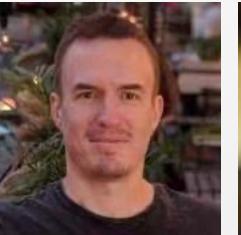
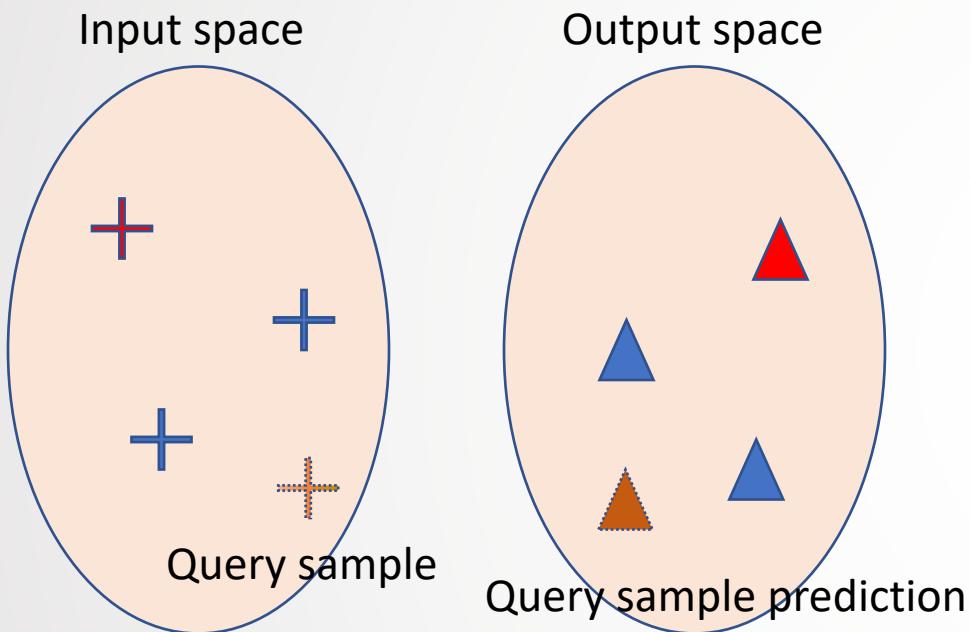


Uncertainty Estimation for Dense Prediction Tasks

**Jing Zhang, Yuchao Dai, Deng-Ping Fan, Nick Barnes, Peyman
Moghadam, Christian Walder, Mehrtash Harandi**

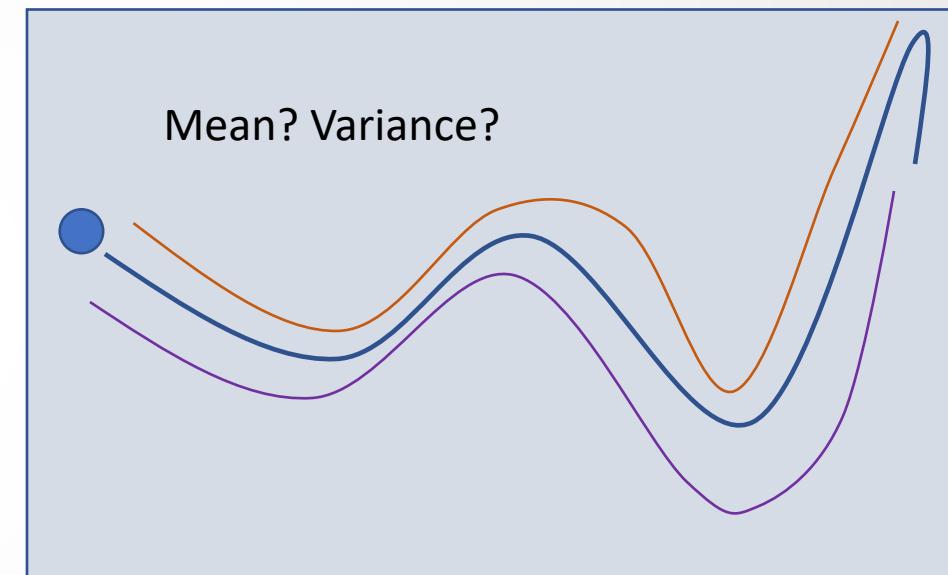


Uncertainty is inherent within Machine Learning



Easy sample?

Hard sample?



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- Motivation
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 - ✓ Ensemble solutions
 - ✓ Generative model solutions
 - ✓ Bayesian latent variable model solutions
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- 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 → Classification
- Salient object detection → Classification
- Monocular depth estimation → Regression

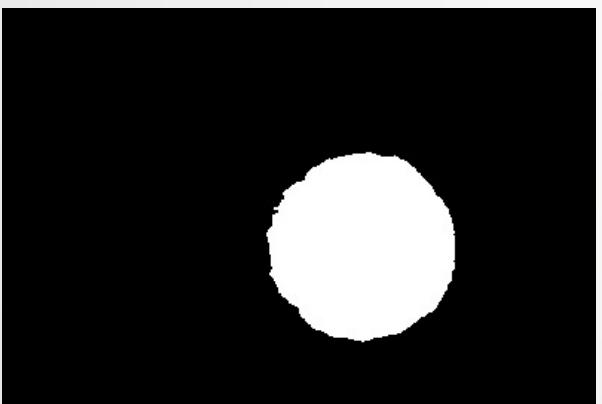
Motivation

- Which one is salient?



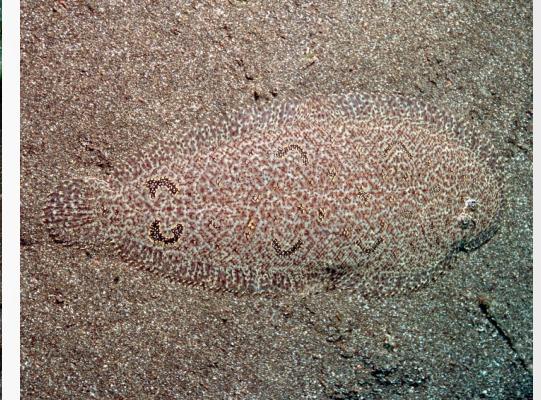
Motivation

- Which one is salient?



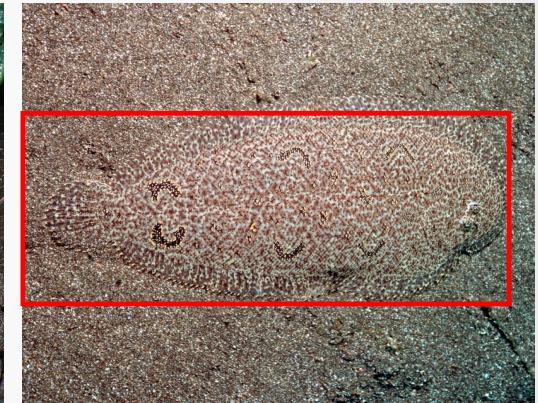
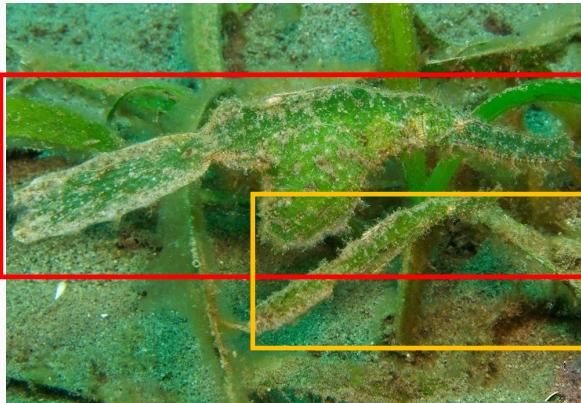
Motivation

- Where is the camouflaged object



Motivation

- Where is the camouflaged object



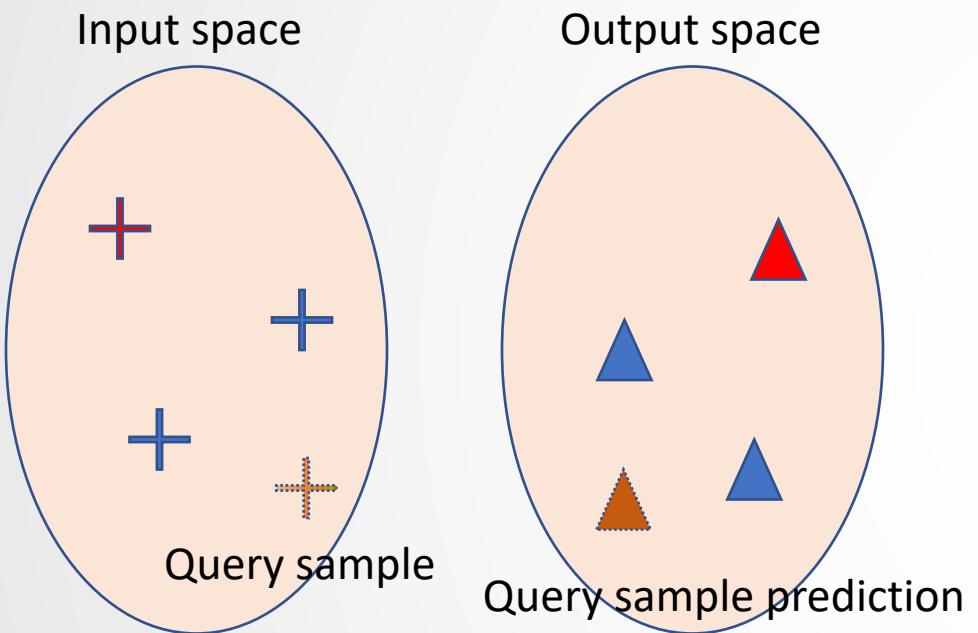
Motivation

- What's the exact distance?

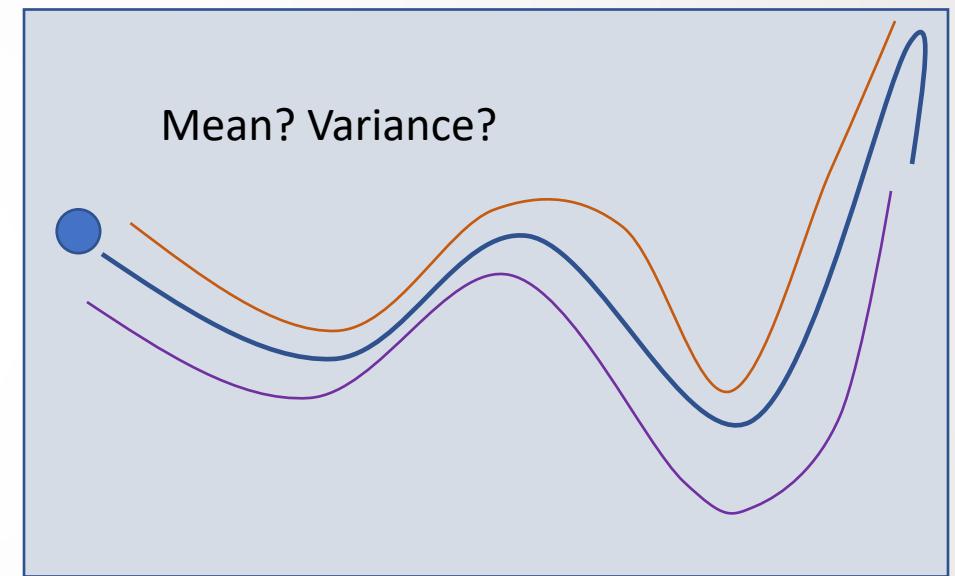
Motivation

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

Uncertainty: a mechanism to understand model limitations



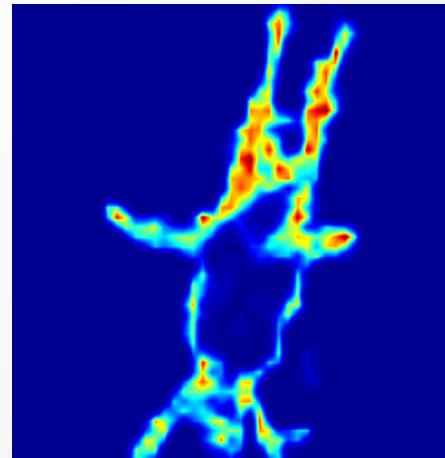
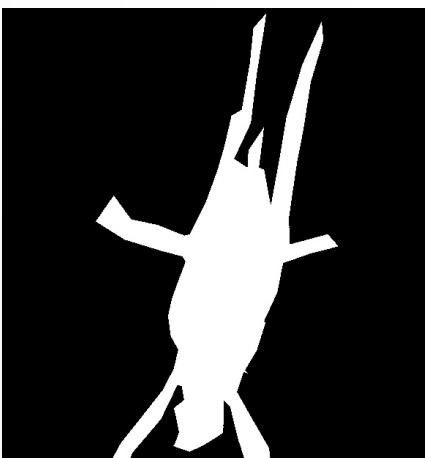
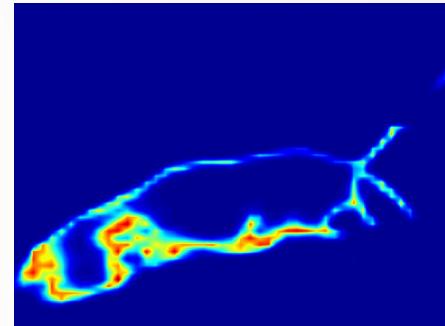
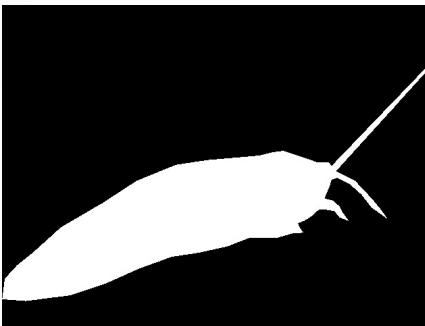
Confidence of $p(y|x)$?



Variance of prediction?

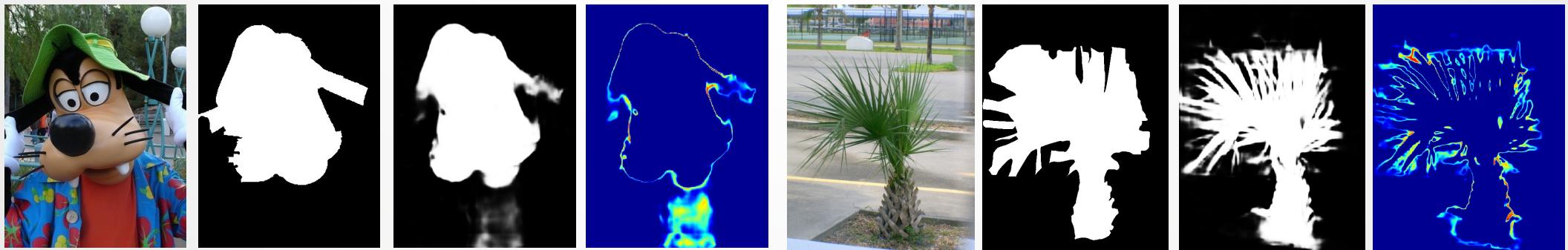
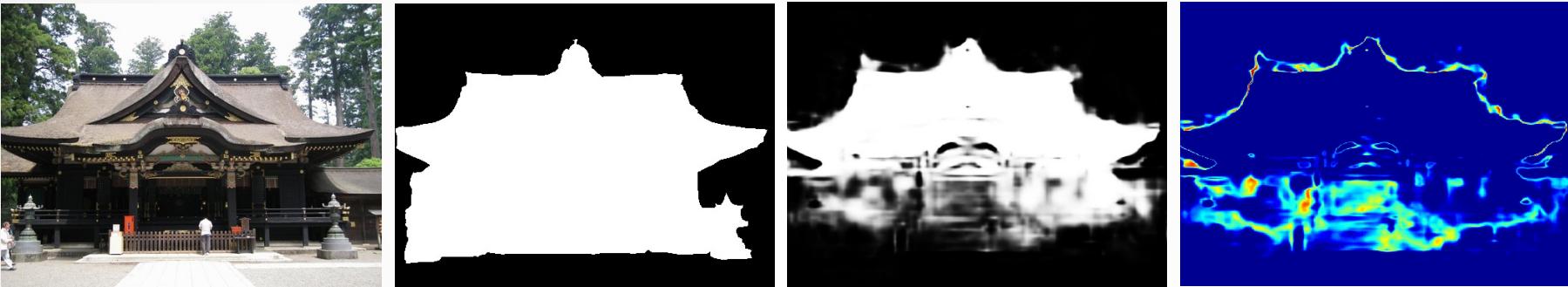
Motivation

- Camouflaged object detection



Motivation

- Salient object detection



Motivation

- Monocular depth estimation

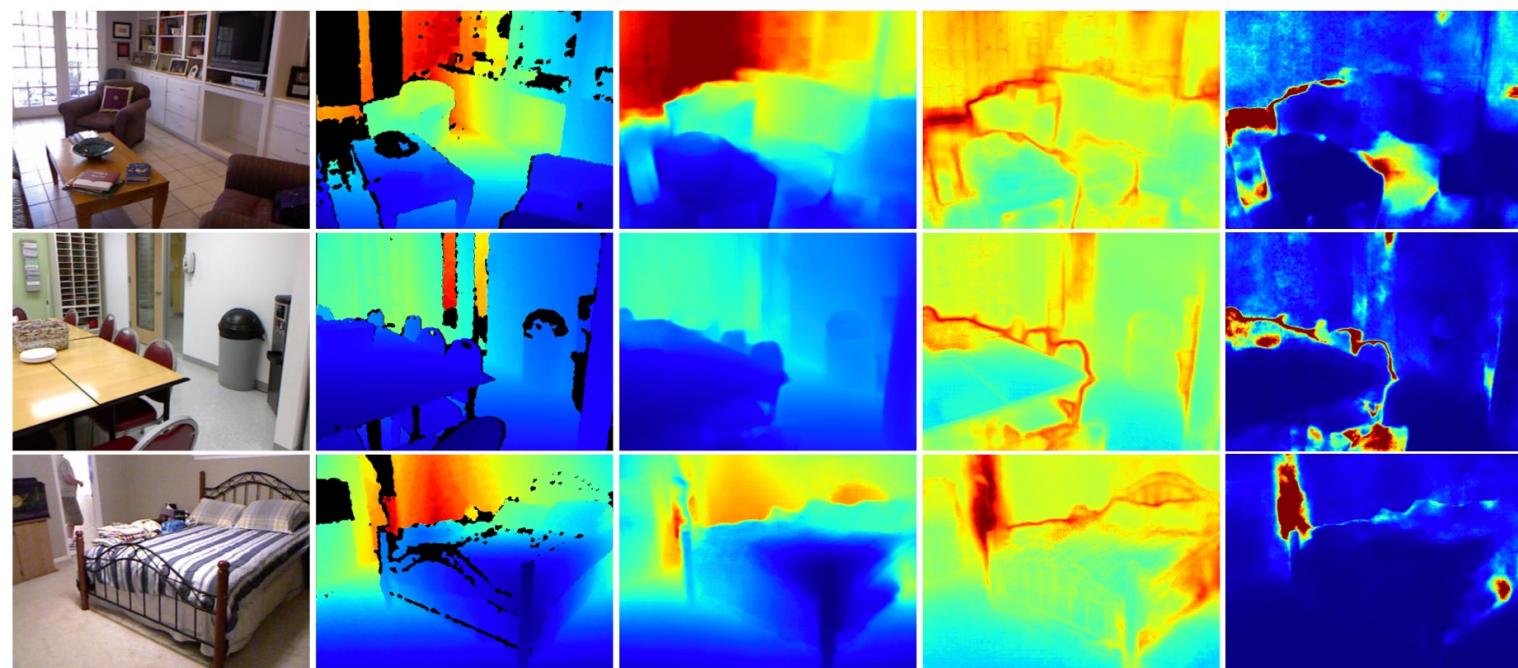
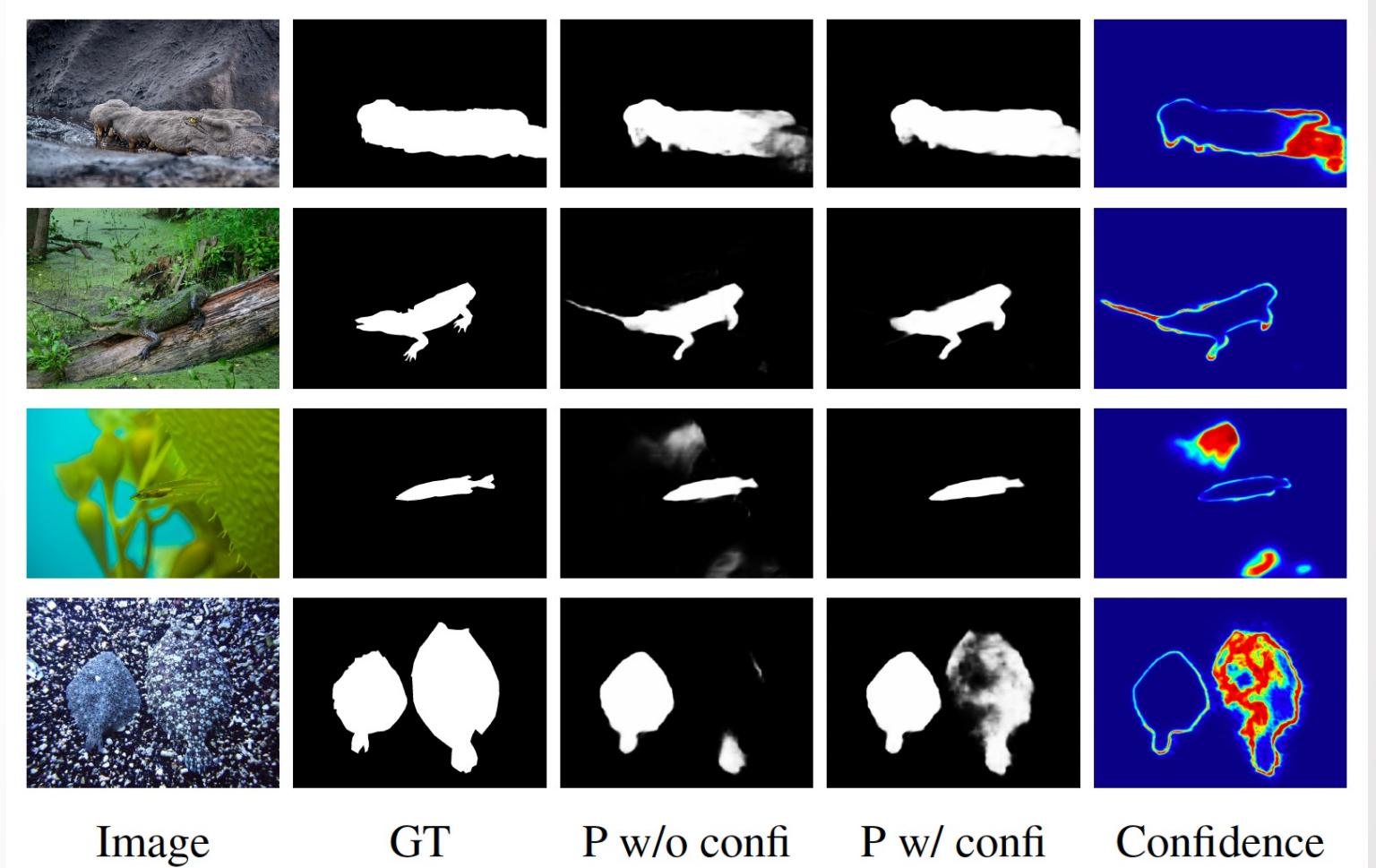


Figure 5: NYUv2 Depth results. From left: input image, ground truth, depth regression, aleatoric uncertainty, and epistemic uncertainty.

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

Motivation

- Well-calibrated model
- Hard-negative mining



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Background

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

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

Ambiguity comes from θ and the representativeness of the sampled dataset D .

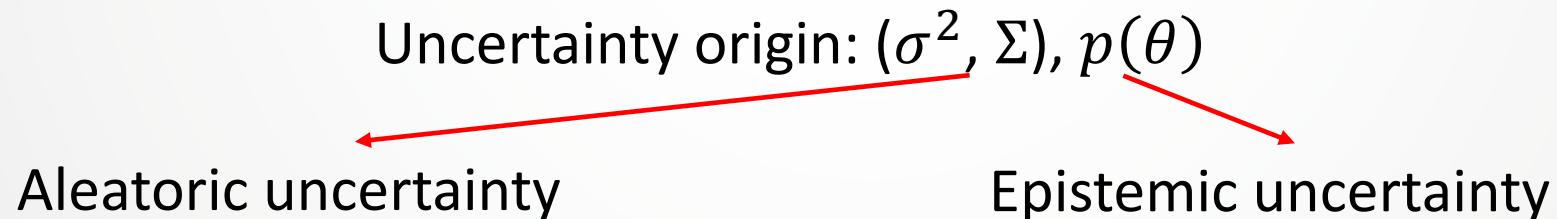
Background

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:

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



1. A. D. Kiureghian and O. Ditlevsen. “Aleatory or epistemic? does it matter?.
2. A. Kendall and Y. Gal. What uncertainties do we need in bayesiandeep learning for computer vision? 2017

Background

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

Aleatoric uncertainty: data related uncertainty

Epistemic uncertainty: model related uncertainty

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.

Image credit: Jonathan Ramkissoon

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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?

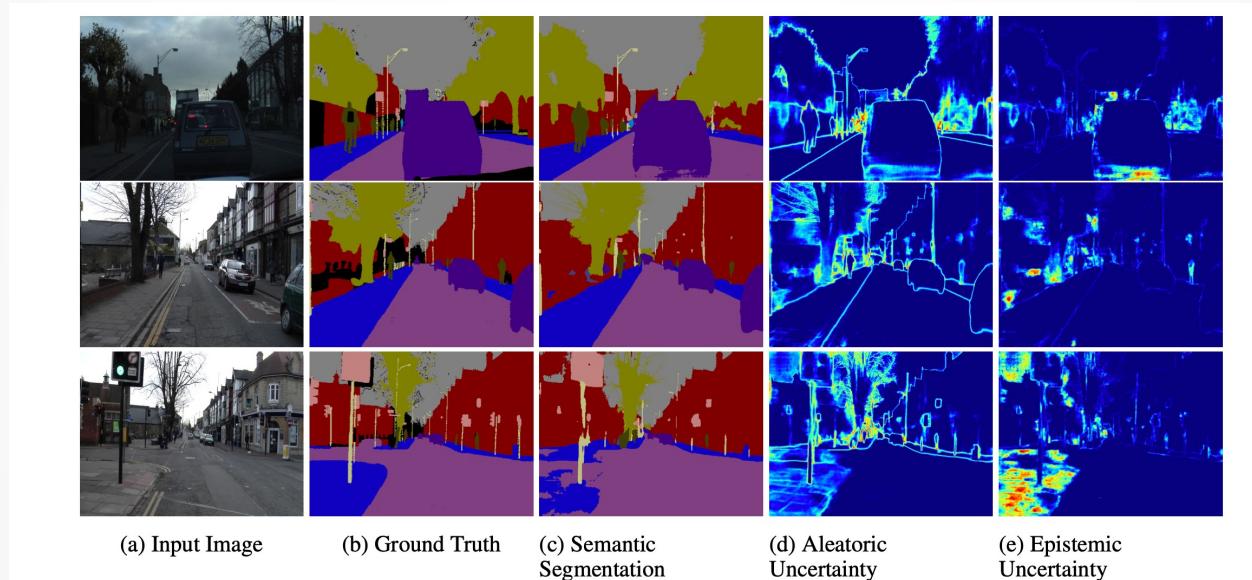


Figure 1: **Illustrating the difference between aleatoric and epistemic uncertainty** for semantic segmentation on the CamVid dataset [8]. *Aleatoric uncertainty* captures noise inherent in the observations. In (d) our model exhibits increased aleatoric uncertainty on object boundaries and for objects 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 bayesiandep learning for computer vision?” by A. Kendall and Y. Gal.

Aleatoric uncertainty modeling

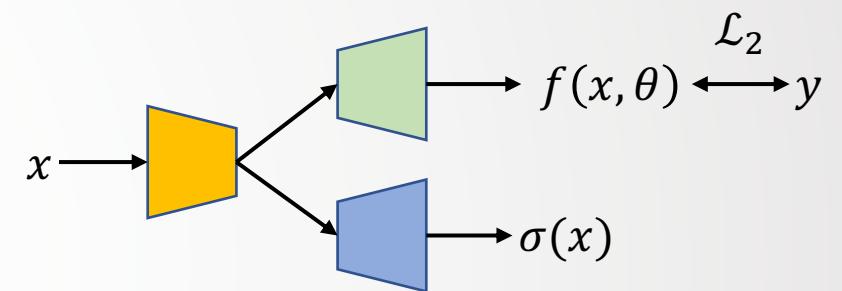
- Image-independent aleatoric uncertainty—homoscedastic uncertainty
- Image conditional aleatoric uncertainty---heteroscedastic uncertainty

Constant vs Learned

Aleatoric Uncertainty:

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

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



Basic assumption: $y = f(x, \theta) + n(x), n(x) \sim \mathcal{N}(0, \sigma(x)^2)$

For numerical stability, define $s_i = \log(\sigma(x)^2)$:

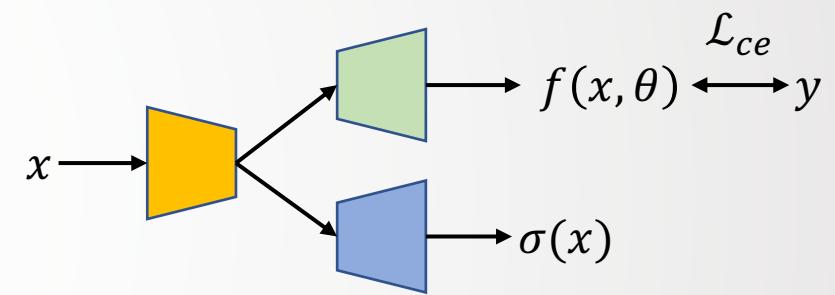
$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^N \left(\frac{1}{2} \exp(-s_i) \mathcal{L}_2 + \frac{1}{2} s_i \right)$$

$$U_a = \sigma(x)^2$$

Aleatoric Uncertainty:

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 $T = \exp(\sigma^2)$:

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

Trivial solution:

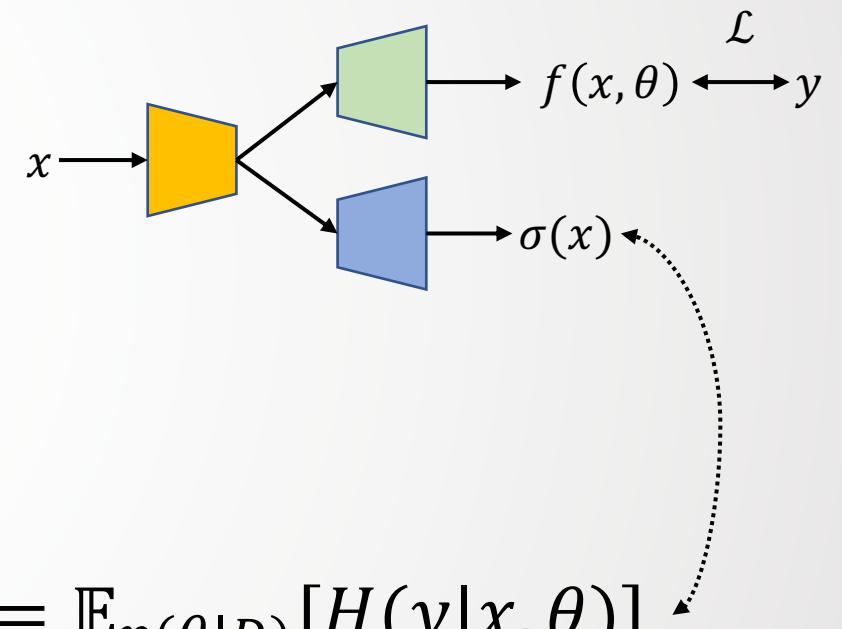
$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^N \left(\frac{1}{2\sigma(x)^2} \mathcal{L}_{ce} + \frac{1}{2} \log(\sigma(x)^2) \right)$$

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

$$\sigma(x)=1 !!$$

Solve it:

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



Epistemic Uncertainty

- Residual of predictive uncertainty and aleatoric uncertainty
- Mutual information of model prediction and model parameters

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

predictive uncertainty $U_p = H(y|x)$

Epistemic Uncertainty

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

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

The predictive uncertainty is then:

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

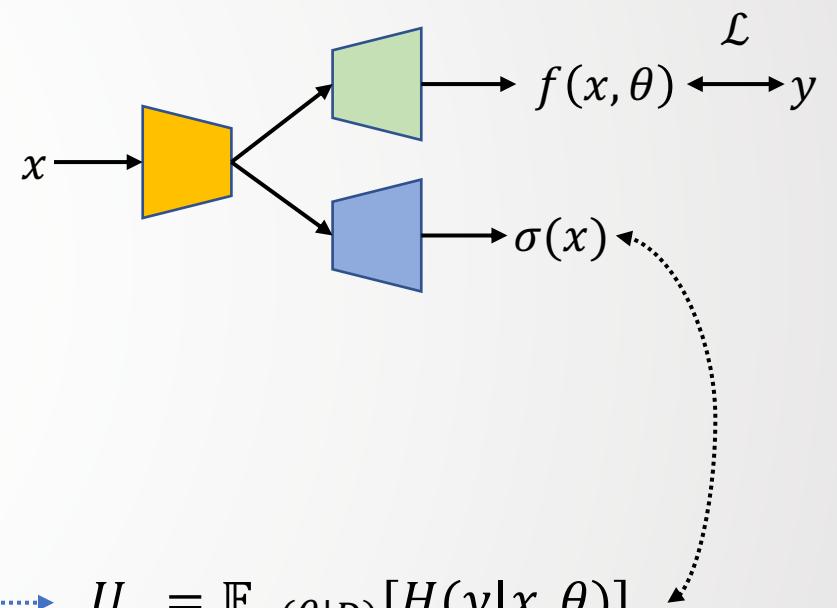
Epistemic Uncertainty

Otherwise:

$$U_p = H(y|x)$$

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

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



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Uncertainty Approximation

- Recall: $U_e = U_p - U_a = H(y|x) - \mathbb{E}_{p(\theta|D)}[H(y|x, \theta)] = I(y, \theta|x)$
- Intractable $p(\theta|D)$
- Approximation for Bayesian posterior inference
 - Variational inference
Approximate $p(\theta|D)$ with easy-controlled distribution $q_\gamma(\theta)$, γ : variational parameters. MC-dropout----Ensemble based solutions
 - MCMC
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
- Bayesian latent variable model solutions

1. Yarin Gal, Zoubin Ghahramani. Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. 2016
2. *Balaji Lakshminarayanan, etc.* Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles. 2017
3. Stefan Depeweg, etc. Decomposition of Uncertainty in Bayesian Deep Learning for Efficient and Risk-sensitive Learning.
4. Kuan-Chieh Wang, etc.. Adversarial distillation of Bayesian neural network posteriors. 2018

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Ensemble Solutions

- 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 θ_t is sampled from the approximate posterior distribution $q_\gamma(\theta)$

Ensemble Solutions

- MC dropout:

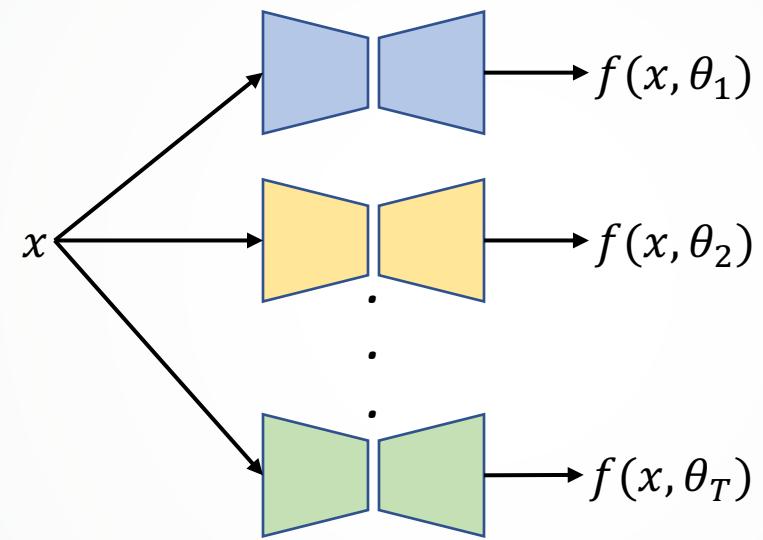
Implementation details: add dropout before every weighted layer during both training and testing.

Pros: easy to implement, no additional parameters

Cons: cannot control the dropout mask, mode collapse issue

Ensemble Solutions

- Deep ensemble



Ensemble Solutions

- Deep ensemble

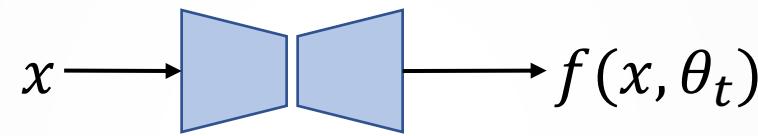
Implementation details: random initialization, multi-network, multi-head.

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



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

Uncertainty computation

- 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

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

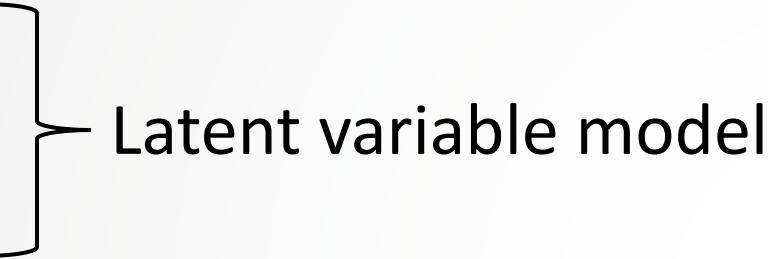
- Epistemic uncertainty

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

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Generative model solutions

- CVAE
 - CGAN
 - ABP
 - EBM: Predictive distribution estimation
- 

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

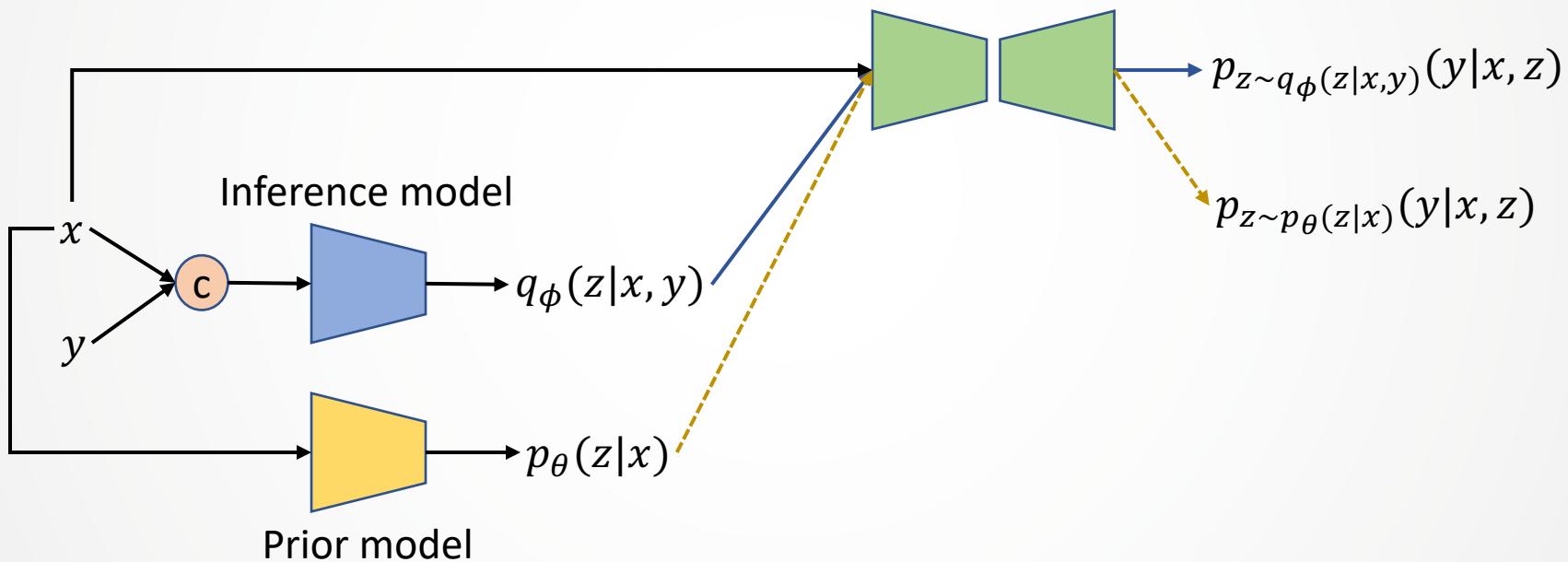
Epistemic uncertainty

Latent variable model solutions

- CVAE
 - CGAN
 - ABP
-
1. Kingma, Diederik and etc. Auto-Encoding Variational Bayes. 2014
 2. Sohn, Kihyuk and etc. Learning Structured Output Representation using Deep Conditional Generative Models. 2015
 3. Goodfellow, Ian and etc. Generative Adversarial Nets. 2014
 4. Mehdi Mirza, Simon Osindero. Conditional Generative Adversarial Nets. 2014
 5. Tian Han. Alternating Back-Propagation for Generator Network. 2016

Latent variable model solutions

- CVAE: conditional directed graph model



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

Latent variable model solutions

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

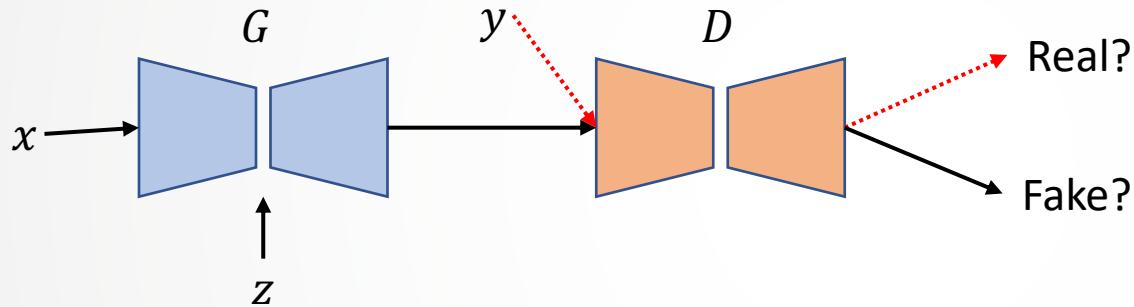
$$\max(\log(D(x)) + \log(1 - D(G(z)))) \text{ or } \min(\mathcal{L}_{ce}(D(x), 1) + \mathcal{L}_{ce}(D(G(z)), 0))$$

- 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.

$$\min(\log(1 - D(G(z))))$$

Latent variable model solutions

- CGAN for dense prediction



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

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

Latent variable model solutions

- ABP: alternating back-propagation, sampling the latent variable directly from the true posterior distribution via Langevin Dynamic based MCMC

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

With:

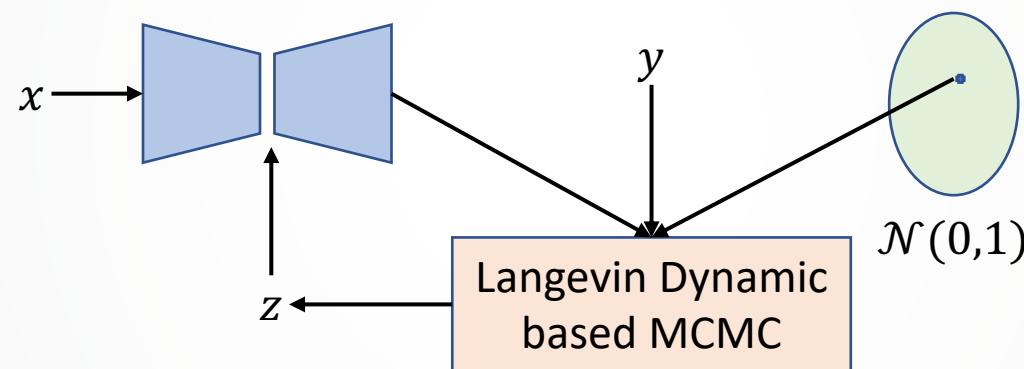
$$\frac{\partial}{\partial z} \log p_\theta(y, z_t | x) = \frac{1}{\sigma^2} (y - f_\theta(x, z)) \frac{\partial}{\partial z} f_\theta(x, z) - z$$

t : time step for Langevin sampling

s : step size

Latent variable model solutions

- 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 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

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_γ is learned and input image x is given, prediction can be achieved via Langevin sampling: $y \sim p_\gamma(y|x)$:

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

Energy-based model solution

- EBM: 1) start point of Langevin sampling, 2) train the energy function U_γ

Start point:

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

Learn U_γ : maximum likelihood estimation

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

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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:

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

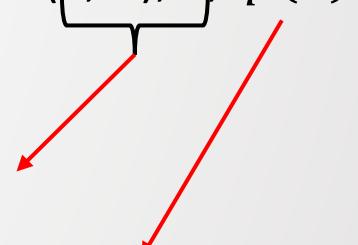
Classification Likelihood:

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

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

Aleatoric uncertainty

Epistemic uncertainty



Uncertainty computation

- 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

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

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Experiments--Uncertainty quality measure?

- Expected calibration error
- Patch accuracy vs patch uncertainty
- Evaluation on out-of-distribution samples

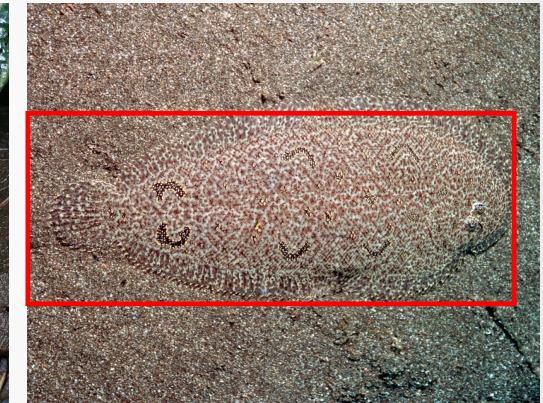
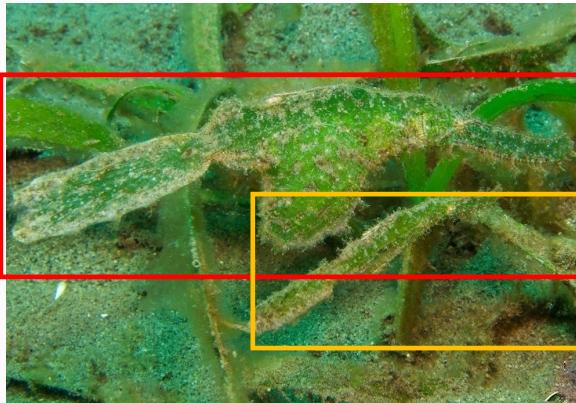
1. Jishnu Mukhoti and Yarin Gal. Evaluating Bayesian Deep Learning Methods for Semantic Segmentation. 2018
2. Chuan Guo and etc. On Calibration of Modern Neural Networks. 2017

Experiments--Tasks

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

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 ↓.

Method	CAMO [82]		CHAMELEON [83]		COD10K [71]		NC4K [84]	
	$F_\beta \uparrow$	$\mathcal{M} \downarrow$						
Base	.757	.079	.848	.029	.731	.035	.803	.048
MD	.767	.080	.842	.028	.731	.035	.803	.048
DE	.729	.088	.846	.030	.718	.037	.796	.051

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

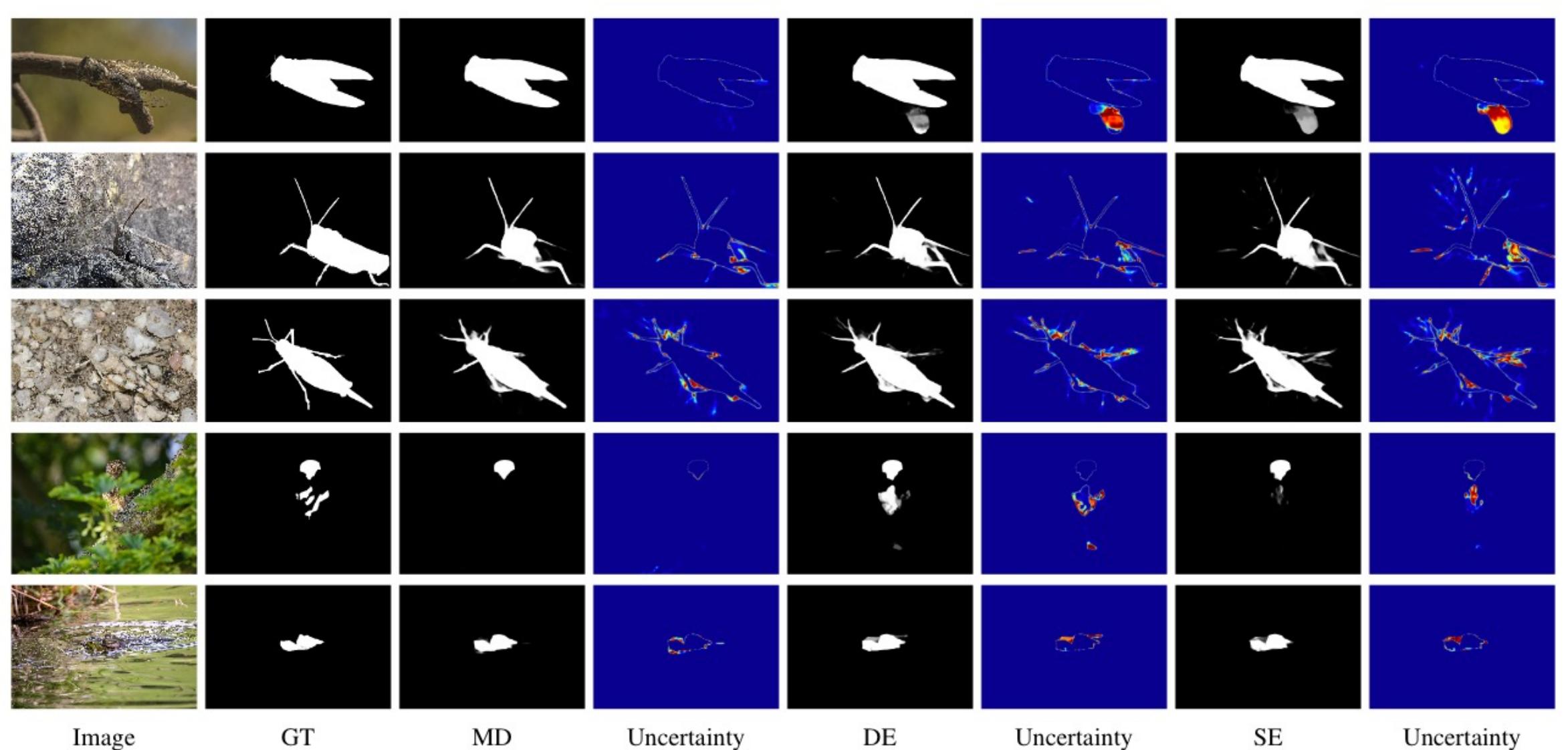
TABLE 3

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

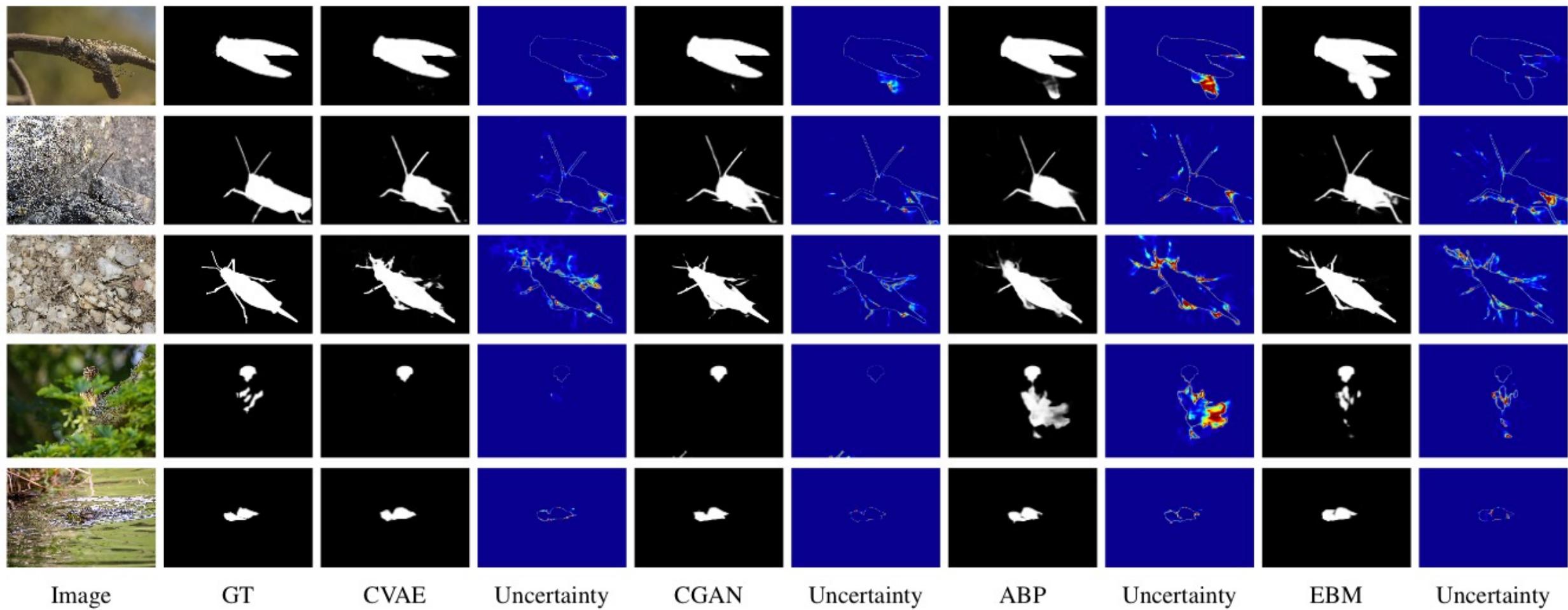
Method	CAMO [82]		CHAMELEON [83]		COD10K [71]		NC4K [84]	
	$F_\beta \uparrow$	$\mathcal{M} \downarrow$						
Base	.757	.079	.848	.029	.731	.035	.731	.035
CVAE	.758	.081	.848	.030	.731	.034	.802	.048
CGAN	.762	.080	.852	.026	.730	.034	.807	.048
ABP	.756	.081	.846	.030	.729	.034	.801	.047
EBM	.777	.076	.844	.031	.721	.038	.796	.050

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

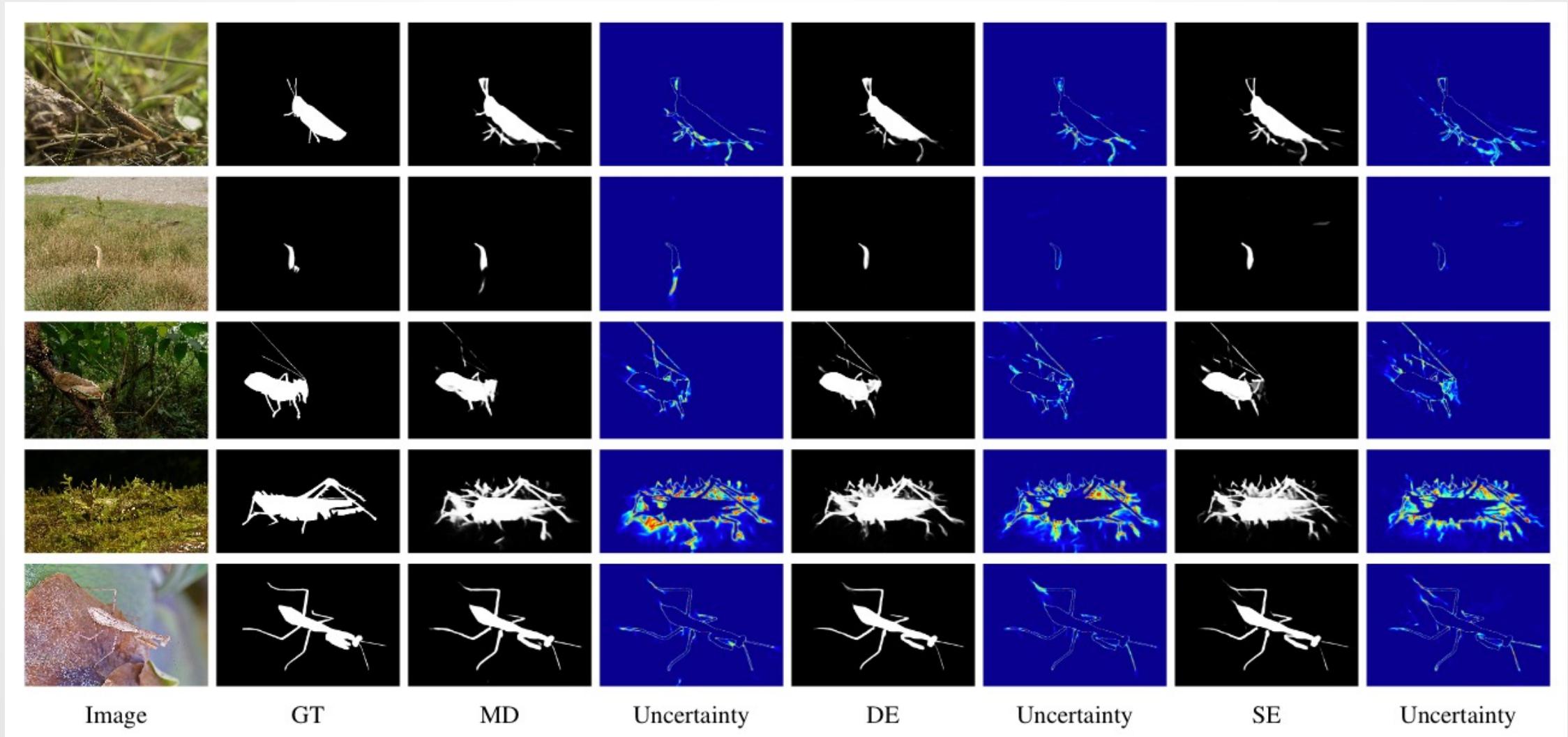
Predictive Uncertainty-Ensemble



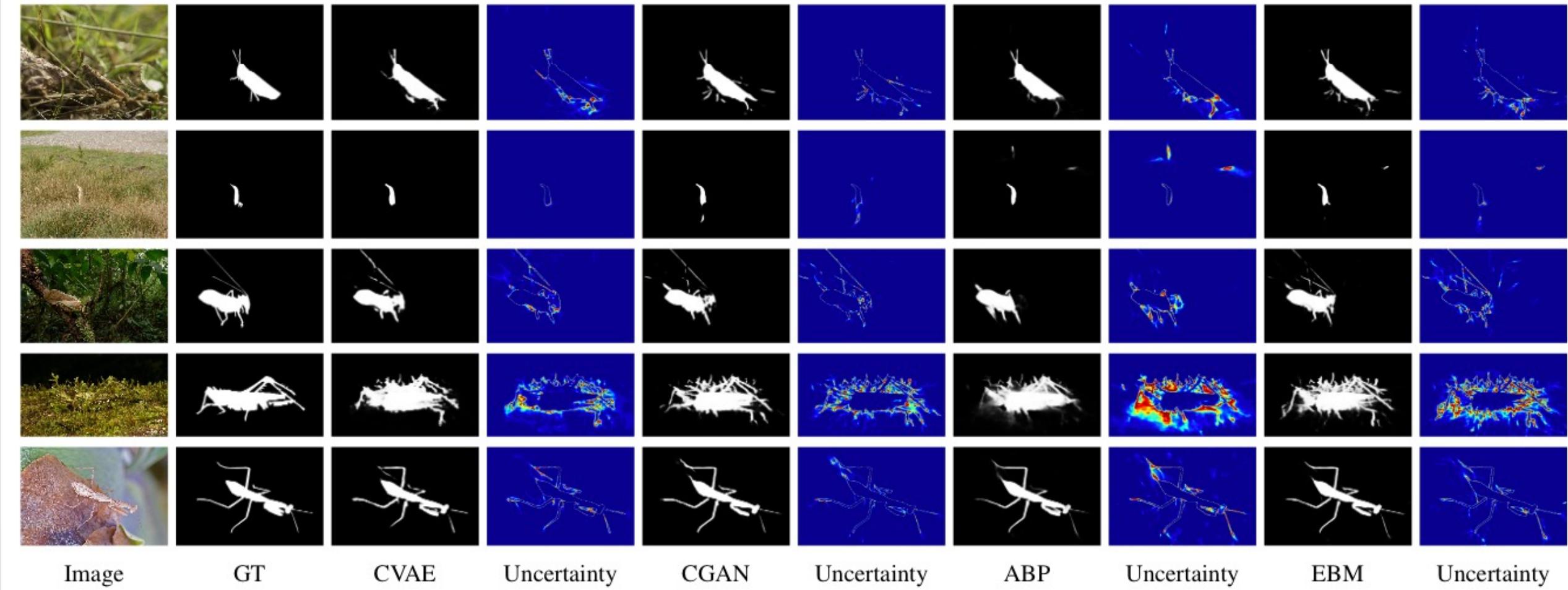
Predictive Uncertainty-Generative Model



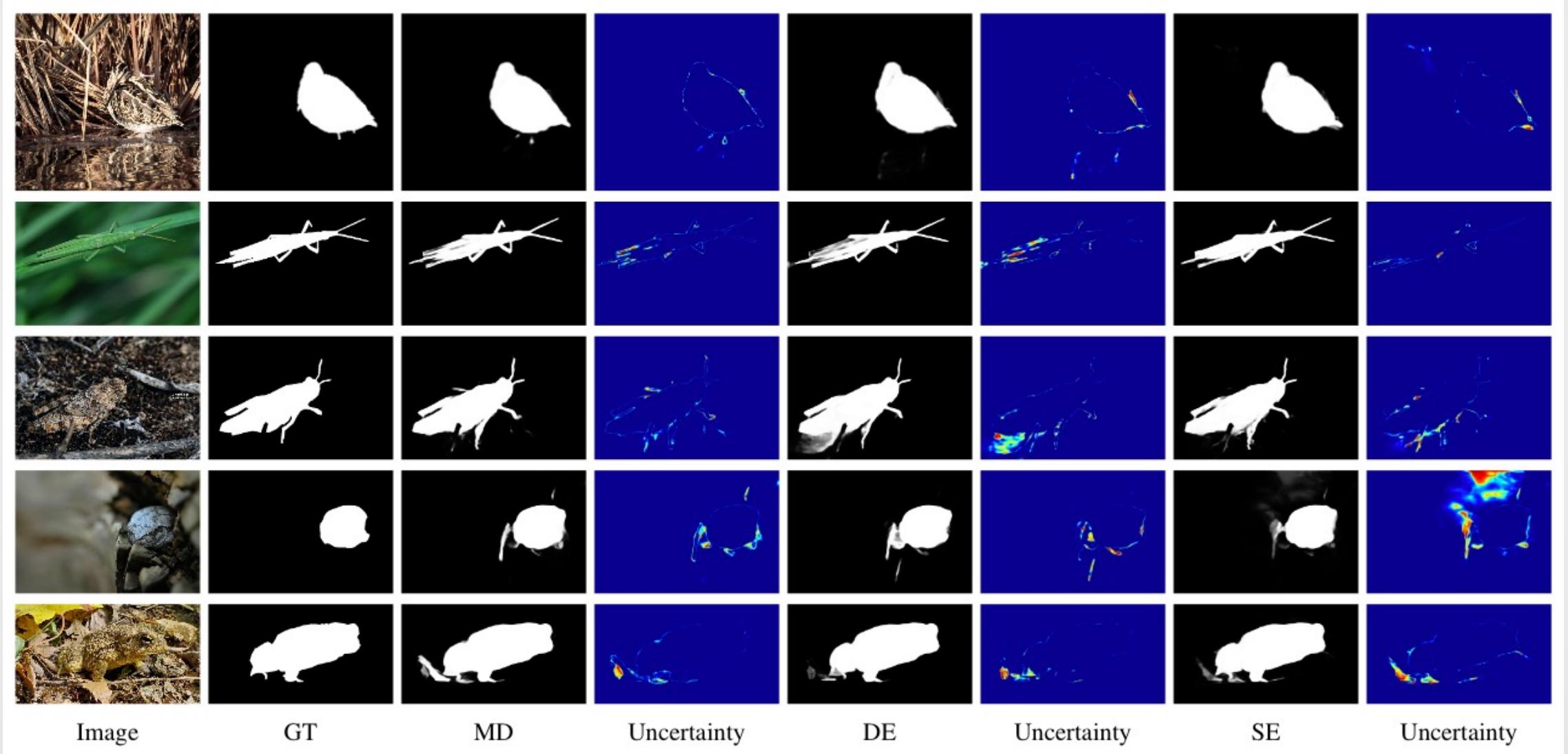
Aleatoric Uncertainty-Ensemble



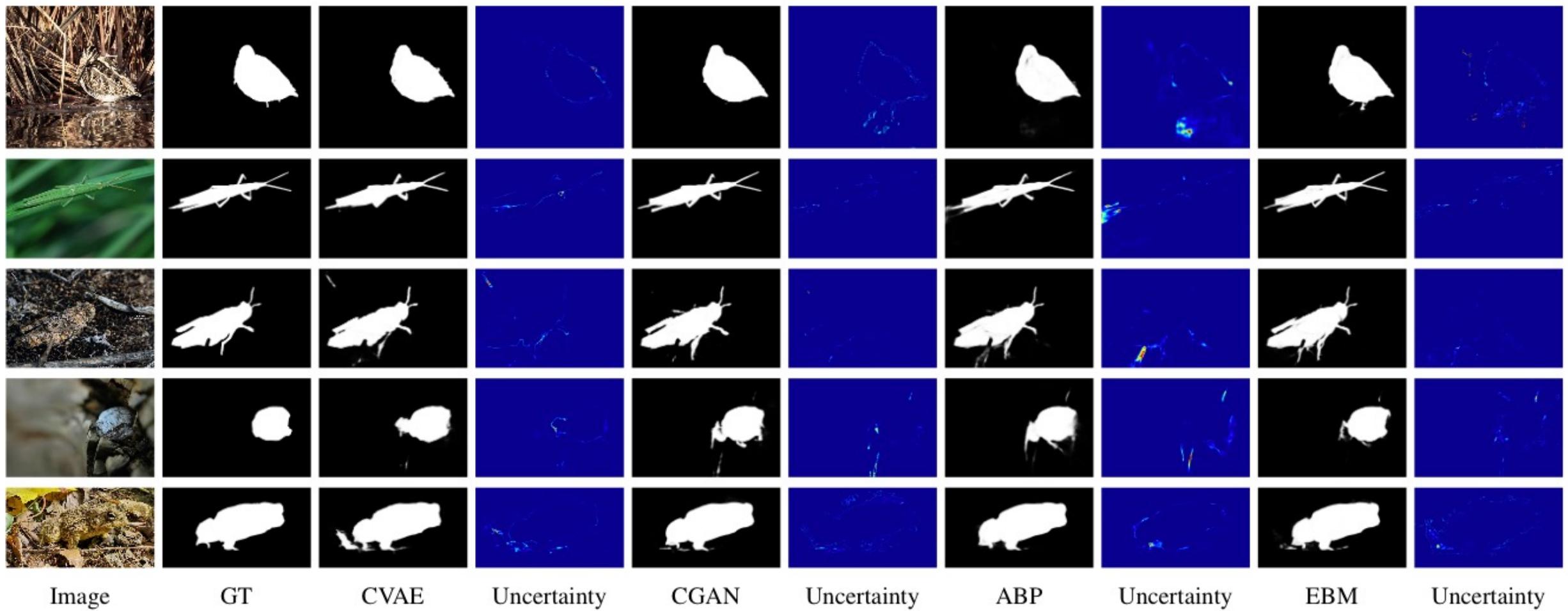
Aleatoric Uncertainty-Generative Model



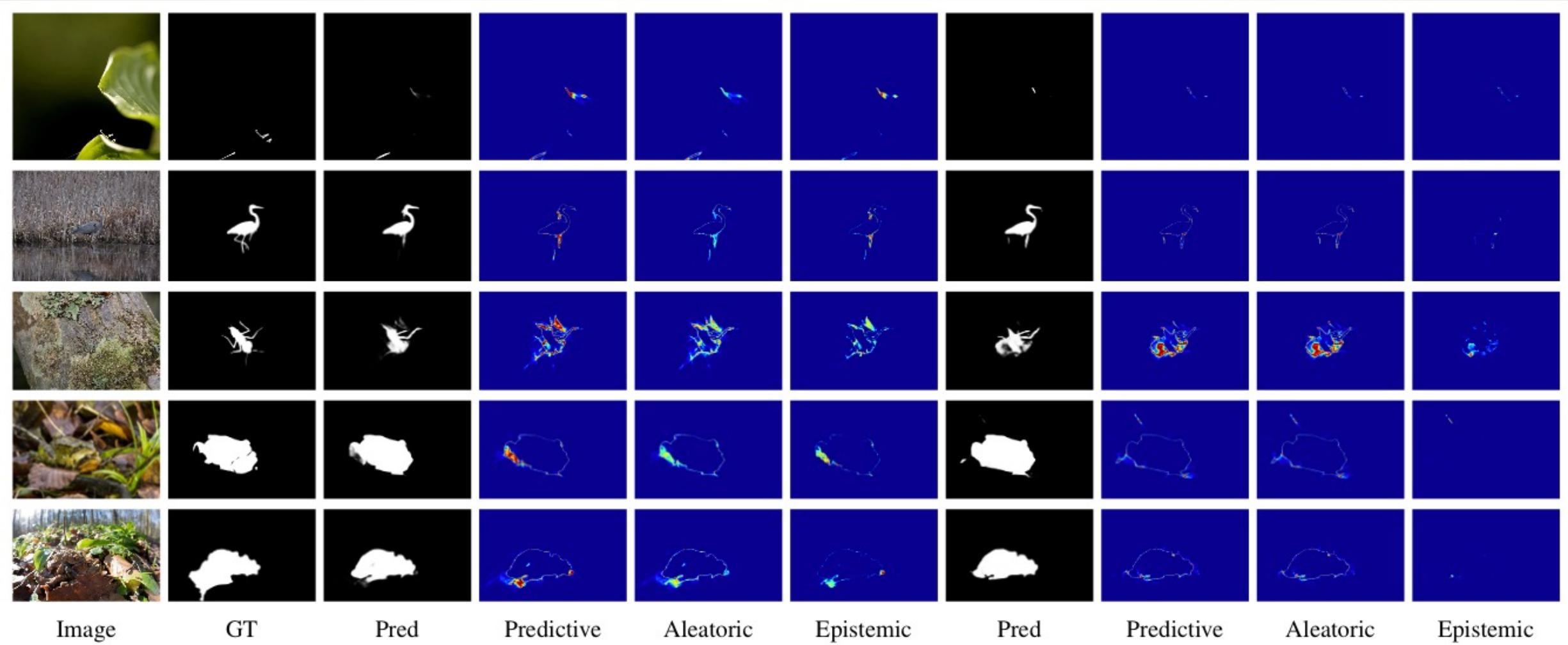
Epistemic Uncertainty-Ensemble



Epistemic Uncertainty-Generative Model



Three types of uncertainty

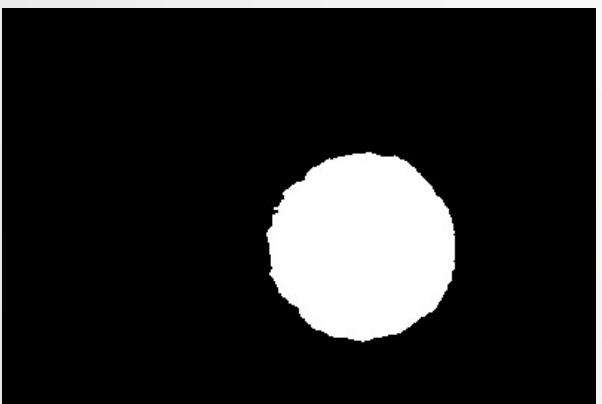


Observations

- 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

TABLE 2

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

Method	DUTS [78]		DUT [79]		HKU-IS [80]		PASCAL [81]	
	$F_\beta \uparrow$	$\mathcal{M} \downarrow$						
Base	.842	.037	.760	.055	.904	.030	.828	.064
MD	.854	.036	.763	.056	.911	.028	.840	.061
DE	.828	.040	.738	.061	.897	.031	.825	.065

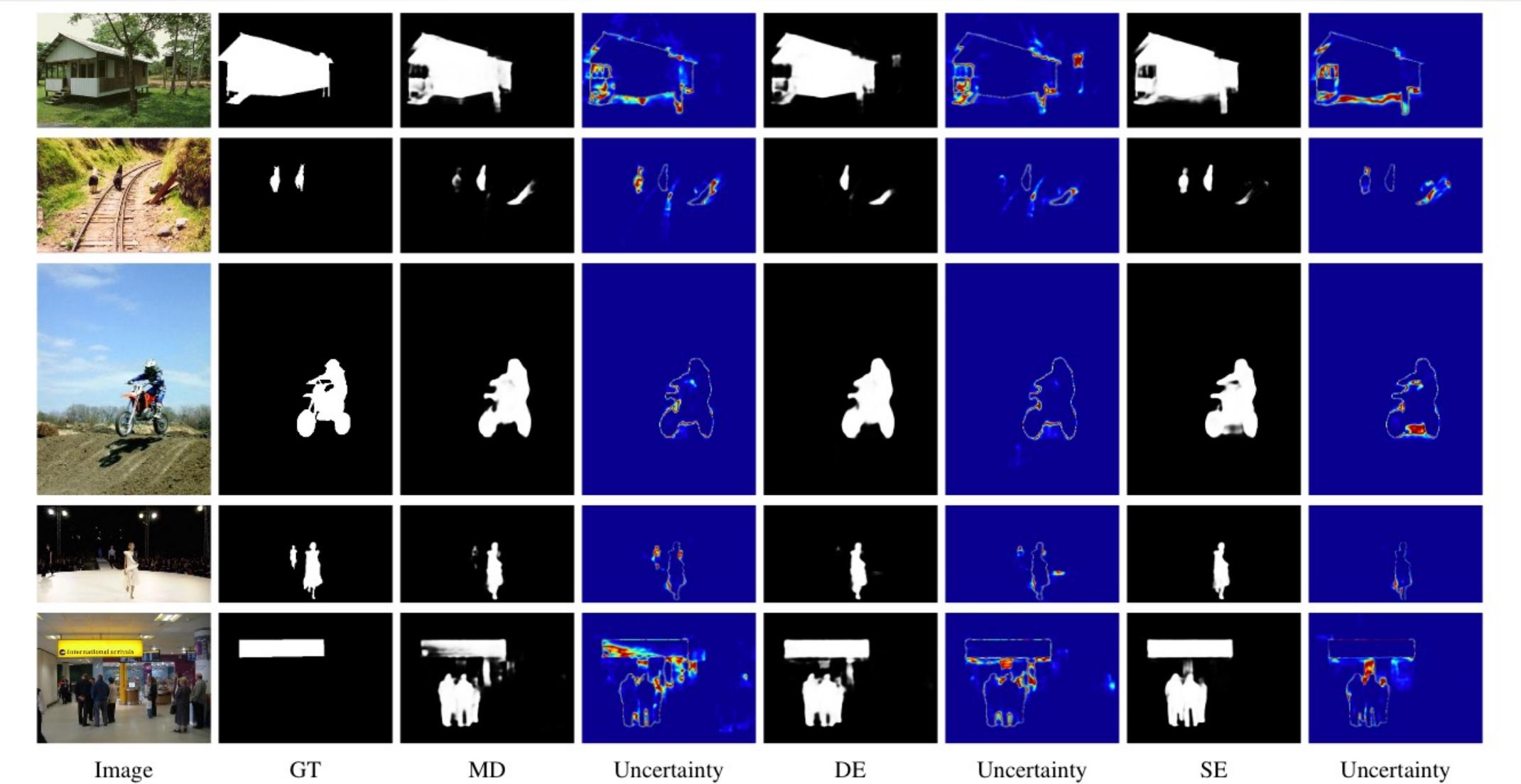
1. Base: the base model
2. MD: MC-dropout
3. DE: deep ensemble

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

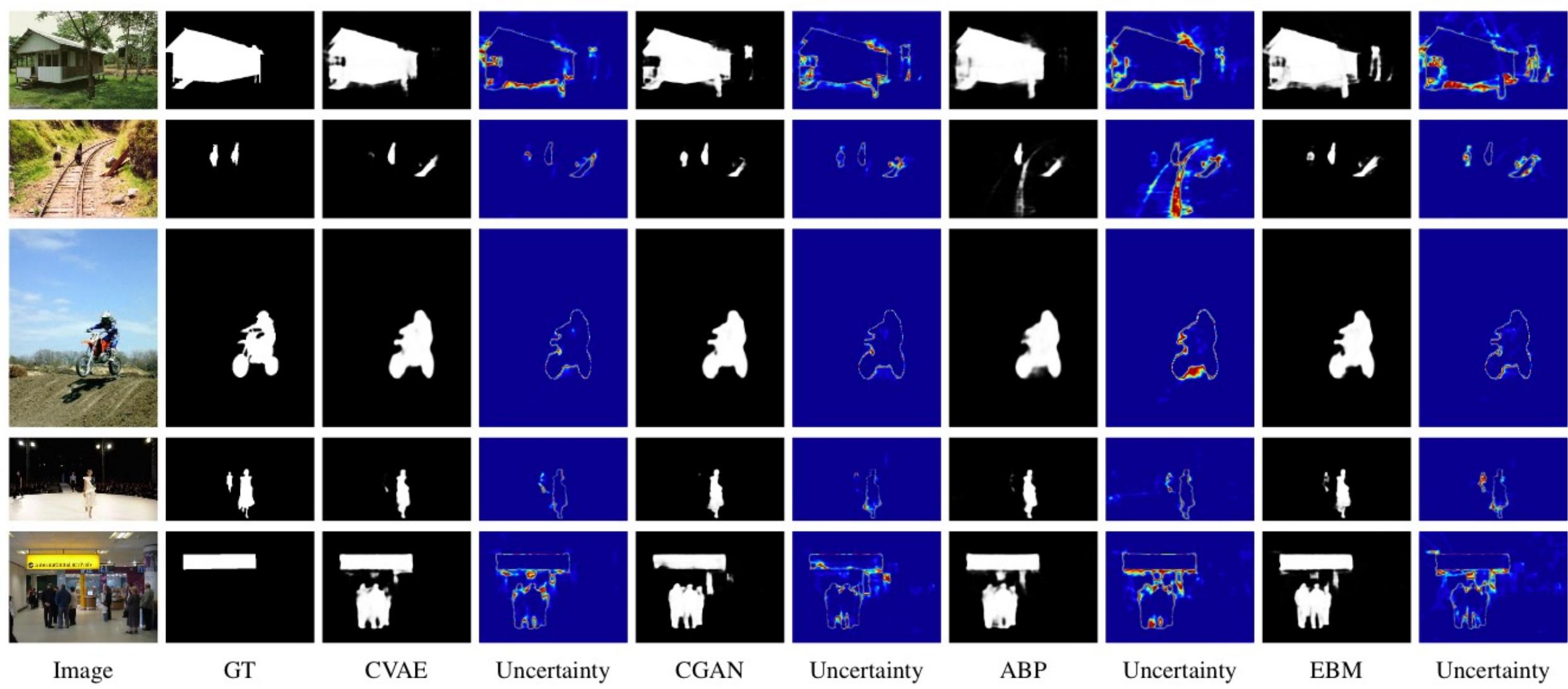
Method	DUTS [79]		DUT [80]		HKU-IS [81]		PASCAL [82]	
	$F_\beta \uparrow$	$\mathcal{M} \downarrow$						
Base	.842	.037	.760	.055	.904	.030	.828	.064
CVAE	.836	.037	.748	.055	.901	.030	.826	.063
CGAN	.846	.035	.752	.054	.905	.029	.828	.063
ABP	.829	.040	.740	.059	.889	.034	.818	.068
EBM	.834	.040	.744	.062	.900	.031	.829	.064

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

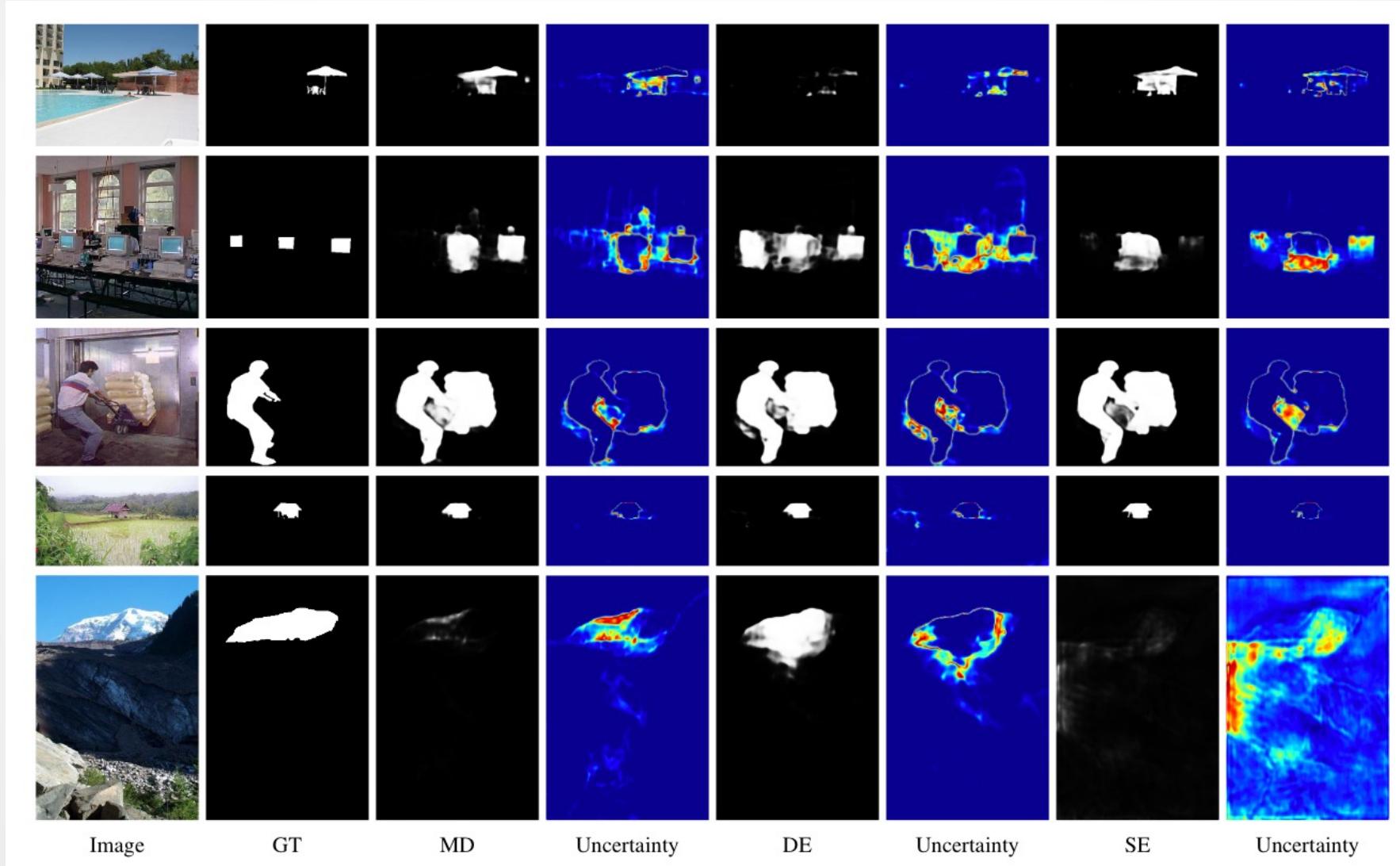
Predictive Uncertainty-Ensemble



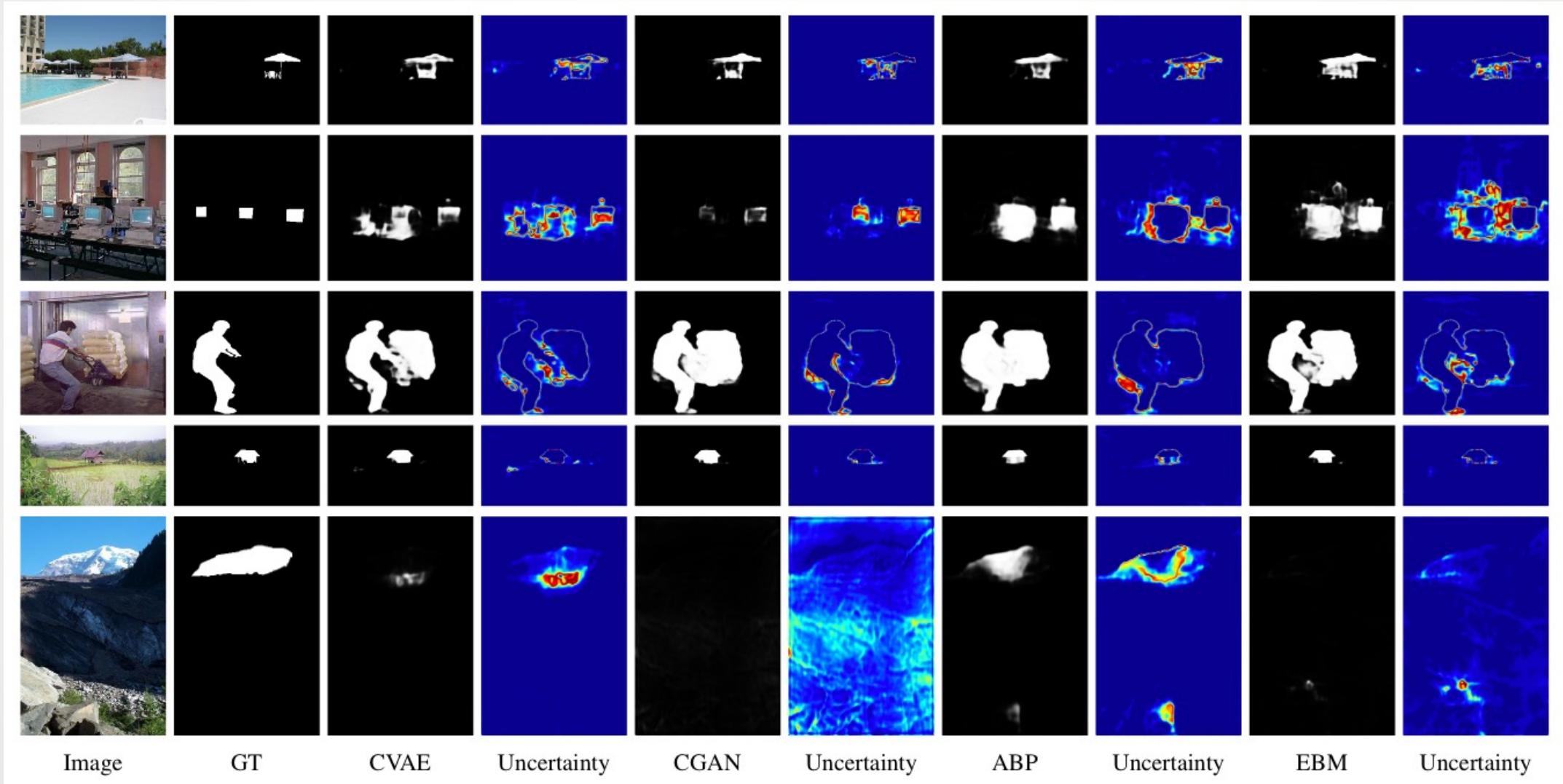
Predictive Uncertainty-Generative Model



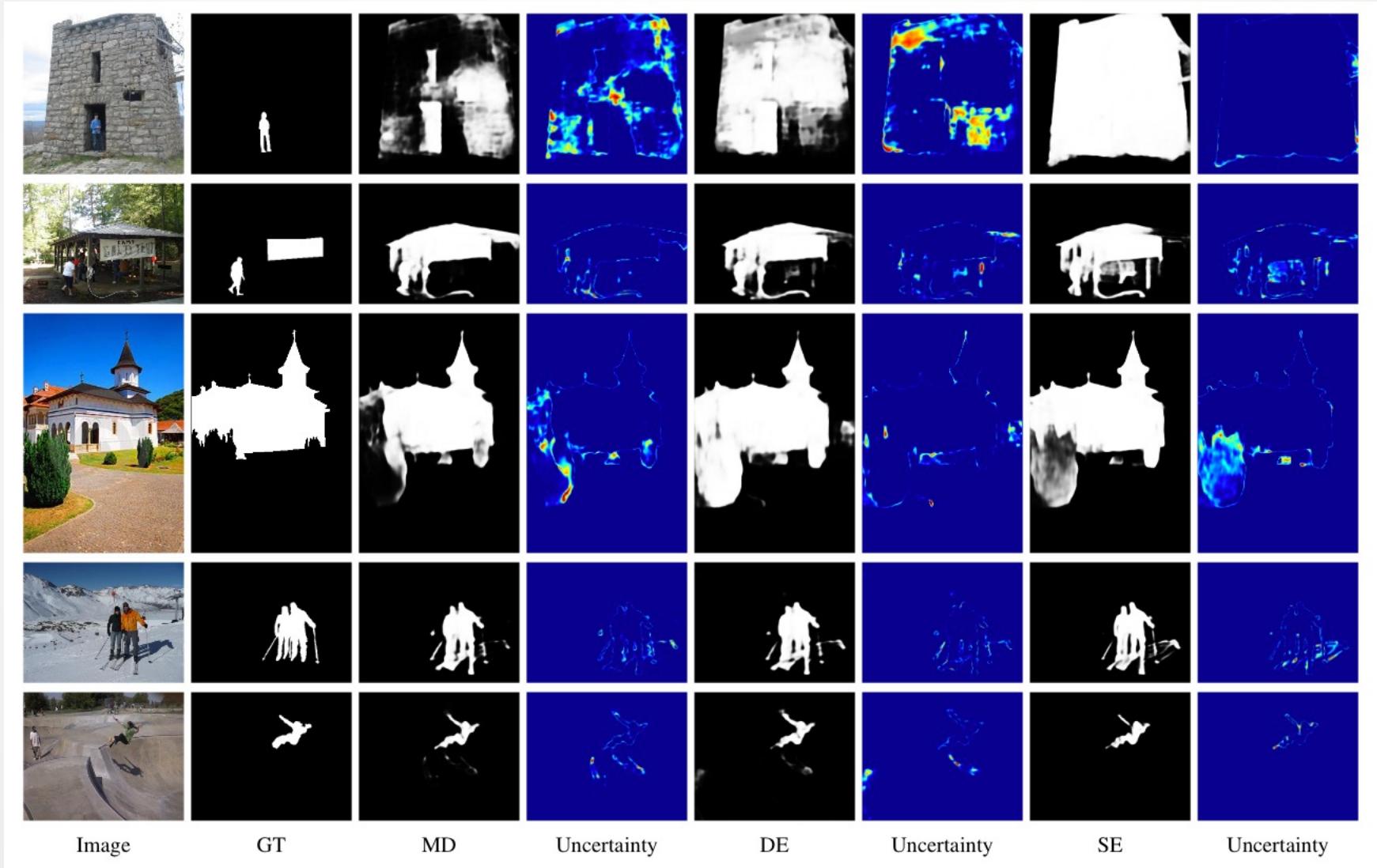
Aleatoric Uncertainty-Ensemble



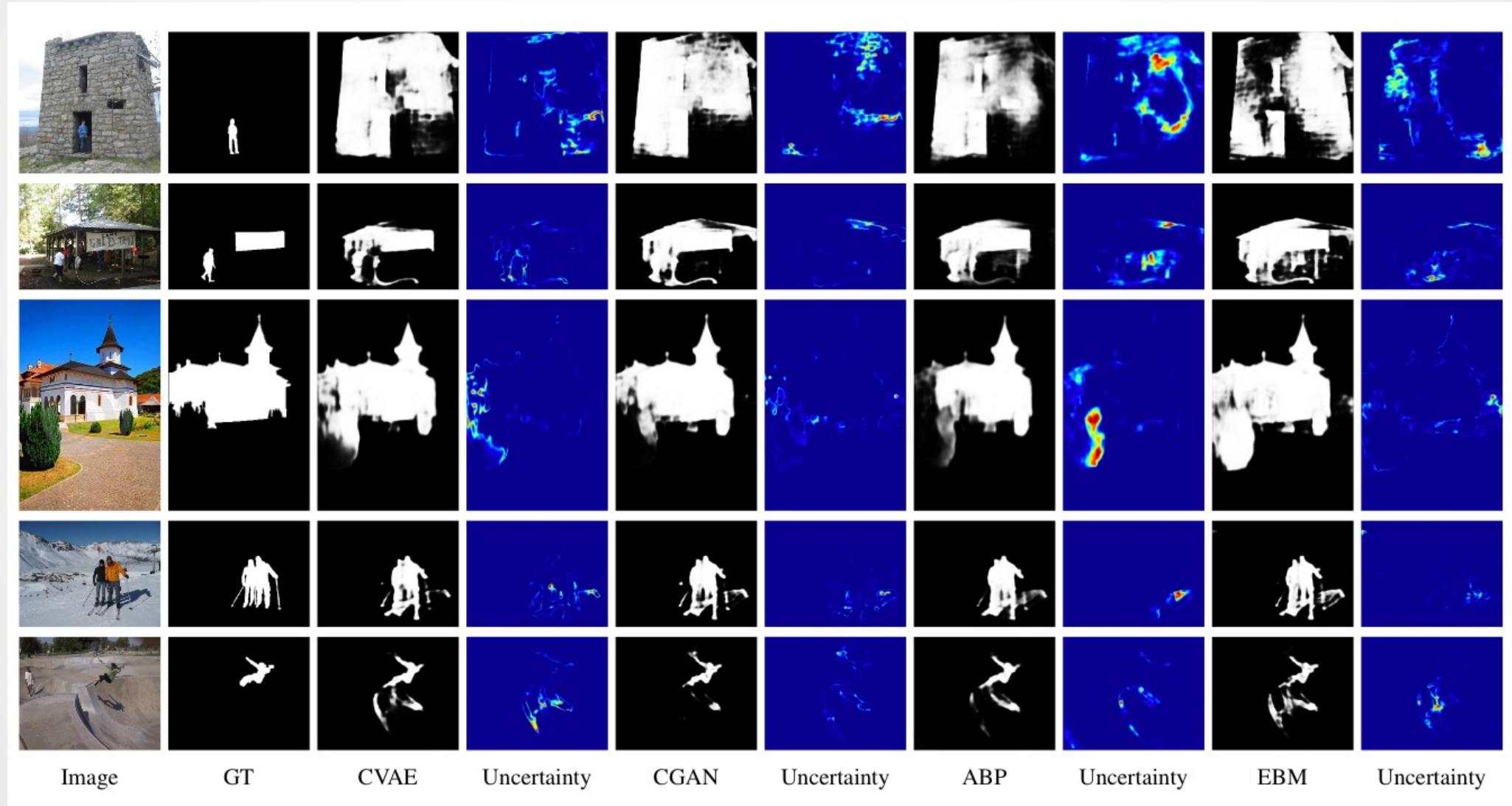
Aleatoric Uncertainty-Generative Model



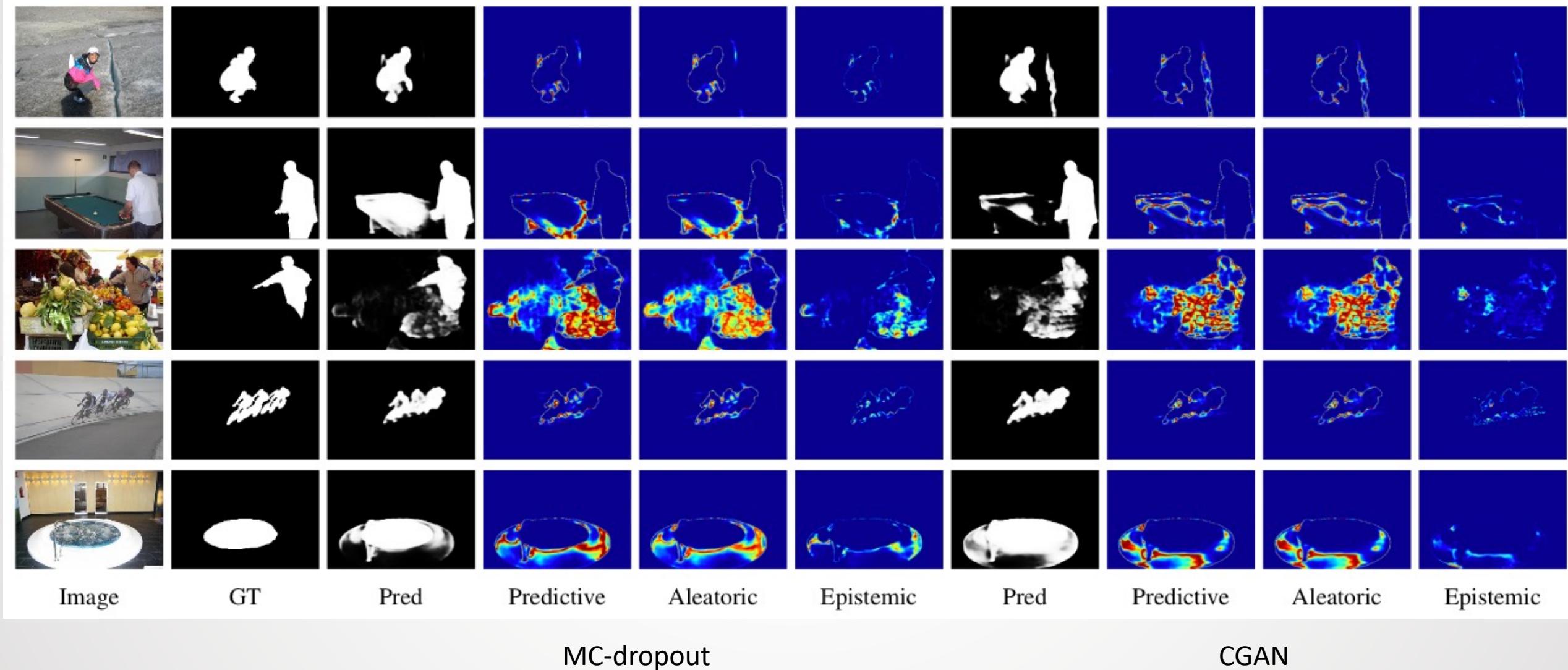
Epistemic Uncertainty-Ensemble



Epistemic Uncertainty-Generative Model



Three types of uncertainty



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
- Effectiveness measure
- Pixel-level uncertainty vs Instance-level uncertainty
- How to effectively use the produced uncertainty

Thanks

Contact: zjnwpw@gmail.com



Code and tutorial material are available



Google scholar