned to real and fake images

\[
\max(\log(D(x)) + \log(1 - D(G(z)))) \quad \text{or} \quad \min(\mathcal{L}_{ce}(D(x), 1) + \mathcal{L}_{ce}(D(G(z)), 0))
\]

• generator learns to generate samples that have a low possibility of being fake by minimizing the log of the inverse probability predicted by the discriminator for fake images.

\[
\min(\log(1 - D(G(z))))
\]
• CGAN for dense prediction

\[ \mathcal{L}_G = \mathcal{L}_{CE}(f_G(x, z), y) + \lambda \mathcal{L}_{CE}(D(f_G(x, z), 1)) \]
\[ \mathcal{L}_D = \mathcal{L}_{CE}(D(y), 1) + \mathcal{L}_{CE}(D(f_G(x, z), 0)) \]

Adversarial Learning for Semi-Supervised Semantic Segmentation. Wei-Chih Hung et. al. BMVC 2018
Explain ABP

• VAE—Inference model is needed
• GAN—Discriminator is needed with no inference model

• ABP—Alternating Back-Propagation
  ➢ Infer the latent variable directly from the true posterior distribution
  ➢ No extra parameters
Alternating Back-Propagation

• Define the generative model as:
  \[ z \sim p(z) = \mathcal{N}(0,1) \]
  \[ y = f_\theta(x, z) + \epsilon, \epsilon \sim \mathcal{N}(0, \Sigma) \]

• The conditional distribution of \( y \) is defined as:
  \[ p_\theta(y|x) = \int p(z)p_\theta(y|x, z)dz \]

• Define the observed data log-likelihood as \( \log(p_\theta(y|x)) \), its gradient is then:
  \[ \frac{\partial}{\partial \theta} \log(p_\theta(y|x)) = \mathbb{E}_{p_\theta(z|x,y)} \left[ \frac{\partial}{\partial \theta} \log(p_\theta(y, z|x)) \right] \]
Alternating Back-Propagation

• The observed data log-likelihood:

\[
\frac{\partial}{\partial \theta} \log(p_\theta(y|x)) = \mathbb{E}_{p_\theta(z|x,y)} \left[ \frac{\partial}{\partial \theta} \log(p_\theta(y, z|x)) \right]
\]

where the expectation term can be approximated with Langevin dynamics based MCMC (a gradient based MCMC) to sample \( z \) from it’s true posterior distribution via:

\[
z_{t+1} = z_t + s^2 \left[ \frac{\partial}{\partial z} \log p_\theta(y, z_t|x) \right] + sN(0,1)
\]

With:

\[
\frac{\partial}{\partial z} \log p_\theta(y, z_t|x) = \frac{1}{\sigma^2} (y - f_\theta(x, z)) \frac{\partial}{\partial z} f_\theta(x, z) - z
\]

\( t \): time step for Langevin sampling \quad \( s \): step size
• ABP for dense prediction

Different from VAE or GAN that involves extra modules (inference model for VAE and discriminator for GAN), ABP sample directly from the true posterior distribution via gradient based MCMC.
Energy-based model

• Latent variable model
  ➢ estimate the distribution of the latent variable
  ➢ Estimate the predictive distribution

• Energy-based model
  ➢ Estimate predictive distribution directly.
Energy-based model solution

• EBM: energy-based model, learns an energy function to assign low energy to in-distribution samples and high energy for others.

• Energy-based model:

\[ p_\gamma(y|x) = \frac{p_\gamma(y, x)}{\int p_\gamma(y, x) dy} = \frac{1}{Z(x; \gamma)} \exp[-U_\gamma(y, x)] \]

\( U_\gamma(y, x) \) : the energy function

\( Z(x; \gamma) = \int \exp[-U_\gamma(y, x)] dy \) : the normalizing constant

A tutorial on energy-based learning. Yann LeCun. 2006
Energy-based model solution

• Energy-based model:

\[
 p_\gamma(y|x) = \frac{p_\gamma(y, x)}{\int p_\gamma(y, x)dy} = \frac{1}{Z(x; \gamma)} \exp[-U_\gamma(y, x)]
\]

When the energy function \( U_\gamma \) is learned and input image \( x \) is given, prediction can be achieved via Langevin sampling: \( y \sim p_\gamma(y|x) \):

\[
y_{t+1} = y_t - \frac{\sigma^2}{2} \frac{\partial U_\gamma(y_t, x)}{\partial y} + \delta \Delta_t, \Delta_t \sim \mathcal{N}(0,1)
\]

Cooperative Training of Descriptor and Generator Networks. Xie, Jianwen et. al. TPAMI. 2018
Energy-based model solution

• EBM: 1) start point of Langevin sampling, 2) train the energy function $U_\gamma$

Start point:
1) Any deterministic model $f_\theta(x)$
2) Any latent variable model $f_\theta(x, z)$

Learn $U_\gamma$ : maximum likelihood estimation

$$
\Delta \gamma \approx \frac{1}{N} \sum_{i=1}^{N} \frac{\partial}{\partial \gamma} U_\gamma(f_\theta(x_i), x_i) - \frac{1}{N} \sum_{i=1}^{N} \frac{\partial}{\partial \gamma} U_\gamma(y_i, x_i)
$$
Outline

• Motivation
• Background
• Aleatoric uncertainty and Epistemic Uncertainty
• Uncertainty Approximation
  ✓ Ensemble solutions
  ✓ Generative model solutions
    ✓ Bayesian latent variable model solutions
• Experiments
• Discussion and Conclusion
Bayesian latent variable model solutions

• Bayesian Neural Network
• Latent variable model

Predictive distribution:

\[ p(y|x) = \int p_\theta(y|x,z)p(\theta)p(z)d\theta dz \]

Regression Likelihood:

\[ p_\theta(y|x,z) = \mathcal{N}(f_\theta(x,z), \Sigma) \]

Classification Likelihood:

\[ p_\theta(y|x,z) = \text{Softmax}(f_\theta(x,z)/\exp(\sigma^2)) \]

Uncertainty origin: \((\varepsilon, \Sigma), z, p(\theta)\)

Aleatoric uncertainty

Epistemic uncertainty
Generative model based Uncertainty computation—regression

- Aleatoric uncertainty: \( U_a = \frac{1}{T} \sum_{t=1}^{T} H(y|x, \theta_t) \), or \( U_a = \sigma(x)^2 \)
- Epistemic uncertainty:
  \[
  U_e = \mathbb{E}_{p(\theta|D)}[p(y|x, \theta)^2] - (\mathbb{E}_{p(\theta|D)}[p(y|x, \theta)])^2
  \]
  or
  \[
  U_e = H\left(\frac{1}{T} \sum_{t=1}^{T} p(y|x, \theta_t)\right) - \frac{1}{T} \sum_{t=1}^{T} H(y|x, \theta_t)
  \]
- Predictive uncertainty:
  \[
  U_p = U_a + U_e
  \]
Generative model based Uncertainty computation--classification

- Aleatoric uncertainty
  \[ U_a = \frac{1}{T} \sum_{t=1}^{T} H(y|x, \theta_t), \text{ or } U_a = \sigma(x)^2 \]

- Predictive uncertainty
  \[ U_p = H\left(\frac{1}{T} \sum_{t=1}^{T} p(y|x, \theta_t)\right) \]

- Epistemic uncertainty
  \[ U_e = H\left(\frac{1}{T} \sum_{t=1}^{T} p(y|x, \theta_t)\right) - \frac{1}{T} \sum_{t=1}^{T} H(y|x, \theta_t) \]
Break
Outline

• Motivation
• Background
• Aleatoric uncertainty and Epistemic Uncertainty
• Uncertainty Approximation
  ✓ Ensemble solutions
  ✓ Generative model solutions
  ✓ Bayesian latent variable model solutions
• Experiments
• Discussion and Conclusion
Experiments--Uncertainty quality measure?

• Expected calibration error
  ➢ On Calibration of Modern Neural Networks. Chuan Guo et. al. ICML. 2017

• Patch accuracy vs patch uncertainty

• Evaluation on out-of-distribution samples
Experiments--Tasks

• Camouflaged object detection
• Salient object detection
COD

- Where is the camouflaged object
Camouflaged object detection

**TABLE 1**
Ensemble based solutions for **camouflaged object detection**. ↑ indicates the higher the score the better, and vice versa for ↓.

<table>
<thead>
<tr>
<th>Method</th>
<th>CAMO [82]</th>
<th>CHAMELEON [83]</th>
<th>COD10K [71]</th>
<th>NC4K [84]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$F_\beta \uparrow$</td>
<td>$\mathcal{M} \downarrow$</td>
<td>$F_\beta \uparrow$</td>
<td>$\mathcal{M} \downarrow$</td>
</tr>
<tr>
<td>Base</td>
<td>.757</td>
<td>.079</td>
<td>.848</td>
<td>.029</td>
</tr>
<tr>
<td>MD</td>
<td>.767</td>
<td>.080</td>
<td>.842</td>
<td>.028</td>
</tr>
<tr>
<td>DE</td>
<td>.729</td>
<td>.088</td>
<td>.846</td>
<td>.030</td>
</tr>
</tbody>
</table>

**TABLE 3**
Generative model based solutions for **camouflaged object detection**. ↑ indicates the higher the score the better, and vice versa for ↓.

<table>
<thead>
<tr>
<th>Method</th>
<th>CAMO [82]</th>
<th>CHAMELEON [83]</th>
<th>COD10K [71]</th>
<th>NC4K [84]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$F_\beta \uparrow$</td>
<td>$\mathcal{M} \downarrow$</td>
<td>$F_\beta \uparrow$</td>
<td>$\mathcal{M} \downarrow$</td>
</tr>
<tr>
<td>Base</td>
<td>.757</td>
<td>.079</td>
<td>.848</td>
<td>.029</td>
</tr>
<tr>
<td>CVAE</td>
<td>.758</td>
<td>.081</td>
<td>.848</td>
<td>.030</td>
</tr>
<tr>
<td>CGAN</td>
<td>.762</td>
<td>.080</td>
<td>.852</td>
<td>.026</td>
</tr>
<tr>
<td>ABP</td>
<td>.756</td>
<td>.081</td>
<td>.846</td>
<td>.030</td>
</tr>
<tr>
<td>EBM</td>
<td>.777</td>
<td>.076</td>
<td>.844</td>
<td>.031</td>
</tr>
</tbody>
</table>

1. **Base**: the base model
2. **CVAE**: the CVAE based framework
3. **CGAN**: the CGAN based framework
4. **ABP**: the ABP based framework
5. **EBM**: the EBM based framework
Predictive Uncertainty-Ensemble
Predictive Uncertainty-Generative Model
Aleatoric Uncertainty-Ensemble
Aleatoric Uncertainty-Generative Model
Epistemic Uncertainty-Ensemble
Epistemic Uncertainty-Generative Model
Three types of uncertainty

<table>
<thead>
<tr>
<th>Image</th>
<th>GT</th>
<th>Pred</th>
<th>Predictive</th>
<th>Aleatoric</th>
<th>Epistemic</th>
<th>Pred</th>
<th>Predictive</th>
<th>Aleatoric</th>
<th>Epistemic</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Observations

• Aleatoric uncertainty focus on inherent noise, i.e. object boundaries
• Epistemic uncertainty highlight challenging pixels, representing our ignorance about which model generated the given dataset.
• COD: **aleatoric uncertainty** vs epistemic uncertainty
SOD

• Which one is salient?
Salient object detection

1. Base: the base model
2. MD: MC-dropout
3. DE: deep ensemble

TABLE 2
Ensemble based solutions for **salient object detection**. ↑ indicates the higher the score the better, and vice versa for ↓.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$F_B$ ↑ $M$ ↓</td>
<td>$F_B$ ↑ $M$ ↓</td>
<td>$F_B$ ↑ $M$ ↓</td>
<td>$F_B$ ↑ $M$ ↓</td>
</tr>
<tr>
<td>Base</td>
<td>.842 .037</td>
<td>.760 .055</td>
<td>.904 .030</td>
<td>.828 .064</td>
</tr>
<tr>
<td>MD</td>
<td>.854 .036</td>
<td>.763 .056</td>
<td>.911 .028</td>
<td>.840 .061</td>
</tr>
<tr>
<td>DE</td>
<td>.828 .040</td>
<td>.738 .061</td>
<td>.897 .031</td>
<td>.825 .065</td>
</tr>
</tbody>
</table>

TABLE 4
Generative model based solutions for **salient object detection**. ↑ indicates the higher the score the better, and vice versa for ↓.

<table>
<thead>
<tr>
<th>Method</th>
<th>DUTS [78]</th>
<th>DUT [80]</th>
<th>HKU-IS [81]</th>
<th>PASCAL [82]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$F_B$ ↑ $M$ ↓</td>
<td>$F_B$ ↑ $M$ ↓</td>
<td>$F_B$ ↑ $M$ ↓</td>
<td>$F_B$ ↑ $M$ ↓</td>
</tr>
<tr>
<td>Base</td>
<td>.842 .037</td>
<td>.760 .055</td>
<td>.904 .030</td>
<td>.828 .064</td>
</tr>
<tr>
<td>CVAE</td>
<td>.836 .037</td>
<td>.748 .055</td>
<td>.901 .030</td>
<td>.826 .063</td>
</tr>
<tr>
<td>CGAN</td>
<td>.846 .035</td>
<td>.752 .054</td>
<td>.905 .029</td>
<td>.828 .063</td>
</tr>
<tr>
<td>ABP</td>
<td>.829 .040</td>
<td>.740 .059</td>
<td>.889 .034</td>
<td>.818 .068</td>
</tr>
<tr>
<td>EBM</td>
<td>.834 .040</td>
<td>.744 .062</td>
<td>.900 .031</td>
<td>.829 .064</td>
</tr>
</tbody>
</table>

1. Base: the base model
2. CVAE: the CVAE based framework
3. CGAN: the CGAN based framework
4. ABP: the ABP based framework
5. EBM: the EBM based framework
Predictive Uncertainty-Ensemble
Predictive Uncertainty-Generative Model
Aleatoric Uncertainty-Ensemble
Aleatoric Uncertainty-Generative Model
Epistemic Uncertainty-Ensemble
Epistemic Uncertainty-Generative Model
Three types of uncertainty

<table>
<thead>
<tr>
<th>Image</th>
<th>GT</th>
<th>Pred</th>
<th>Predictive</th>
<th>Aleatoric</th>
<th>Epistemic</th>
<th>Pred</th>
<th>Predictive</th>
<th>Aleatoric</th>
<th>Epistemic</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

MC-dropout

CGAN
Observations

- Aleatoric uncertainty focus on inherent noise, i.e. object boundaries.
- Epistemic uncertainty highlight challenging pixels, representing our ignorance about which model generated the given dataset.
- SOD: aleatoric uncertainty vs epistemic uncertainty
Discussion

• Sampling-free uncertainty estimation
• Pixel-level uncertainty vs Instance-level uncertainty
• How to effectively use the produced uncertainty
• Model calibration and uncertainty estimation
• Out-of-distribution detection and uncertainty estimation
• Multi-modal/multi-task learning
• Semi-/weakly-supervised learning
• Effectiveness measure
Thanks

Contact: zjnwpu@gmail.com

Thanks Bushfire CoE for the support.

Code and tutorial material are available.