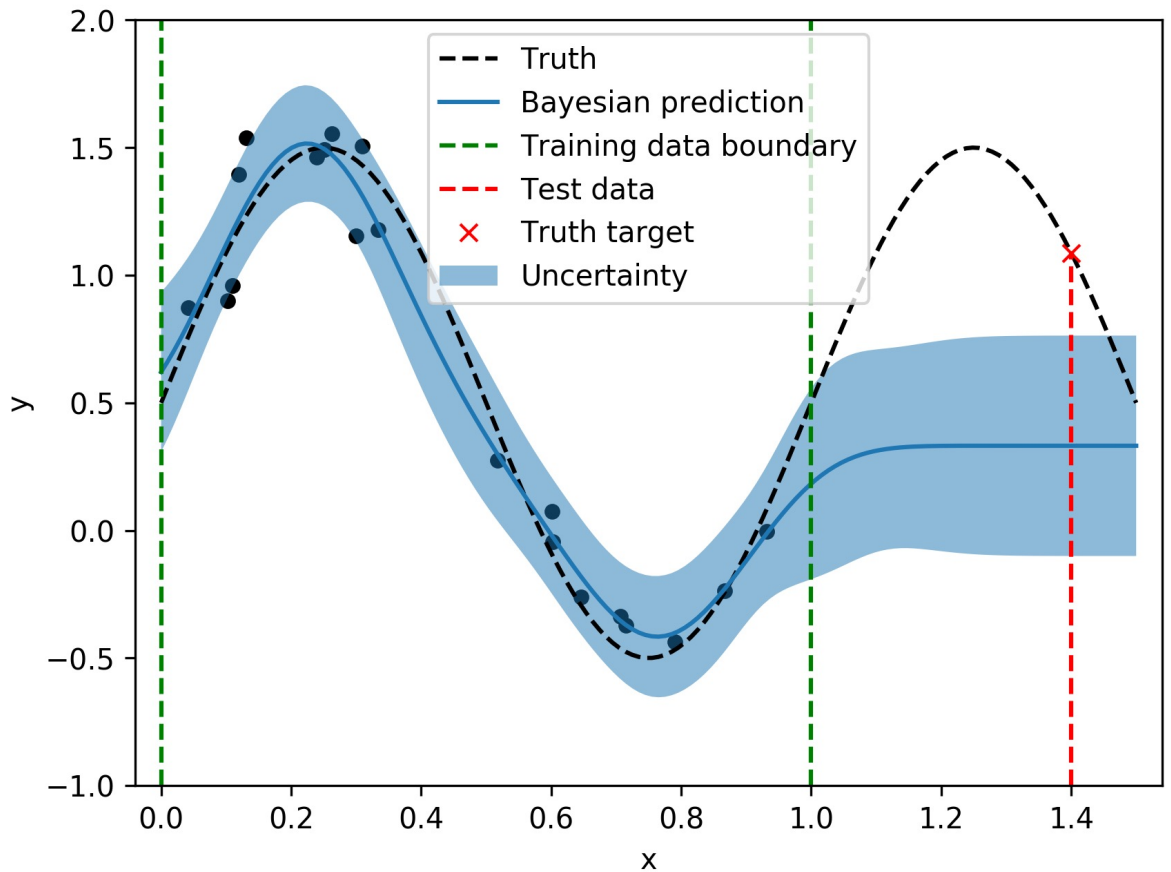


# Bayesian meta-learning

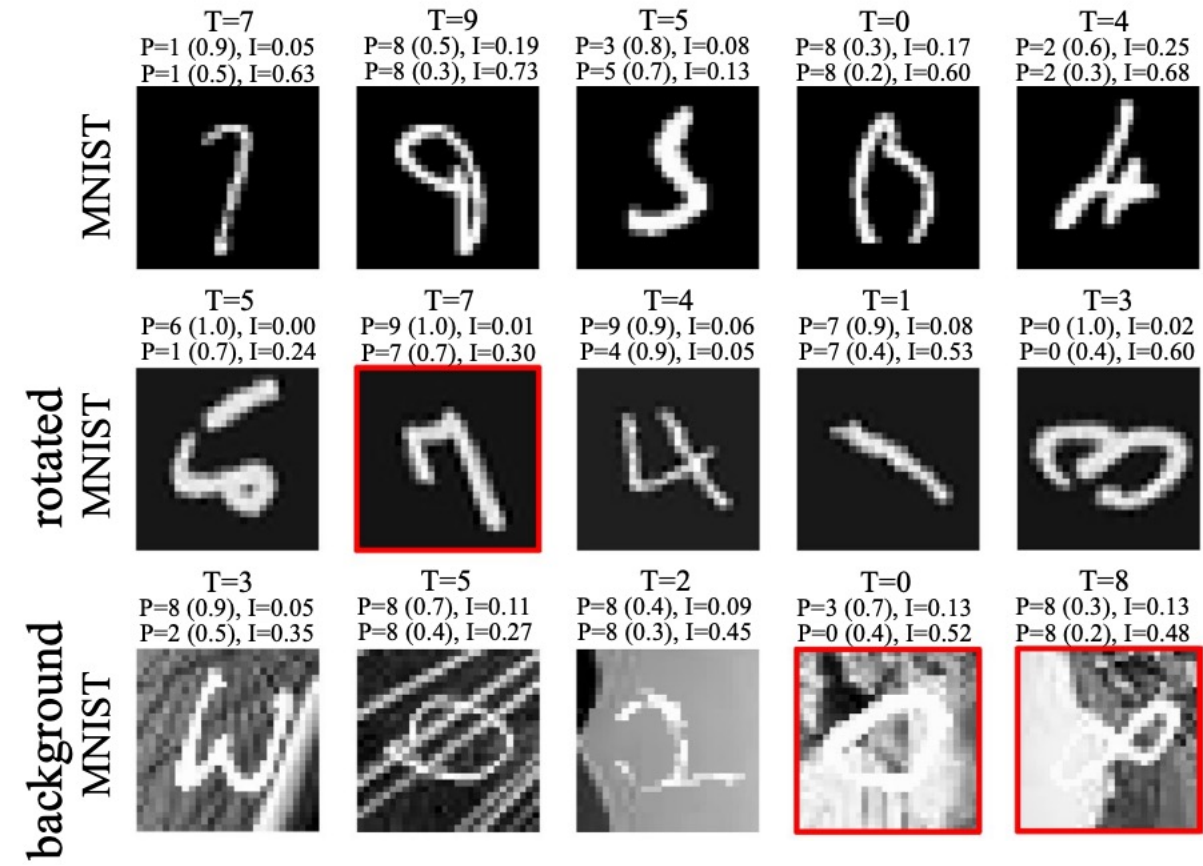
HoUston Learning Algorithms (HULA) Lab  
Presented by Pengyu (Ben) Yuan

UNIVERSITY of HOUSTON | ENGINEERING

# Uncertainty exists everywhere



Regression problem: High uncertainty when outside of training distribution

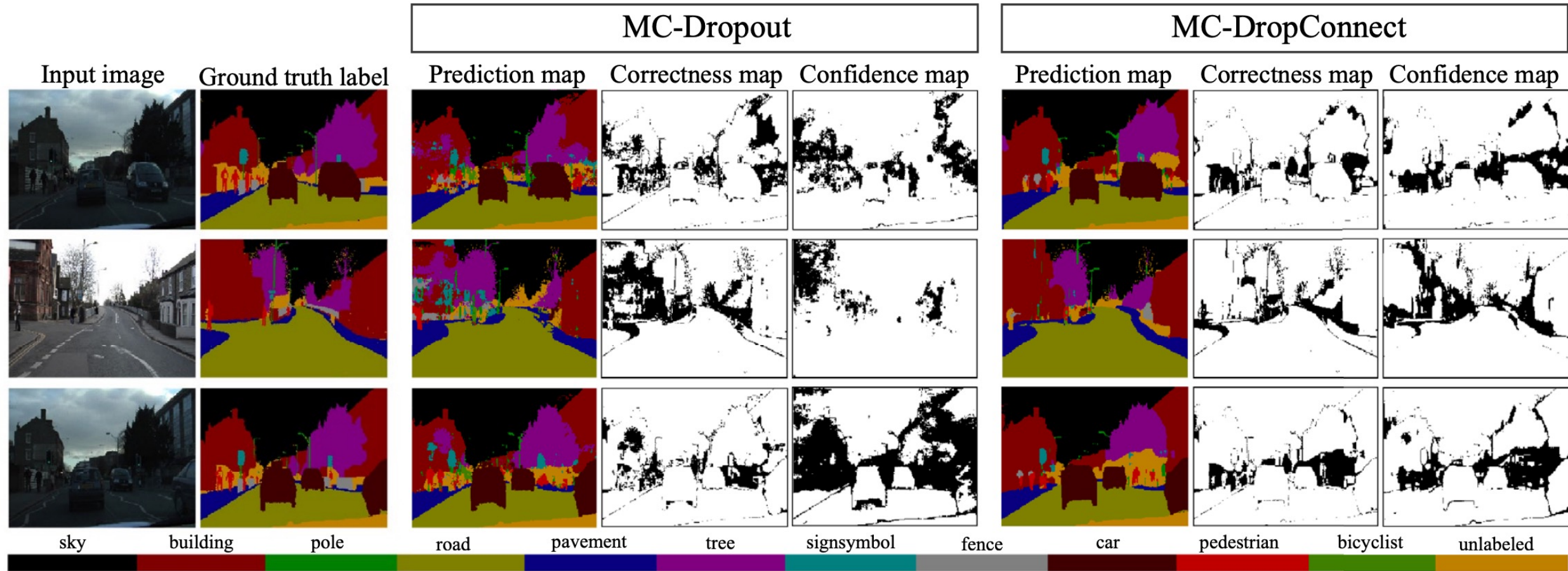


Classification problem: Correcting wrong prediction when use uncertainty

<https://www.nature.com/articles/s41598-020-134854-x>

# Uncertainty exists everywhere

Cam Vid



Segmentation problem: High correlation between uncertainty and correctness

<https://www.nature.com/articles/s41598-020-18485-4>



# Deterministic meta-learning

- Learner's parameter (deterministic)

$$p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta^*) \approx \delta(\phi_i^*)$$

where

$$\phi_i^* = \arg \max_{\phi_i} \log p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta^*)$$

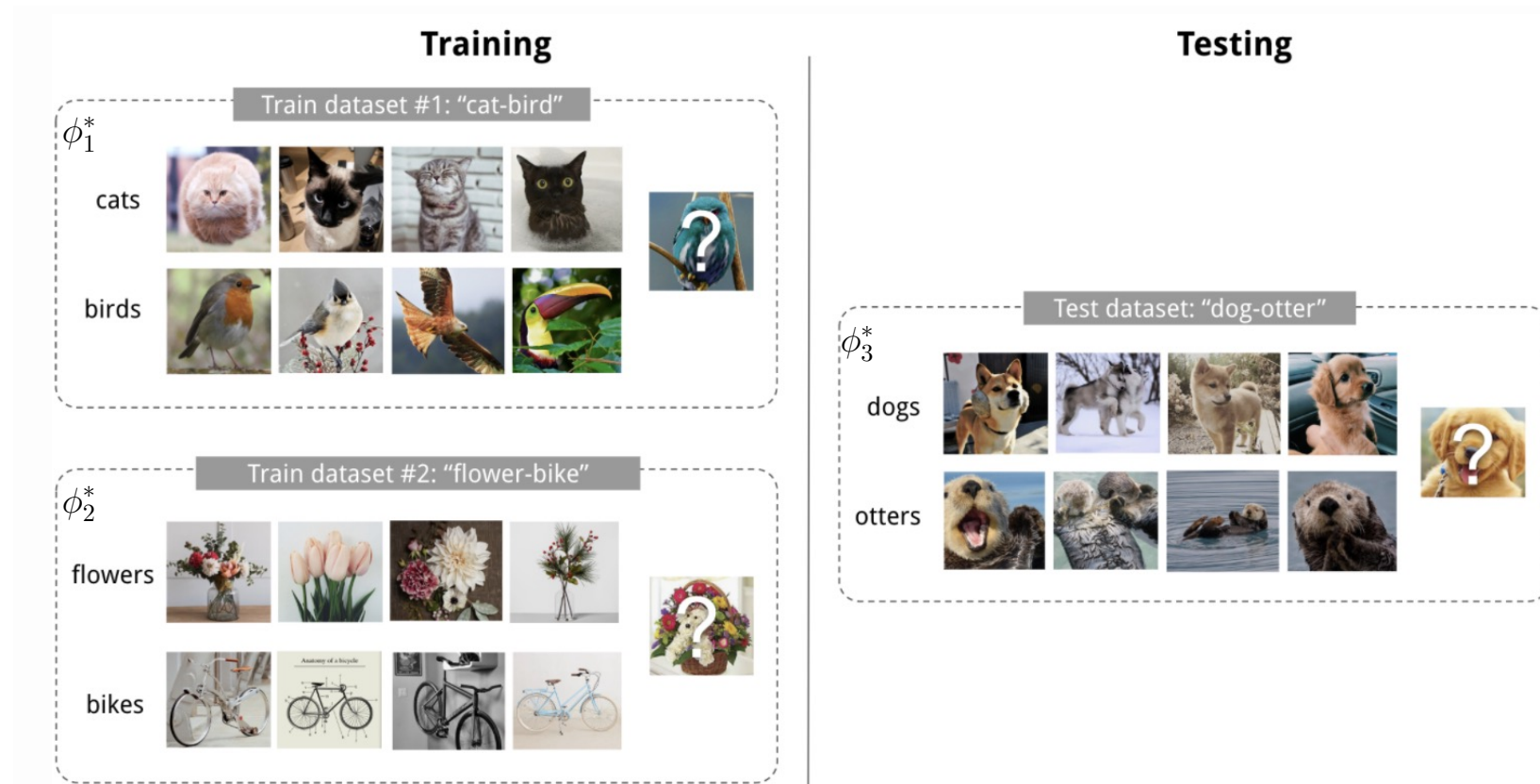
- Problems:

- $\phi_i^*$  is a point estimate (MAP)
- There is no uncertainty in the prediction:

$$y^{\text{te}} = g_{\phi^*}(x^{\text{te}})$$

where  $g$  is the learner's network

- Few shot learning is ambiguous, easily overfitting



Can we get a distribution of  $p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta^*)$  ?

So 
$$p(y^{\text{te}} | x^{\text{te}}, \mathcal{D}^{\text{tr}}, \theta^*) = \int_{\Phi} p(y^{\text{te}} | x^{\text{te}}, \phi) p(\phi | \mathcal{D}^{\text{tr}}, \theta^*) d\phi$$

$\phi_i^*$  is a set of classifier parameters for  $\mathcal{D}_i$

# Deterministic meta-learning

- Meta parameter (deterministic)

$$p(\theta \mid \mathcal{D}_{\text{meta-train}}) \approx \delta(\theta^*)$$

where

$$\theta^* = \arg \max_{\theta} \log p(\theta \mid \mathcal{D}_{\text{meta-train}})$$

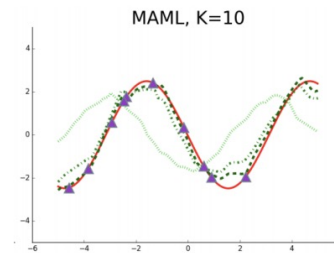
- Problems:

- $\theta^*$  is also a point estimate (MAP)
- When the number of tasks is small, there is high uncertainty in the meta parameters. Leads to **meta-overfitting**
- Learner's parameters are affected by meta parameters:

$$p(\phi_i \mid \mathcal{D}_i^{\text{tr}}, \theta)$$

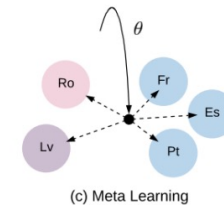
Thus, it can also affect the distribution of the prediction.

What information might  $\theta$  contain...



...in a toy sinusoid problem?

$\theta$  corresponds to family of sinusoid functions (everything but phase and amplitude)



...in multi-language machine translation?

$\theta$  corresponds to the family of all language pairs

$\theta$  is the shared latent information from  $\mathcal{D}_{\text{meta-train}}$

# Why Bayesian in meta-learning?

Bayesian method can:

- give us a distribution over prediction
- prevent overfitting problem
- update model gradually by using online learning

In meta-learning scenario, it can:

- Learn **safety-critical** few-shot model (especially in medical imaging)
- Learn to **actively annotate** new samples (active learning)
- Learn to **explore** in meta reinforcement learning



# Bayesian tools

How ?

- Learn distribution over learner's parameters:  $\delta(\phi_i^*) \rightarrow p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta^*)$
- Learn distribution over meta parameters:  $\delta(\theta^*) \rightarrow p(\theta | \mathcal{D}_{\text{meta-train}})$
- Can be either one or both

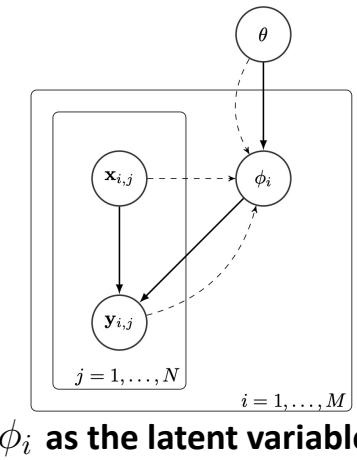
Bayesian toolboxes:

- Latent variable models + variational inference
  - approximate likelihood of latent variable model with variational lower bound
- Bayesian ensembles
  - particle-based representation: train separate models on bootstraps of the data
- Bayesian neural networks
  - explicit distribution over the space of network parameters
- ...

<https://openreview.net/pdf?id=rkgpy3C5tX>

[http://cs330.stanford.edu/fall2020/slides/cs330\\_bayesian\\_meta\\_learning\\_2020.pdf](http://cs330.stanford.edu/fall2020/slides/cs330_bayesian_meta_learning_2020.pdf)

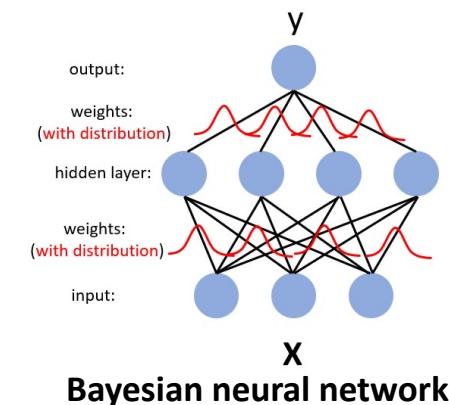
[https://www.researchgate.net/publication/328757994\\_A\\_Batched\\_Scalable\\_Multi-Objective\\_Bayesian\\_Optimization\\_Algorithm](https://www.researchgate.net/publication/328757994_A_Batched_Scalable_Multi-Objective_Bayesian_Optimization_Algorithm)



Single donkey



An ensemble of donkey



# Outline

- Introduction
  - Why Bayesian meta-learning?
  - The evidence lower bound (ELBO)
- Bayesian meta-learning approaches based on
  - Amortized variational inference
    - Black-box
    - Optimization
  - Bayesian ensembles
  - Bayesian neural networks
- Bayesian meta-learning evaluation
  - Qualitative visualization
  - Quantitative evaluation
  - Active-learning evaluation





# Outline

- Introduction
  - Why Bayesian meta-learning?
  - The evidence lower bound (ELBO)
- Bayesian meta-learning approaches based on
  - Amortized variational inference
    - Black-box
    - Optimization
  - Bayesian ensembles
  - Bayesian neural networks
- Bayesian meta-learning evaluation
  - Qualitative visualization
  - Quantitative evaluation
  - Active-learning evaluation



# The evidence lower bound (ELBO)

- What is ELBO?

It is an optimization function used in variational inference.

$$q(\phi) = \arg \max_q ELBO \quad \text{where} \quad ELBO = \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi$$

$\phi$  – parameters

$\mathcal{D}$  – observations

$q(\phi)$  – variational distribution



# The evidence lower bound (ELBO)

- What is ELBO?

It is an optimization function used in variational inference.

$$q(\phi) = \arg \max_q ELBO \quad \text{where} \quad ELBO = \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi$$

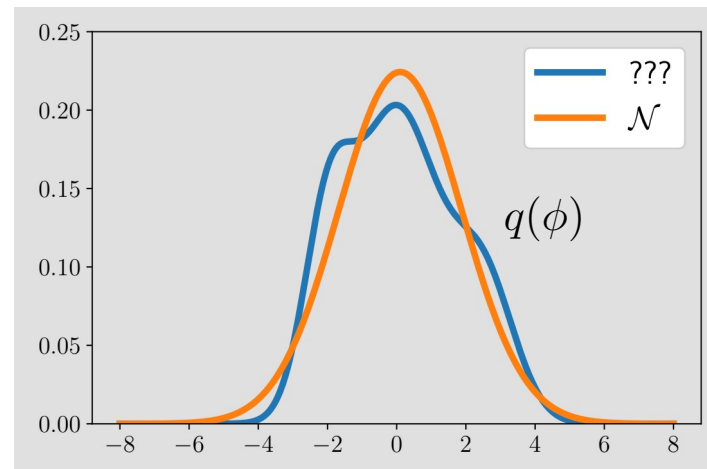
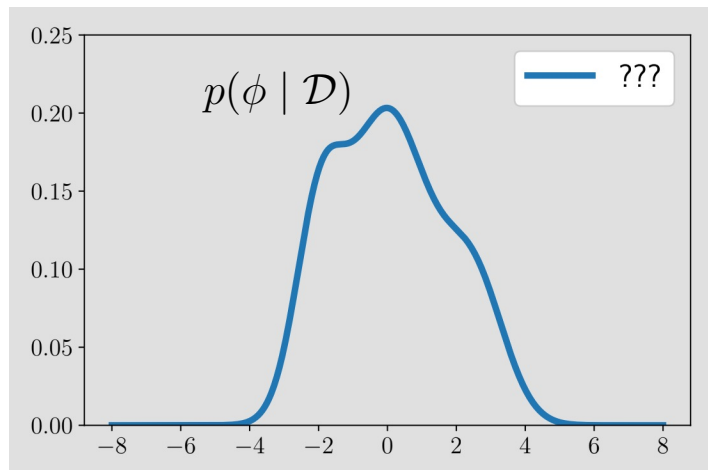
$\phi$  – parameters

$\mathcal{D}$  – observations

$q(\phi)$  – variational distribution

- What is variational inference (VI)?

Approximating a posterior distribution with some easy to manipulate distribution like the Gaussian



$$q(\phi) \rightarrow p(\phi | \mathcal{D})$$



# The evidence lower bound (ELBO)

- What is ELBO?

It is an optimization function used in variational inference.

$$q(\phi) = \arg \max_q ELBO \quad \text{where} \quad ELBO = \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi$$

$\phi$  – parameters  
 $\mathcal{D}$  – observations  
 $q(\phi)$  – variational distribution

- What is variational inference (VI)?

Approximating a posterior distribution with some easy to manipulate distribution like the Gaussian

$$q(\phi) \xrightarrow{\text{Approx.}} p(\phi | \mathcal{D})$$

- Why do we need VI?

It is intractable to calculate the true posterior distribution

$$p(\phi | \mathcal{D}) = \frac{p(\mathcal{D}, \phi)}{p(\mathcal{D})} = \frac{p(\mathcal{D} | \phi)p(\phi)}{p(\mathcal{D})} = \frac{p(\mathcal{D} | \phi)p(\phi)}{\int_{\Phi} p(\mathcal{D} | \phi)p(\phi) d\phi}$$

because it is impossible to consider all configurations  $\phi$  of the neural network.

$p(\phi | \mathcal{D})$  – true posterior distribution  
 $p(\mathcal{D} | \phi)$  – likelihood  
 $p(\phi)$  – prior distribution



# The evidence lower bound (ELBO)

- What is ELBO?

It is an optimization function used in variational inference.

$$q(\phi) = \arg \max_q ELBO \quad \text{where} \quad ELBO = \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi$$

$\phi$  – parameters  
 $\mathcal{D}$  – observations  
 $q(\phi)$  – variational distribution

- What is variational inference (VI)?

Approximating a posterior distribution with some easy to manipulate distribution like the Gaussian

$$q(\phi) \xrightarrow{\text{Approx.}} p(\phi | \mathcal{D})$$

- Why do we need VI?

It is intractable to calculate the true posterior distribution

$$p(\phi | \mathcal{D}) = \frac{p(\mathcal{D}, \phi)}{p(\mathcal{D})} = \frac{p(\mathcal{D} | \phi)p(\phi)}{p(\mathcal{D})} = \frac{p(\mathcal{D} | \phi)p(\phi)}{\int_{\Phi} p(\mathcal{D} | \phi)p(\phi) d\phi}$$

- Why do we need posterior distribution?

To get distribution (uncertainty) over predictions:

$$p(y^{\text{te}} | x^{\text{te}}, \mathcal{D}^{\text{tr}}) = \int_{\Phi} p(y^{\text{te}} | x^{\text{te}}, \phi) p(\phi | \mathcal{D}^{\text{tr}}) d\phi$$

$p(\phi | \mathcal{D})$  – true posterior distribution  
 $p(\mathcal{D} | \phi)$  – likelihood  
 $p(\phi)$  – prior distribution



# The evidence lower bound (ELBO)

- Why optimizing the ELBO can help to approximate the true posterior distribution?

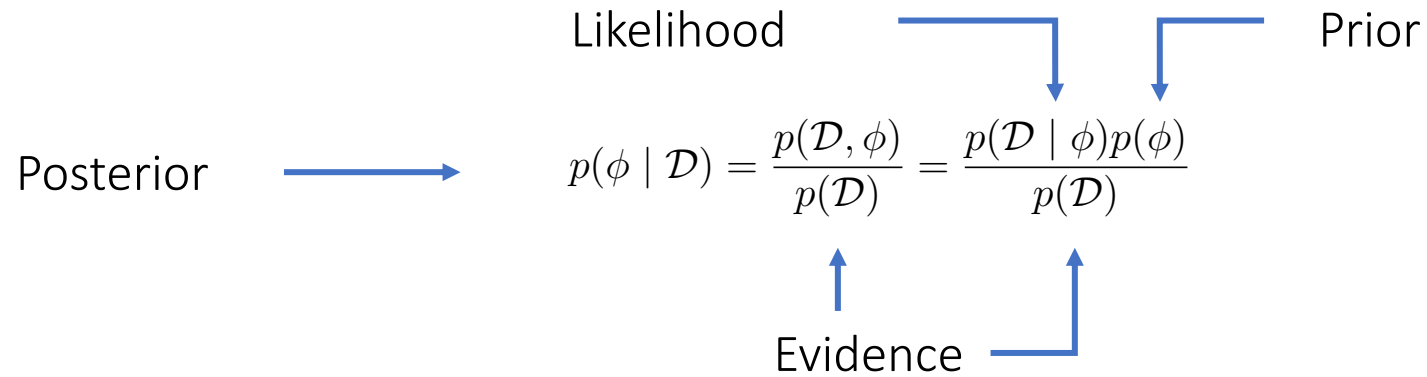
Look at the Bayesian rule:

Posterior  $\longrightarrow$

$$p(\phi | \mathcal{D}) = \frac{p(\mathcal{D}, \phi)}{p(\mathcal{D})} = \frac{p(\mathcal{D} | \phi)p(\phi)}{p(\mathcal{D})}$$

Likelihood  $\longleftarrow$   $\longleftarrow$  Prior

Evidence  $\longleftarrow$   $\longleftarrow$



$q(\phi)$  – variational distribution  
 $p(\phi | \mathcal{D})$  – true posterior distribution  
 $p(\mathcal{D} | \phi)$  – likelihood  
 $p(\phi)$  – prior distribution  
 $p(\mathcal{D})$  – evidence



# The evidence lower bound (ELBO)

- Why optimizing the ELBO can help to approximate the true posterior distribution?

Look at the Bayesian rule:

Posterior  $\longrightarrow$

$$p(\phi | \mathcal{D}) = \frac{p(\mathcal{D}, \phi)}{p(\mathcal{D})} = \frac{p(\mathcal{D} | \phi)p(\phi)}{p(\mathcal{D})}$$

Likelihood  $\longleftarrow$   $\longleftarrow$  Prior

Evidence  $\longleftarrow$   $\longleftarrow$

Log evidence:

$$\ln p(\mathcal{D}) = ELBO + \underbrace{KL(q(\phi) || p(\phi | \mathcal{D}))}_{\geq 0} \geq ELBO \quad KL(\cdot || \cdot) \geq 0$$

Difference between the variational distribution  
and true posterior distribution

Evidence is fixed by data, thus

$$q(\phi) = \arg \min_q KL(q(\phi) || p(\phi | \mathcal{D})) = \arg \max_q ELBO$$

$q(\phi)$  – variational distribution  
 $p(\phi | \mathcal{D})$  – true posterior distribution  
 $p(\mathcal{D} | \phi)$  – likelihood  
 $p(\phi)$  – prior distribution  
 $p(\mathcal{D})$  – evidence



# The evidence lower bound (ELBO)

- Let's get a closer look at ELBO

$$\max_q ELBO = \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi$$

$q(\phi)$  – variational distribution

$p(\phi | \mathcal{D})$  – true posterior distribution

$p(\mathcal{D} | \phi)$  – likelihood

$p(\phi)$  – prior distribution

$p(\mathcal{D})$  – evidence





# The evidence lower bound (ELBO)

- Let's get a closer look at ELBO

$$\begin{aligned}\max_q ELBO &= \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi \\ &= \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}|\phi)p(\phi)}{q(\phi)} d\phi\end{aligned}$$

$q(\phi)$  – variational distribution

$p(\phi | \mathcal{D})$  – true posterior distribution

$p(\mathcal{D} | \phi)$  – likelihood

$p(\phi)$  – prior distribution

$p(\mathcal{D})$  – evidence



# The evidence lower bound (ELBO)

- Let's get a closer look at ELBO

$$\begin{aligned}\max_q ELBO &= \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi \\ &= \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}|\phi)p(\phi)}{q(\phi)} d\phi \\ &= \int_{\Phi} q(\phi) \ln p(\mathcal{D} | \phi) - \int_{\Phi} q(\phi) \ln \frac{q(\phi)}{p(\phi)} d\phi\end{aligned}$$

$q(\phi)$  – variational distribution  
 $p(\phi | \mathcal{D})$  – true posterior distribution  
 $p(\mathcal{D} | \phi)$  – likelihood  
 $p(\phi)$  – prior distribution  
 $p(\mathcal{D})$  – evidence



# The evidence lower bound (ELBO)

- Let's get a closer look at ELBO

$$\begin{aligned}\max_q ELBO &= \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi \\ &= \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}|\phi)p(\phi)}{q(\phi)} d\phi \\ &= \int_{\Phi} q(\phi) \ln p(\mathcal{D} | \phi) - \int_{\Phi} q(\phi) \ln \frac{q(\phi)}{p(\phi)} d\phi \\ &= \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))\end{aligned}$$

$q(\phi)$  – variational distribution  
 $p(\phi | \mathcal{D})$  – true posterior distribution  
 $p(\mathcal{D} | \phi)$  – likelihood  
 $p(\phi)$  – prior distribution  
 $p(\mathcal{D})$  – evidence



# The evidence lower bound (ELBO)

- Let's get a closer look at ELBO

$$\begin{aligned}\max_q ELBO &= \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}, \phi)}{q(\phi)} d\phi \\ &= \int_{\Phi} q(\phi) \ln \frac{p(\mathcal{D}|\phi)p(\phi)}{q(\phi)} d\phi \\ &= \int_{\Phi} q(\phi) \ln p(\mathcal{D} | \phi) - \int_{\Phi} q(\phi) \ln \frac{q(\phi)}{p(\phi)} d\phi \\ &= \underbrace{\mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)]}_{\text{Samples from } q(\phi) \text{ to perform original tasks}} - \underbrace{KL(q(\phi) || p(\phi))}_{\text{Regularization term}}\end{aligned}$$

Samples from  $q(\phi)$  to perform original tasks

Regularization term

$q(\phi)$  – variational distribution  
 $p(\phi | \mathcal{D})$  – true posterior distribution  
 $p(\mathcal{D} | \phi)$  – likelihood  
 $p(\phi)$  – prior distribution  
 $p(\mathcal{D})$  – evidence



# The evidence lower bound (ELBO)

- More about ELBO

$$\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$$

evidence

variational distribution

likelihood

prior distribution



# The evidence lower bound (ELBO)

- More about ELBO

$$\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$$

evidence      variational distribution      likelihood      prior distribution

variational distribution can be any form:

$$q(\phi) \Rightarrow q(\phi | \mathcal{D}), q(\phi | \theta)$$

For example  $q(\phi | \theta) \xrightarrow{\text{Approx.}} p(\phi | \mathcal{D})$  :  $\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi | \theta)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi | \theta) || p(\phi))$



# The evidence lower bound (ELBO)

- More about ELBO

$$\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$$

evidence      variational distribution      likelihood      prior distribution

variational distribution can be any form:

$$q(\phi) \Rightarrow q(\phi | \mathcal{D}), q(\phi | \theta)$$

For example  $q(\phi | \theta) \xrightarrow{\text{Approx.}} p(\phi | \mathcal{D})$  :  $\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi | \theta)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi | \theta) || p(\phi))$

posterior can be conditioned on other variables:

$$p(\phi | \mathcal{D}) \Rightarrow p(\phi | \mathcal{D}, \theta)$$

For example  $q(\phi) \xrightarrow{\text{Approx.}} p(\phi | \mathcal{D}, \theta)$  :  $\ln p(\mathcal{D} | \theta) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi, \theta)] - KL(q(\phi) || p(\phi | \theta))$



# The evidence lower bound (ELBO)

- Problem of ELBO:

$$\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$$

evidence      variational distribution      likelihood      prior distribution

**1. Cannot optimizing  $q(\phi)$  directly, reparameterization trick is required.**

- Variational distribution has variational parameters  $\lambda$ , i.e.  $q(\phi) = q_{\lambda}(\phi)$        $\lambda = \{\mu, \sigma^2\}$
- It is in general difficult to calculate the derivative  $\nabla_{\lambda} \mathbb{E}_{q_{\lambda}(\phi)}$





# The evidence lower bound (ELBO)

- Problem of ELBO:

$$\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$$

The diagram shows the ELBO equation with four terms:  $\ln p(\mathcal{D})$ ,  $\mathbb{E}_{q(\phi)}$ ,  $\ln p(\mathcal{D} | \phi)$ , and  $KL(q(\phi) || p(\phi))$ . Blue arrows point from each term to a label below it: 'evidence' for  $\ln p(\mathcal{D})$ , 'variational distribution' for  $\mathbb{E}_{q(\phi)}$ , 'likelihood' for  $\ln p(\mathcal{D} | \phi)$ , and 'prior distribution' for  $KL(q(\phi) || p(\phi))$ . A blue line also connects the 'variational distribution' and 'prior distribution' labels, indicating the KL divergence between them.

## 1. Cannot optimizing $q(\phi)$ directly, reparameterization trick is required.

- Variational distribution has variational parameters  $\lambda$ , i.e.  $q(\phi) = q_{\lambda}(\phi)$   $\lambda = \{\mu, \sigma^2\}$
- It is in general difficult to calculate the derivative  $\nabla_{\lambda} \mathbb{E}_{q_{\lambda}(\phi)}$

To see that, set  $f_{\lambda}(\phi, \mathcal{D}) = \ln p(\mathcal{D} | \phi)$ , then

$$\begin{aligned} \nabla_{\lambda} \mathbb{E}_{q_{\lambda}(\phi)} [f_{\lambda}(\phi, \mathcal{D})] &= \nabla_{\lambda} \left[ \int_{\Phi} q_{\lambda}(\phi) f_{\lambda}(\phi, \mathcal{D}) d\phi \right] \\ &= \int_{\Phi} \nabla_{\lambda} [q_{\lambda}(\phi) f_{\lambda}(\phi, \mathcal{D})] d\phi \\ &= \int_{\Phi} f_{\lambda}(\phi, \mathcal{D}) \nabla_{\lambda} q_{\lambda}(\phi) d\phi + \int_{\Phi} q_{\lambda}(\phi) \nabla_{\lambda} f_{\lambda}(\phi, \mathcal{D}) d\phi \\ &= \underbrace{\int_{\Phi} f_{\lambda}(\phi, \mathcal{D}) \nabla_{\lambda} q_{\lambda}(\phi) d\phi}_{\text{What about this?}} + \mathbb{E}_{q_{\lambda}(\phi)} [\nabla_{\lambda} f_{\lambda}(\phi, \mathcal{D})] \end{aligned}$$



# The evidence lower bound (ELBO)

- Problem of ELBO:

$$\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$$

## 1. Cannot optimizing $q(\phi)$ directly, reparameterization trick is required.

- Variational distribution has variational parameters  $\lambda$ , i.e.  $q(\phi) = q_\lambda(\phi)$       $\lambda = \{\mu, \sigma^2\}$
- It is in general difficult to calculate the derivative  $\nabla_\lambda \mathbb{E}_{q_\lambda(\phi)}$

To see that, set  $f_\lambda(\phi, \mathcal{D}) = \ln p(\mathcal{D} | \phi)$ , then

$$\phi \sim N(\mu, \sigma^2)$$

reparameterization



$$\phi = \mu + \sigma\epsilon, \text{ where } \epsilon \sim N(0, \mathbf{I})$$

$$f_\lambda(\phi, \mathcal{D}) = f(g_\lambda(\epsilon, \mathcal{D}))$$

$$\nabla_\lambda \mathbb{E}_{q_\lambda(\phi)} [f_\lambda(\phi, \mathcal{D})] = \underbrace{\int_{\Phi} f_\lambda(\phi, \mathcal{D}) \nabla_\lambda q_\lambda(\phi) d\phi}_{\text{What about this?}} + \mathbb{E}_{q_\lambda(\phi)} [\nabla_\lambda f_\lambda(\phi, \mathcal{D})]$$

$$\begin{aligned} \nabla_\lambda \mathbb{E}_{q_\lambda(\phi)} [f_\lambda(\phi, \mathcal{D})] &= \nabla_\lambda \mathbb{E}_{p(\epsilon)} [f(g_\lambda(\epsilon, \mathcal{D}))] \\ &= \mathbb{E}_{p(\epsilon)} [\nabla_\lambda f(g_\lambda(\epsilon, \mathcal{D}))] \end{aligned}$$



# The evidence lower bound (ELBO)

- Problem of ELBO:

$$\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$$

evidence      variational distribution      likelihood      prior distribution

## 2. Can only model Gaussian variational distribution $q(\phi)$

- Variational distribution needs to be simple
- Reparameterization trick gives us Gaussian distribution
- KL divergence has analytic solution when both distributions are Gaussian



# The evidence lower bound (ELBO)

Basic ideas: maximize ELBO to use  $q(\phi)$  to approximate  $p(\phi | \mathcal{D})$

- During training:

1. Sample model parameters from  $q(\phi)$
2. Maximize the likelihood of the observation  $p(\mathcal{D} | \phi)$  while minimize the gap between the  $q(\phi)$  and  $p(\phi)$

$$\max \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$$

- During test:

1. Sample model parameters from  $q(\phi)$
2. Use it as the true posterior distribution for prediction

$$\begin{aligned} p(y^{\text{te}} | x^{\text{te}}, \mathcal{D}^{\text{tr}}) &= \int_{\Phi} p(y^{\text{te}} | x^{\text{te}}, \phi) p(\phi | \mathcal{D}^{\text{tr}}) d\phi \\ &\approx \int_{\Phi} p(y^{\text{te}} | x^{\text{te}}, \phi) q(\phi) d\phi \end{aligned}$$



# Outline

- Introduction
  - Why Bayesian meta-learning?
  - The evidence lower bound (ELBO)
- Bayesian meta-learning approaches based on
  - Amortized variational inference
    - Black-box
    - Optimization
  - Bayesian ensembles
  - Bayesian neural networks
- Bayesian meta-learning evaluation
  - Qualitative visualization
  - Quantitative evaluation
  - Active-learning evaluation



# Amortized variational inference

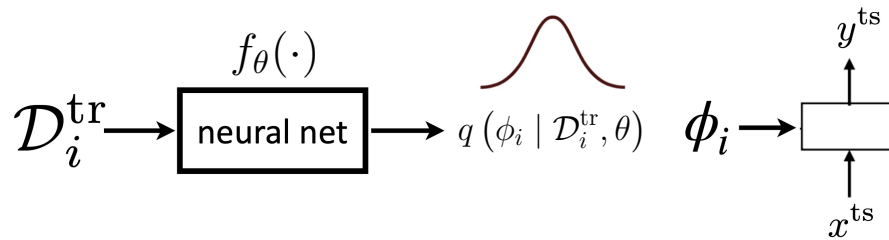
For dataset  $\mathcal{D}_i$ , the posterior distribution we need is:  $p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)$

The variational distribution we used:  $q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) \sim N(\mu_i, \sigma_i^2)$

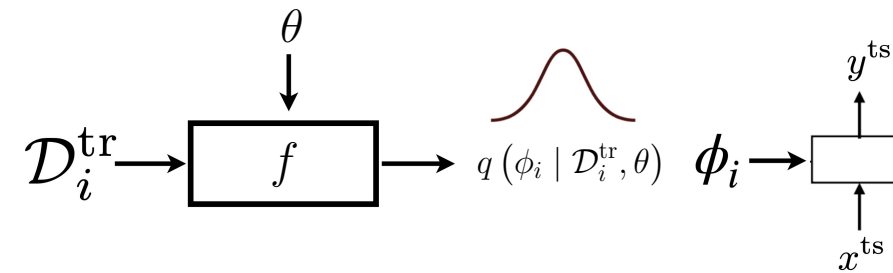
## Amortized Variational Inference

1. Introduce a parameterized model or function that outputs the variational parameters of the approximate posteriors.

$$\lambda = \{\mu_i, \sigma_i^2\} = f_{\theta}(\mathcal{D}_i^{\text{tr}})$$



$$\lambda = \{\mu_i, \sigma_i^2\} = f(\mathcal{D}_i^{\text{tr}}, \theta)$$



2. Variational parameter  $\lambda$  is determined by meta parameter  $\theta$ , thus **optimizing variational parameter is the same as optimizing the meta parameter**. This optimization is done by doing gradient descent on the **loss function for the variational inference**.

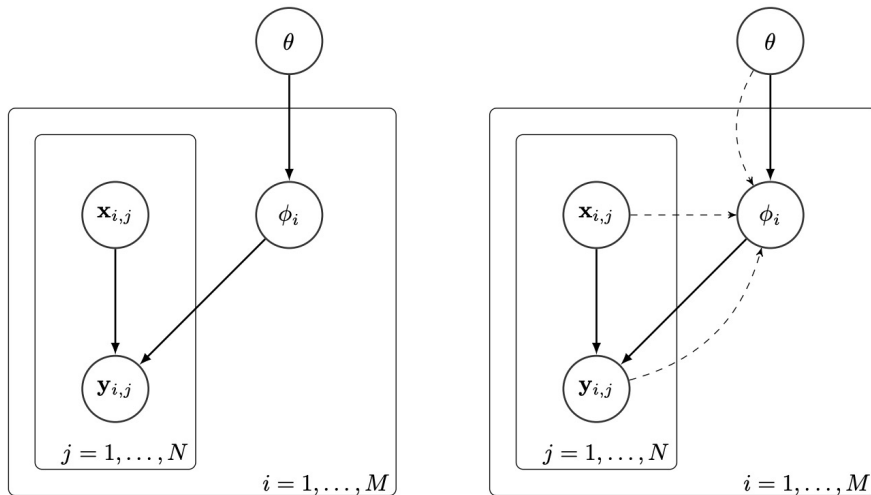


# Amortized variational inference

- What is the loss function for the variational inference in meta-learning?

Variational inference:  $\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$

Because of the meta-learning, we have additional meta-parameter  $\theta$



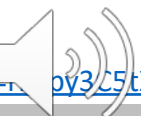
By replacing:

$$q(\phi) \Rightarrow q(\phi | \mathcal{D}^{tr}, \theta)$$

$$p(\phi | \mathcal{D}) \Rightarrow p(\phi | \mathcal{D}, \theta)$$

We have:

$$\max_{\theta} ELBO = \max_{\theta} \mathbb{E}_{q(\phi | \mathcal{D}^{tr}, \theta)}[\ln p(\mathcal{D} | \phi, \theta)] - KL(q(\phi | \mathcal{D}^{tr}, \theta) || p(\phi | \theta))$$

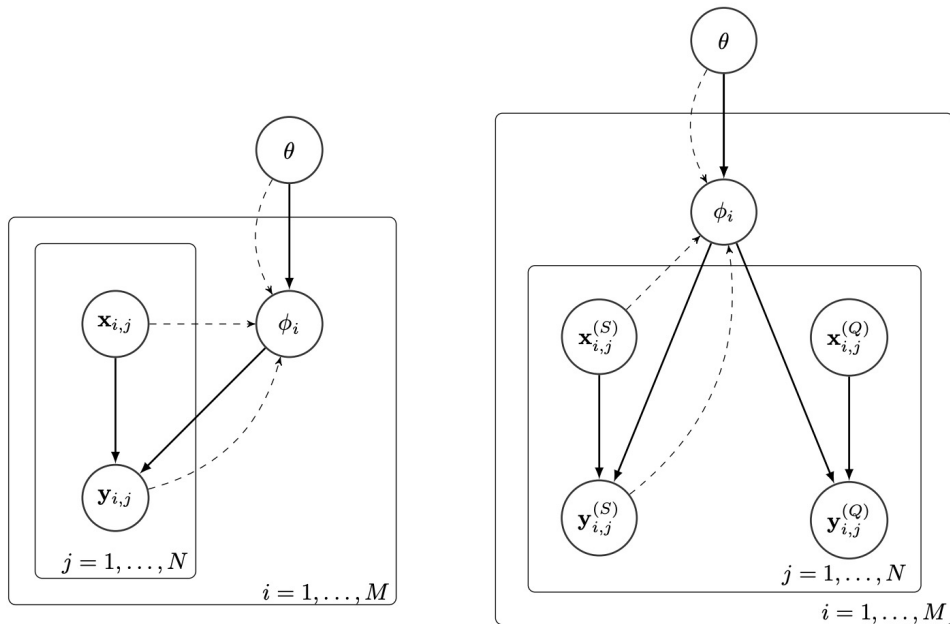


# Amortized variational inference

- What is the loss function for the variational inference in meta-learning?

Variational inference:  $\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$

Because of the meta-learning, we have additional meta-parameter  $\theta$



By replacing:  $q(\phi) \Rightarrow q(\phi | \mathcal{D}^{tr}, \theta)$   $p(\phi | \mathcal{D}) \Rightarrow p(\phi | \mathcal{D}, \theta)$

We have:  $\max_{\theta} ELBO = \max_{\theta} \mathbb{E}_{q(\phi | \mathcal{D}^{tr}, \theta)}[\ln p(\mathcal{D} | \phi, \theta)] - KL(q(\phi | \mathcal{D}^{tr}, \theta) || p(\phi | \theta))$

Approximating the posterior of test data:  $p(\phi | \mathcal{D}, \theta) \Rightarrow p(\phi | \mathcal{D}^{te}, \theta)$

We have:  $\max_{\theta} ELBO = \max_{\theta} \mathbb{E}_{q(\phi | \mathcal{D}^{tr}, \theta)}[\ln p(\mathcal{D}^{te} | \phi, \theta)] - KL(q(\phi | \mathcal{D}^{tr}, \theta) || p(\phi | \theta))$

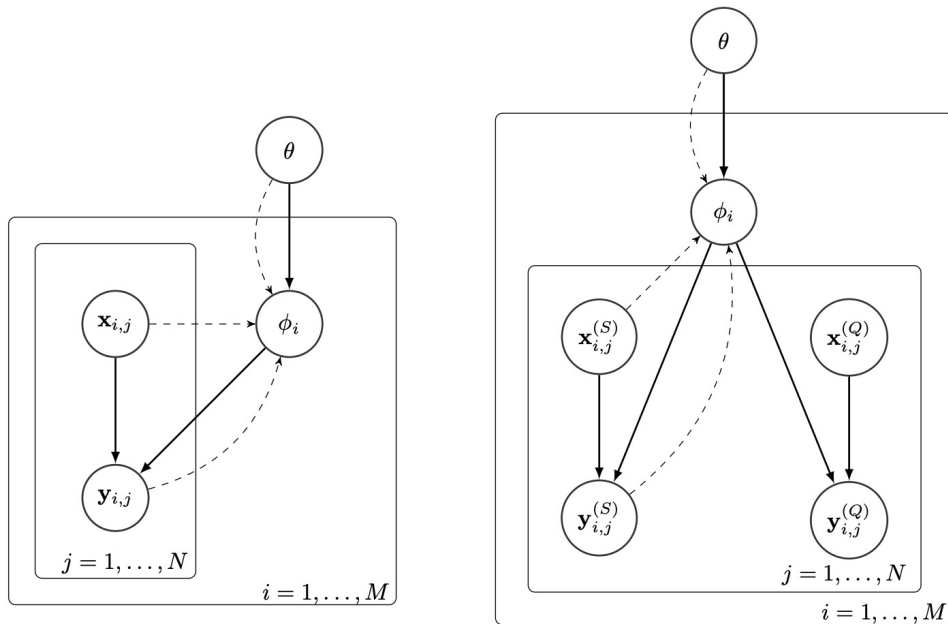


# Amortized variational inference

- What is the loss function for the variational inference in meta-learning?

Variational inference:  $\ln p(\mathcal{D}) \geq ELBO = \mathbb{E}_{q(\phi)}[\ln p(\mathcal{D} | \phi)] - KL(q(\phi) || p(\phi))$

Because of the meta-learning, we have additional meta-parameter  $\theta$



By replacing:  $q(\phi) \Rightarrow q(\phi | \mathcal{D}^{tr}, \theta)$   $p(\phi | \mathcal{D}) \Rightarrow p(\phi | \mathcal{D}, \theta)$

We have:  $\max_{\theta} ELBO = \max_{\theta} \mathbb{E}_{q(\phi | \mathcal{D}^{tr}, \theta)}[\ln p(\mathcal{D} | \phi, \theta)] - KL(q(\phi | \mathcal{D}^{tr}, \theta) || p(\phi | \theta))$

Approximating the posterior of test data:  $p(\phi | \mathcal{D}, \theta) \Rightarrow p(\phi | \mathcal{D}^{te}, \theta)$

We have:  $\max_{\theta} ELBO = \max_{\theta} \mathbb{E}_{q(\phi | \mathcal{D}^{tr}, \theta)}[\ln p(\mathcal{D}^{te} | \phi, \theta)] - KL(q(\phi | \mathcal{D}^{tr}, \theta) || p(\phi | \theta))$

For all tasks, the final objective is:

$$\max_{\theta} \mathbb{E}_{p(\mathcal{D}_i)} \left[ \mathbb{E}_{q(\phi_i | \mathcal{D}_i^{tr}, \theta)} [\ln p(\mathcal{D}_i^{te} | \phi_i, \theta)] - KL(q(\phi_i | \mathcal{D}_i^{tr}, \theta) || p(\phi_i | \theta)) \right]$$

↓  
ELBO for  $\mathcal{D}_i$

# Amortized variational inference

Different way to model  $q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) \sim N(\mu_i, \sigma_i^2)$

$$\max_{\theta} \mathbb{E}_{p(\mathcal{D}_i)} [\mathbb{E}_{q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)} [\ln p(\mathcal{D}_i^{\text{te}} | \phi_i, \theta)] - KL(q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) || p(\phi_i | \theta))]$$

Two parametric meta-learning approaches:

Deterministic version

Bayesian version

- Black-box based.

**Key idea:** Train a neural network to represent

$$q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)$$

$$\phi_i = f_{\theta}(\mathcal{D}_i^{\text{tr}})$$

$$\lambda = \{\mu_i, \sigma_i^2\} = f(\mathcal{D}_i^{\text{tr}}, \theta)$$

- Optimization based (normally using gradient descent).

**Key idea:** Acquire  $\phi_i$  through optimization on  $\mathcal{D}_i^{\text{tr}}$ ,

meta parameter  $\theta$  serves as a prior

$$\phi_i = \arg \max_{\phi_i} \log p(\mathcal{D}_i^{\text{tr}} | \phi_i) + \log p(\phi_i | \theta)$$

$$\lambda_i = \arg \max_{\lambda_i} \log p(\mathcal{D}_i^{\text{tr}} | \phi_i) + \log p(\phi_i | \theta)$$



# Amortized variational inference

- Black-box based approach (VERSA)

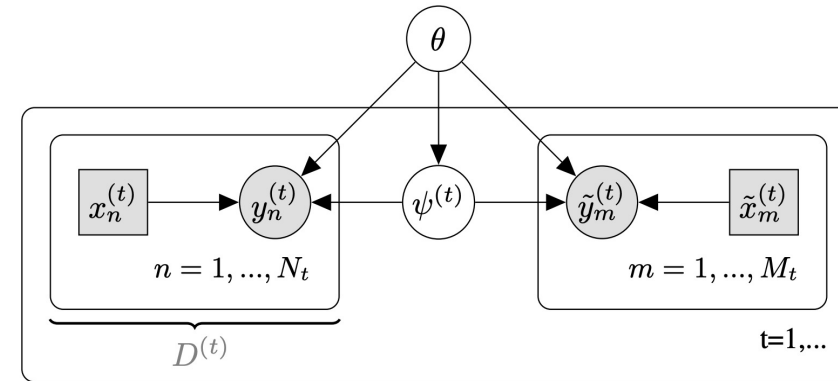
$$\lambda = \{\mu_i, \sigma_i^2\} = f(\mathcal{D}_i^{\text{tr}}, \theta)$$

- Meta learner has two components:

- Feature extraction network  $\theta$
- Amortization network  $\phi$

- Meta parameter  $\{\theta, \phi\}$

- Learner's parameter  $\psi^{(t)} = \{W^{(t)}, b^{(t)}\}$



Training data  $D^{(t)} = \{(x_n^{(t)}, y_n^{(t)})\}_{n=1}^{N_t}$ , and test data  $\{(\tilde{x}_m^{(t)}, \tilde{y}_m^{(t)})\}_{m=1}^{M_t}$

task specific parameters  $\{\psi^{(t)}\}_{t=1}^T$        $\psi^{(t)} = \{W^{(t)}, b^{(t)}\}$

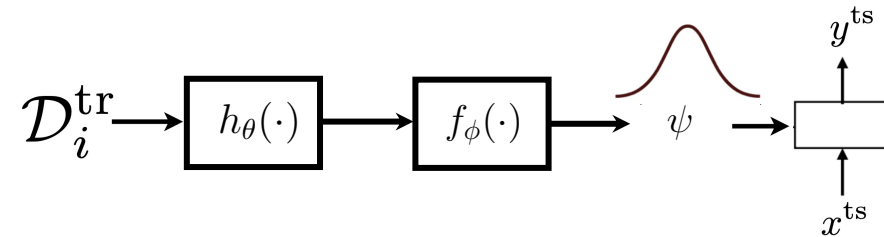
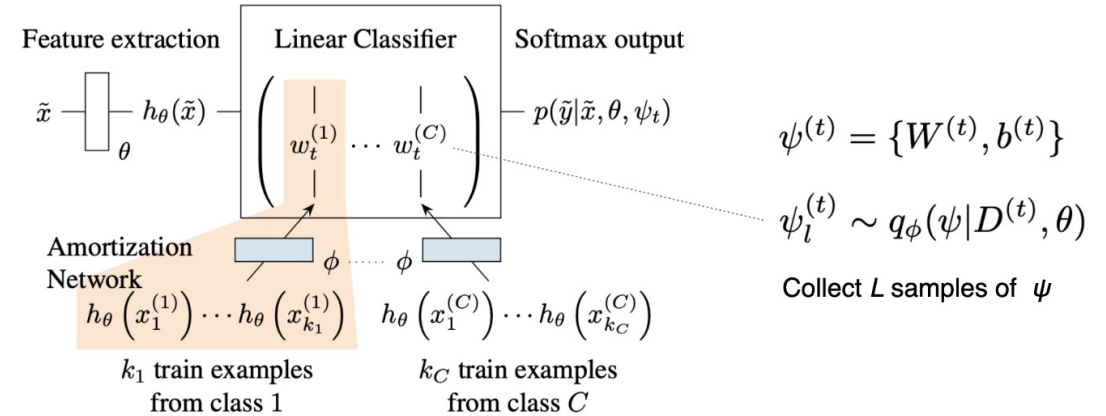
# Amortized variational inference

- Black-box based approach (VERSA)

$$\lambda = \{\mu_i, \sigma_i^2\} = f(\mathcal{D}_i^{\text{tr}}, \theta)$$

- Meta learner has two components:
  - Feature extraction network  $\theta$
  - Amortization network  $\phi$
- Meta parameter  $\{\theta, \phi\}$
- Learner's parameter  $\psi^{(t)} = \{W^{(t)}, b^{(t)}\}$
- Approximate the posterior with

$$\psi_i^{(t)} \sim q_\phi(\psi | D^{(t)}, \theta)$$



# Amortized variational inference

- Black-box based approach (VERSA)

$$\lambda = \{\mu_i, \sigma_i^2\} = f(\mathcal{D}_i^{\text{tr}}, \theta)$$

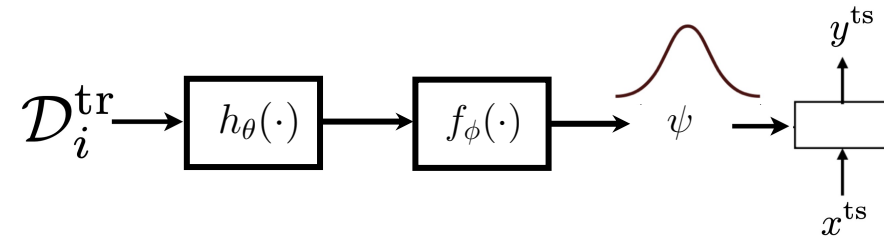
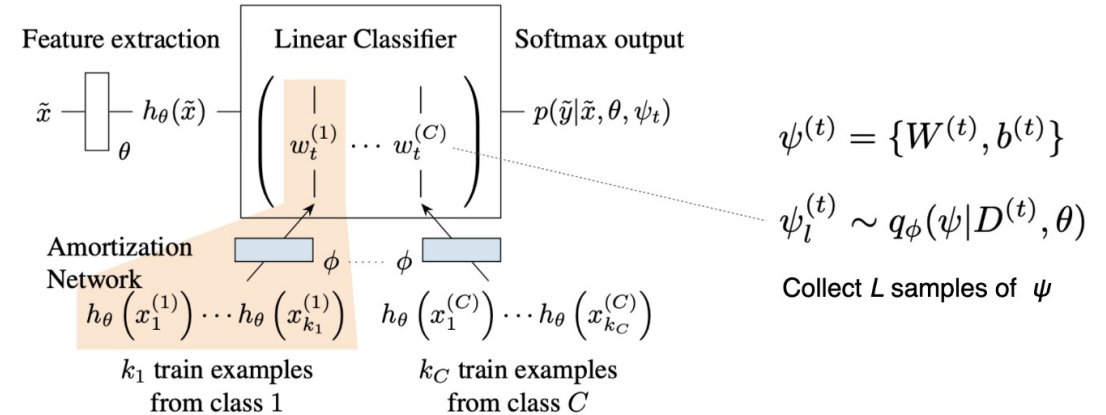
- Meta learner has two components:
  - Feature extraction network  $\theta$
  - Amortization network  $\phi$
- Meta parameter  $\{\theta, \phi\}$
- Learner's parameter  $\psi^{(t)} = \{W^{(t)}, b^{(t)}\}$
- Approximate the posterior with

$$\psi_i^{(t)} \sim q_\phi(\psi | D^{(t)}, \theta)$$

- Objective function

$$\hat{\mathcal{L}}(\theta, \phi) = \frac{1}{MT} \sum_{M,T} \log \frac{1}{L} \sum_{l=1}^L p(\tilde{y}_m^{(t)} | \tilde{x}_m^{(t)}, \psi_l^{(t)}, \theta), \quad \text{with } \psi_l^{(t)} \sim q_\phi(\psi | D^{(t)}, \theta)$$

$$\max_{\theta} \mathbb{E}_{p(\mathcal{D}_i)} [\mathbb{E}_{q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)} [\ln p(\mathcal{D}_i^{\text{te}} | \phi_i, \theta)] - KL(q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) || p(\phi_i | \theta))]$$



$$\begin{aligned} \delta(\phi_i^*) & p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta^*) \\ \delta(\theta^*) & p(\theta | \mathcal{D}_{\text{meta-train}}) \end{aligned}$$

<https://arxiv.org/pdf/1805.0921.pdf>

<https://jonathan-hui.medium.com/meta-learning-bayesian-meta-learning-weak-supervision-09f2eff3>

# Amortized variational inference

- Black-box based approach (VERSA)

$$\lambda = \{\mu_i, \sigma_i^2\} = f(\mathcal{D}_i^{\text{tr}}, \theta)$$

- Meta learner has two components:

- Feature extraction network  $\theta$
- Amortization network  $\phi$

- Meta parameter  $\{\theta, \phi\}$

- Learner's parameter  $\psi^{(t)} = \{W^{(t)}, b^{(t)}\}$

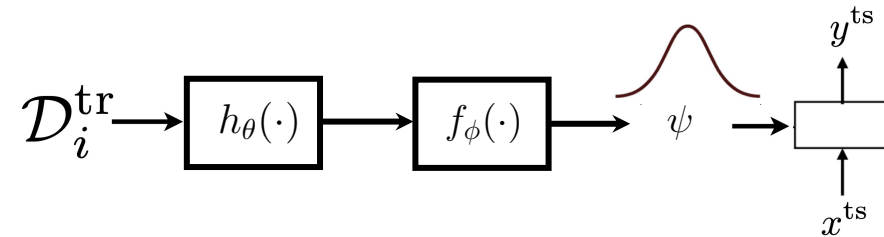
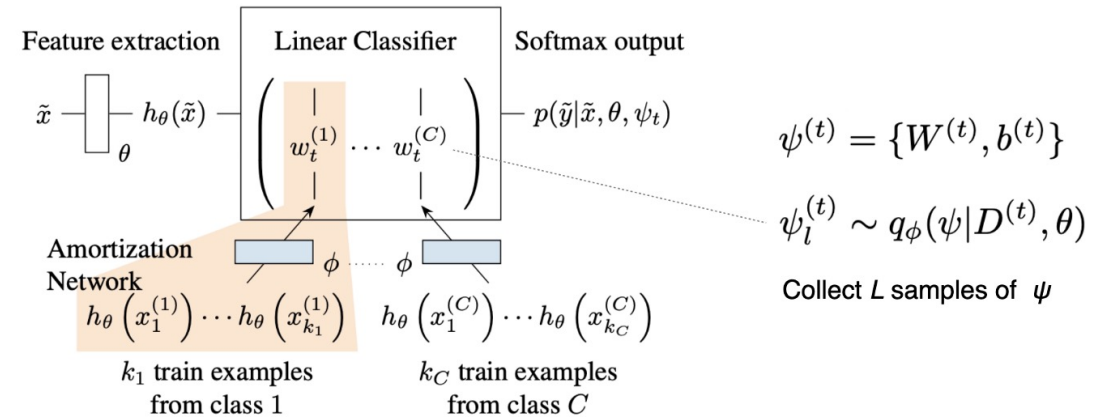
- Approximate the posterior with

$$\psi_i^{(t)} \sim q_\phi(\psi | D^{(t)}, \theta)$$

- Objective function

$$\hat{\mathcal{L}}(\theta, \phi) = \frac{1}{MT} \sum_{M,T} \log \frac{1}{L} \sum_{l=1}^L p(\tilde{y}_m^{(t)} | \tilde{x}_m^{(t)}, \psi_l^{(t)}, \theta), \quad \text{with } \psi_l^{(t)} \sim q_\phi(\psi | D^{(t)}, \theta)$$

$$\max_{\theta} \mathbb{E}_{p(\mathcal{D}_i)} [\mathbb{E}_{q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)} [\ln p(\mathcal{D}_i^{\text{te}} | \phi_i, \theta)] - KL(q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) || p(\phi_i | \theta))]$$



$\delta(\phi_i^*)$	X	$p(\phi_i   \mathcal{D}_i^{\text{tr}}, \theta^*)$	✓
$\delta(\theta^*)$	✓	$p(\theta   \mathcal{D}_{\text{meta-train}})$	X

<https://arxiv.org/pdf/1805.0921.pdf>

<https://jonathan-hui.medium.com/meta-learning-bayesian-meta-learning-weak-supervision-09f2eff3>

# Amortized variational inference

- Optimization based approach ([Amortized Bayesian Meta-Learning](#))

- Recall objective function:

$$\max_{\theta} \mathbb{E}_{p(\mathcal{D}_i)} \left[ \mathbb{E}_{q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)} [\ln p(\mathcal{D}_i^{\text{te}} | \phi_i, \theta)] - KL(q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) || p(\phi_i | \theta)) \right]$$

- $q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)$  is achieved by SGD on the mean and variance using  $\mathcal{D}_i^{\text{tr}}$

$$\lambda_i = \arg \max_{\lambda_i} \log p(\mathcal{D}_i^{\text{tr}} | \phi_i) + \log p(\phi_i | \theta)$$

$$q_{\theta}(\phi_i | \mathcal{D}_i^{(S)}) = \mathcal{N}(\phi_i; \mu_{\lambda}^{(K)}, \sigma_{\lambda}^{2(K)})$$

- SGD:

1.  $\lambda^{(0)} = \lambda^{(init)}$
2. for  $k = 0, \dots, K - 1$ , set  
 $\lambda^{(k+1)} = \lambda^{(k)} - \alpha \nabla_{\lambda^{(k)}} \mathcal{L}_{\mathcal{D}}(\lambda^{(k)}, \theta)$

- $\lambda^{(init)}$  is  $\theta$  like MAML, SGD is the inner loop optimization

# Amortized variational inference

- Optimization based approach (Amortized Bayesian Meta-Learning)

$$\begin{aligned} \delta(\phi_i^*) & p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta^*) \\ \delta(\theta^*) & p(\theta | \mathcal{D}_{\text{meta-train}}) \end{aligned}$$

---

## Algorithm 1 Meta-training

---

**Input:** Number of update steps  $K$ , Number of total episodes  $M$ , Inner learning rate  $\alpha$ , Outer learning rate  $\beta$

```

1: Initialize  $\theta = \{\mu_\theta, \sigma_\theta^2\}$ 
2:  $p(\theta) = \mathcal{N}(\mu; \mathbf{0}, \mathbf{I}) \cdot \prod_{l=1}^D \text{Gamma}(\tau_l; a_0, b_0)$ 
3: for  $i = 1$  to  $M$  do
4:    $\mathcal{D}_i = \{\mathcal{D}_i^{(S)}, \mathcal{D}_i^{(Q)}\}$ 
5:    $\mu_\lambda^{(0)} \leftarrow \mu_\theta; \sigma_\lambda^{2(0)} \leftarrow \sigma_\theta^2$ 
6:   for  $k = 0$  to  $K - 1$  do
7:      $\lambda^{(k)} \leftarrow \{\mu_\lambda^{(k)}, \sigma_\lambda^{2(k)}\}$ 
8:      $\mu_\lambda^{(k+1)} \leftarrow \mu_\lambda^{(k)} - \alpha \nabla_{\mu_\lambda^{(k)}} \mathcal{L}_{\mathcal{D}_i^{(S)}}(\lambda^{(k)}, \theta)$ 
9:      $\sigma_\lambda^{2(k+1)} \leftarrow \sigma_\lambda^{2(k)} - \alpha \nabla_{\sigma_\lambda^{2(k)}} \mathcal{L}_{\mathcal{D}_i^{(S)}}(\lambda^{(k)}, \theta)$ 
10:  end for
11:   $\lambda^{(K)} \leftarrow \{\mu_\lambda^{(K)}, \sigma_\lambda^{2(K)}\}$ 
12:   $q(\theta) = \mathbb{1}\{\mu = \mu_\theta\} \cdot \mathbb{1}\{\sigma^2 = \sigma_\theta^2\}$ 
13:   $\mu_\theta \leftarrow \mu_\theta - \beta \nabla_{\mu_\theta} [\mathcal{L}_{\mathcal{D}_i}(\lambda^{(K)}, \theta) + \frac{1}{M} \text{KL}(q(\theta) \| p(\theta))]$ 
14:   $\sigma_\theta^2 \leftarrow \sigma_\theta^2 - \beta \nabla_{\sigma_\theta^2} [\mathcal{L}_{\mathcal{D}_i}(\lambda^{(K)}, \theta) + \frac{1}{M} \text{KL}(q(\theta) \| p(\theta))]$ 
15: end for

```

SGD

---

## Algorithm 2 Meta-evaluation

---

**Input:** Number of update steps  $K$ , Dataset  $\mathcal{D} = \{\mathcal{D}^{(S)}, \mathcal{D}^{(Q)}\}$ , Parameters  $\theta = \{\mu_\theta, \sigma_\theta^2\}$ , Inner learning rate  $\alpha$

```

1:  $\mu_\lambda^{(0)} \leftarrow \mu_\theta; \sigma_\lambda^{2(0)} \leftarrow \sigma_\theta^2$ 
2: for  $k = 0$  to  $K - 1$  do
3:    $\lambda^{(k)} \leftarrow \{\mu_\lambda^{(k)}, \sigma_\lambda^{2(k)}\}$ 
4:    $\mu_\lambda^{(k+1)} \leftarrow \mu_\lambda^{(k)} - \alpha \nabla_{\mu_\lambda^{(k)}} \mathcal{L}_{\mathcal{D}^{(S)}}(\lambda^{(k)}, \theta)$ 
5:    $\sigma_\lambda^{2(k+1)} \leftarrow \sigma_\lambda^{2(k)} - \alpha \nabla_{\sigma_\lambda^{2(k)}} \mathcal{L}_{\mathcal{D}^{(S)}}(\lambda^{(k)}, \theta)$ 
6: end for
7:
8:  $q_\theta(\phi | D^{(S)}) = \mathcal{N}(\phi; \mu_\lambda^{(K)}, \sigma_\lambda^{2(K)})$ 
9: Evaluate  $D^{(Q)}$  using  $\mathbb{E}_{q_\theta(\phi | D^{(S)})} [p(D^{(Q)} | \phi)]$ 

```

---



# Amortized variational inference

- Optimization based approach (Amortized Bayesian Meta-Learning)

$\delta(\phi_i^*)$	X	$p(\phi_i   \mathcal{D}_i^{\text{tr}}, \theta^*)$	✓
$\delta(\theta^*)$	X	$p(\theta   \mathcal{D}_{\text{meta-train}})$	✓

---

## Algorithm 1 Meta-training

---

**Input:** Number of update steps  $K$ , Number of total episodes  $M$ , Inner learning rate  $\alpha$ , Outer learning rate  $\beta$

```

1: Initialize  $\theta = \{\mu_\theta, \sigma_\theta^2\}$ 
2:  $p(\theta) = \mathcal{N}(\mu; \mathbf{0}, \mathbf{I}) \cdot \prod_{l=1}^D \text{Gamma}(\tau_l; a_0, b_0)$ 
3: for  $i = 1$  to  $M$  do
4:    $\mathcal{D}_i = \{\mathcal{D}_i^{(S)}, \mathcal{D}_i^{(Q)}\}$ 
5:    $\mu_\lambda^{(0)} \leftarrow \mu_\theta; \sigma_\lambda^{2(0)} \leftarrow \sigma_\theta^2$ 
6:   for  $k = 0$  to  $K - 1$  do
7:      $\lambda^{(k)} \leftarrow \{\mu_\lambda^{(k)}, \sigma_\lambda^{2(k)}\}$ 
8:      $\mu_\lambda^{(k+1)} \leftarrow \mu_\lambda^{(k)} - \alpha \nabla_{\mu_\lambda^{(k)}} \mathcal{L}_{\mathcal{D}_i^{(S)}}(\lambda^{(k)}, \theta)$ 
9:      $\sigma_\lambda^{2(k+1)} \leftarrow \sigma_\lambda^{2(k)} - \alpha \nabla_{\sigma_\lambda^{2(k)}} \mathcal{L}_{\mathcal{D}_i^{(S)}}(\lambda^{(k)}, \theta)$ 
10:  end for
11:   $\lambda^{(K)} \leftarrow \{\mu_\lambda^{(K)}, \sigma_\lambda^{2(K)}\}$ 
12:   $q(\theta) = \mathbb{1}\{\mu = \mu_\theta\} \cdot \mathbb{1}\{\sigma^2 = \sigma_\theta^2\}$ 
13:   $\mu_\theta \leftarrow \mu_\theta - \beta \nabla_{\mu_\theta} [\mathcal{L}_{\mathcal{D}_i}(\lambda^{(K)}, \theta) + \frac{1}{M} \text{KL}(q(\theta) \| p(\theta))]$ 
14:   $\sigma_\theta^2 \leftarrow \sigma_\theta^2 - \beta \nabla_{\sigma_\theta^2} [\mathcal{L}_{\mathcal{D}_i}(\lambda^{(K)}, \theta) + \frac{1}{M} \text{KL}(q(\theta) \| p(\theta))]$ 
15: end for

```

SGD

---

## Algorithm 2 Meta-evaluation

---

**Input:** Number of update steps  $K$ , Dataset  $\mathcal{D} = \{\mathcal{D}^{(S)}, \mathcal{D}^{(Q)}\}$ , Parameters  $\theta = \{\mu_\theta, \sigma_\theta^2\}$ , Inner learning rate  $\alpha$

```

1:  $\mu_\lambda^{(0)} \leftarrow \mu_\theta; \sigma_\lambda^{2(0)} \leftarrow \sigma_\theta^2$ 
2: for  $k = 0$  to  $K - 1$  do
3:    $\lambda^{(k)} \leftarrow \{\mu_\lambda^{(k)}, \sigma_\lambda^{2(k)}\}$ 
4:    $\mu_\lambda^{(k+1)} \leftarrow \mu_\lambda^{(k)} - \alpha \nabla_{\mu_\lambda^{(k)}} \mathcal{L}_{\mathcal{D}^{(S)}}(\lambda^{(k)}, \theta)$ 
5:    $\sigma_\lambda^{2(k+1)} \leftarrow \sigma_\lambda^{2(k)} - \alpha \nabla_{\sigma_\lambda^{2(k)}} \mathcal{L}_{\mathcal{D}^{(S)}}(\lambda^{(k)}, \theta)$ 
6: end for
7:
8:  $q_\theta(\phi | \mathcal{D}^{(S)}) = \mathcal{N}(\phi; \mu_\lambda^{(K)}, \sigma_\lambda^{2(K)})$ 
9: Evaluate  $\mathcal{D}^{(Q)}$  using  $\mathbb{E}_{q_\theta(\phi | \mathcal{D}^{(S)})} [p(\mathcal{D}^{(Q)} | \phi)]$ 

```

---

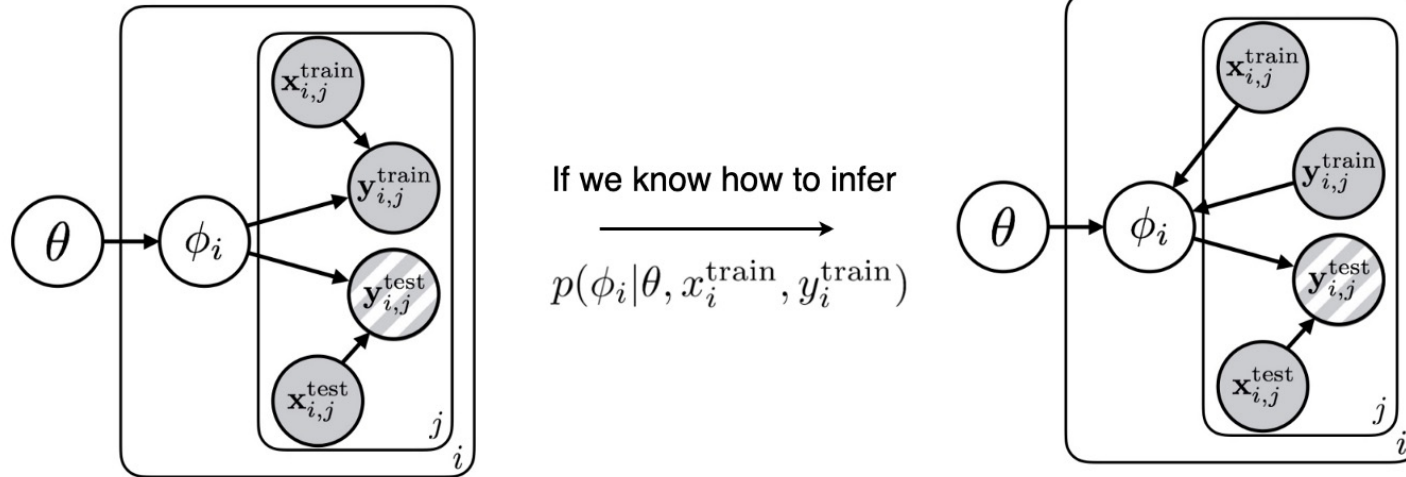
# Amortized variational inference

- Optimization based approach (Probabilistic MAML)

How about approximating posterior distribution directly on  $\theta$  ?

$\delta(\phi_i^*)$	✓	$p(\phi_i   \mathcal{D}_i^{\text{tr}}, \theta^*)$	✗
$\delta(\theta^*)$	✗	$p(\theta   \mathcal{D}_{\text{meta-train}})$	✓

Original graphical model



For example, in MAML,

$p(\phi_i | \mathbf{x}_i^{\text{tr}}, \mathbf{y}_i^{\text{tr}}, \theta) \approx \delta(\phi_i = \phi_i^*)$  where  $\phi_i^*$  is obtained via gradient descent starting from  $\theta$ .

# Amortized variational inference

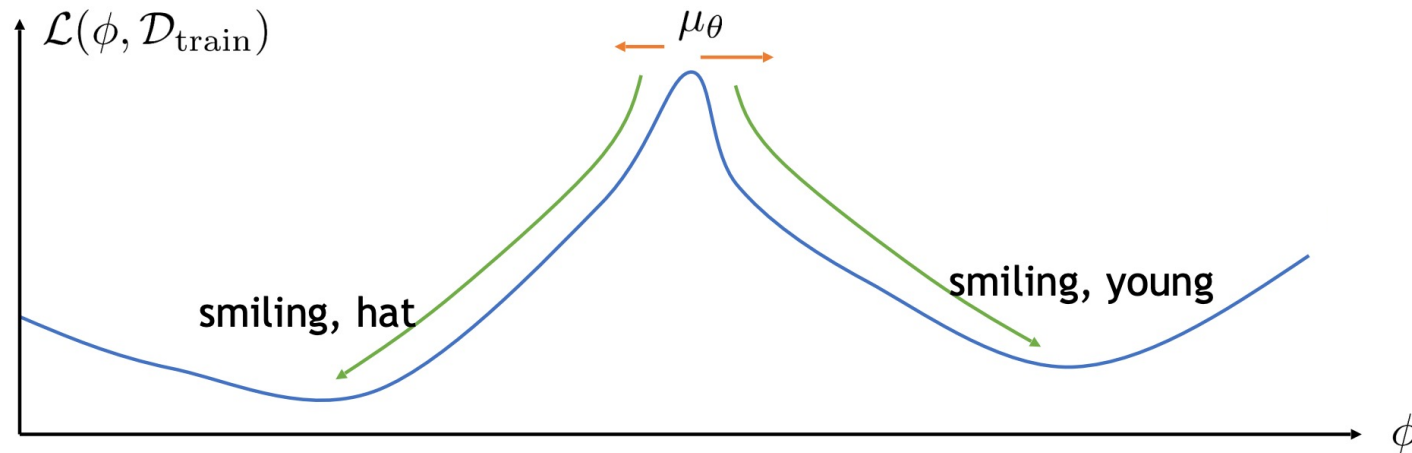
- Optimization based approach (Probabilistic MAML)

$$\theta \sim p(\theta) = \mathcal{N}(\mu_\theta, \Sigma_\theta)$$

**key idea:**  $p(\phi_i | \theta, x_i^{\text{train}}, y_i^{\text{train}}) \approx \delta(\hat{\phi}_i) \quad \hat{\phi}_i \approx \theta + \alpha \nabla_\theta \log p(y_i^{\text{train}} | x_i^{\text{train}}, \theta)$

What does ancestral sampling look like?

1.  $\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$
2.  $\phi_i \sim p(\phi_i | \theta, x_i^{\text{train}}, y_i^{\text{train}}) \approx \hat{\phi}_i = \theta + \alpha \nabla_\theta \log p(y_i^{\text{train}} | x_i^{\text{train}}, \theta)$



# Amortized variational inference

- Optimization based approach (Probabilistic MAML)

---

## Algorithm 1 Meta-training, differences from MAML in red

---

**Require:**  $p(\mathcal{T})$ : distribution over tasks

- 1: initialize  $\Theta := \{\mu_\theta, \sigma_\theta^2, \mathbf{v}_q, \gamma_p, \gamma_q\}$
- 2: **while** not done **do**
- 3:   Sample batch of tasks  $\mathcal{T}_i \sim p(\mathcal{T})$
- 4:   **for all**  $\mathcal{T}_i$  **do**
- 5:      $\mathcal{D}^{\text{tr}}, \mathcal{D}^{\text{test}} = \mathcal{T}_i$
- 6:     Evaluate  $\nabla_{\mu_\theta} \mathcal{L}(\mu_\theta, \mathcal{D}^{\text{test}})$
- 7:     Sample  $\theta \sim q = \mathcal{N}(\mu_\theta - \gamma_q \nabla_{\mu_\theta} \mathcal{L}(\mu_\theta, \mathcal{D}^{\text{test}}), \mathbf{v}_q)$
- 8:     Evaluate  $\nabla_\theta \mathcal{L}(\theta, \mathcal{D}^{\text{tr}})$
- 9:     Compute adapted parameters with gradient descent:  
       $\phi_i = \theta - \alpha \nabla_\theta \mathcal{L}(\theta, \mathcal{D}^{\text{tr}})$
- 10:    Let  $p(\theta | \mathcal{D}^{\text{tr}}) = \mathcal{N}(\mu_\theta - \gamma_p \nabla_{\mu_\theta} \mathcal{L}(\mu_\theta, \mathcal{D}^{\text{tr}}), \sigma_\theta^2)$
- 11:    Compute  $\nabla_\Theta (\sum_{\mathcal{T}_i} \mathcal{L}(\phi_i, \mathcal{D}^{\text{test}})$   
       $+ D_{\text{KL}}(q(\theta | \mathcal{D}^{\text{test}}) || p(\theta | \mathcal{D}^{\text{tr}}))$
- 12:    Update  $\Theta$  using Adam

Posterior distribution on test data  $q(\theta | \mathcal{D}^{\text{test}})$

Minimize the gap between two posterior distribution

---

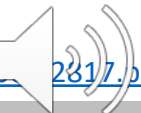
## Algorithm 2 Meta-testing

---

**Require:** training data  $\mathcal{D}_{\mathcal{T}}^{\text{tr}}$  for new task  $\mathcal{T}$

**Require:** learned  $\Theta$

- 1: Sample  $\theta$  from the prior  $p(\theta | \mathcal{D}^{\text{tr}})$
- 2: Evaluate  $\nabla_\theta \mathcal{L}(\theta, \mathcal{D}^{\text{tr}})$
- 3: Compute adapted parameters with gradient descent:  
       $\phi_i = \theta - \alpha \nabla_\theta \mathcal{L}(\theta, \mathcal{D}^{\text{tr}})$

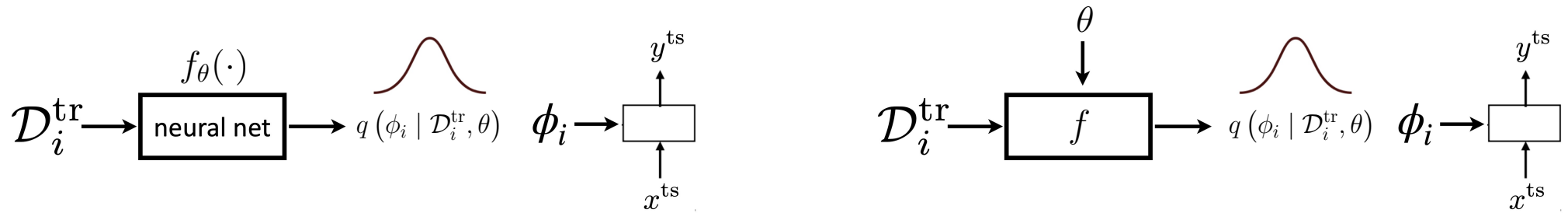


# Amortized variational inference

- Summary

- Latent variable models + variational inference (approximating  $p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta^*)$ )

approximate likelihood of latent variable model with variational lower bound



$$\max_{\theta} \mathbb{E}_{p(\mathcal{D}_i)} [\mathbb{E}_{q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)} [\ln p(\mathcal{D}_i^{\text{te}} | \phi_i, \theta)] - KL(q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) || p(\phi_i | \theta))]$$

**Pros:**

- + can represent non-Gaussian distributions over  $y^{\text{ts}}$
- + produces distribution over functions

**Cons:**

- Can only represent Gaussian distributions  $p(\phi_i | \theta)$

Not always restricting: e.g. if  $p(y_i^{\text{ts}} | x_i^{\text{ts}}, \phi_i, \theta)$  is also conditioned on  $\theta$ .

# Amortized variational inference

- Summary

- Latent variable models + variational inference (approximating  $p(\theta | \mathcal{D}_{\text{meta-train}})$ )

approximate likelihood of latent variable model with variational lower bound

1.  $\theta \sim \mathcal{N}(\mu_\theta, \Sigma_\theta)$

2.  $\phi_i \sim p(\phi_i | \theta, x_i^{\text{train}}, y_i^{\text{train}}) \approx \hat{\phi}_i = \theta + \alpha \nabla_\theta \log p(y_i^{\text{train}} | x_i^{\text{train}}, \theta)$

$$\min_{\lambda_\theta} \left( \sum_{\mathcal{T}_i} \mathcal{L}(\phi_i, \mathcal{D}^{\text{te}}) + KL(q(\theta | \mathcal{D}^{\text{te}}) \| p(\theta | \mathcal{D}^{\text{tr}})) \right)$$

**Pros:** Non-Gaussian posterior, simple at test time, only one model instance.

**Con:** More complex training procedure.



# Outline

- Introduction
  - Why Bayesian meta-learning?
  - The evidence lower bound (ELBO)
- Bayesian meta-learning approaches based on
  - Amortized variational inference
    - Black-box
    - Optimization
  - Bayesian ensembles
  - Bayesian neural networks
- Bayesian meta-learning evaluation
  - Qualitative visualization
  - Quantitative evaluation
  - Active-learning evaluation



# Bayesian ensembles

- Key idea: train separate models on bootstraps of the data

- Ensemble of MAML (EMAML)

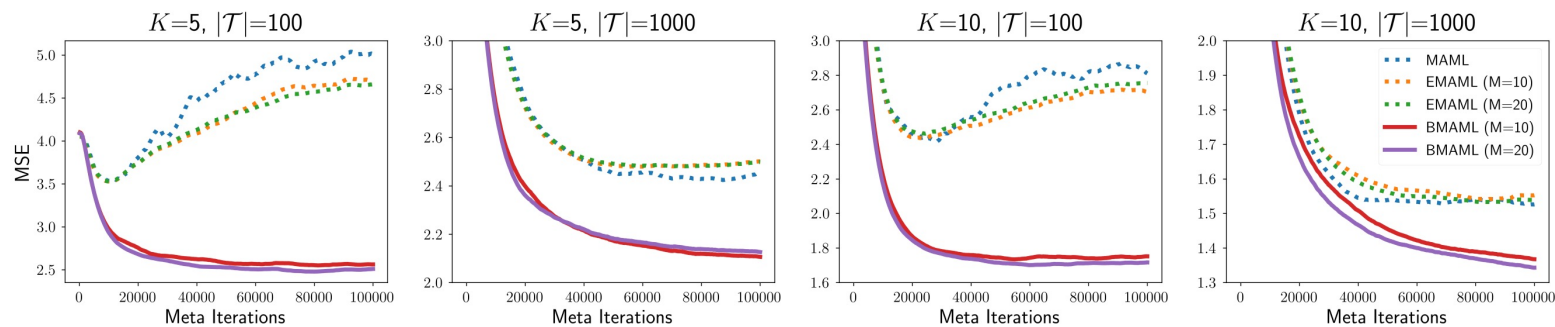
Train  $M$  independent MAML models then take the average

Does not work as the ensemble members are too similar

- Bayesian Meta-Learning with Chaser Loss (BMAML)

Use stein variational gradient descent (SVGD) to push the particles away from one another

Use chaser loss to improve the generalization ability



**Figure 1:** Sinusoidal regression experimental results (meta-testing performance) by varying the number of examples ( $K$ -shot) given for each task and the number of tasks  $|\mathcal{T}|$  used for meta-training.

[http://cs330.stanford.edu/fall2020/slides/cs330\\_bayesian\\_meta\\_learning\\_2020.pdf](http://cs330.stanford.edu/fall2020/slides/cs330_bayesian_meta_learning_2020.pdf)  
<https://proceedings.neurips.cc/paper/2018/file/e1021d43911ca2c1845910d84f40ac/paper.pdf>



# Bayesian ensembles

- Notations
  - Meta parameter  $\theta \Rightarrow \theta_0$
  - Learner's parameter  $\phi \Rightarrow \theta_\tau$
- Stein variational gradient descent (SVGD)

$$\theta_{t+1} \leftarrow \theta_t + \epsilon_t \phi(\theta_t) \quad \text{where} \quad \phi(\theta_t) = \frac{1}{M} \sum_{j=1}^M \left[ \underbrace{k(\theta_t^j, \theta_t)}_{\substack{\text{keep } M \\ \text{models}}} \nabla_{\theta_t^j} \log p(\theta_t^j) + \nabla_{\theta_t^j} \underbrace{k(\theta_t^j, \theta_t)}_{\substack{\text{positive-definite} \\ \text{kernel}}} \right],$$

$\downarrow$  push the models away from one another

- MAML vs. MAML with SVGD

---

### Algorithm 1 MAML

---

Sample a mini-batch of tasks  $\mathcal{T}_t$  from  $p(\mathcal{T})$   
**for** each task  $\tau \in \mathcal{T}_t$  **do**  
     $\theta_\tau \leftarrow \text{GD}_n(\theta_0; \mathcal{D}_\tau^{\text{tm}}, \alpha)$   
**end for**  
 $\theta_0 \leftarrow \theta_0 - \beta \nabla_{\theta_0} \sum_{\tau \in \mathcal{T}_t} \mathcal{L}(\theta_\tau; \mathcal{D}_\tau^{\text{val}})$

---

---

### Algorithm 2 Bayesian Fast Adaptation

---

Sample a mini-batch of tasks  $\mathcal{T}_t$  from  $p(\mathcal{T})$   
**for** each task  $\tau \in \mathcal{T}_t$  **do**  
     $\Theta_\tau(\Theta_0) \leftarrow \text{SVGD}_n(\Theta_0; \mathcal{D}_\tau^{\text{tm}}, \alpha)$   
**end for**  
 $\Theta_0 \leftarrow \Theta_0 - \beta \nabla_{\Theta_0} \sum_{\tau \in \mathcal{T}_t} \mathcal{L}_{\text{BFA}}(\Theta_\tau(\Theta_0); \mathcal{D}_\tau^{\text{val}})$

---

where  $\mathcal{L}_{\text{BFA}}(\Theta_\tau(\Theta_0); \mathcal{D}_\tau^{\text{val}}) = \log \left[ \frac{1}{M} \sum_{m=1}^M p(\mathcal{D}_\tau^{\text{val}} | \theta_\tau^m) \right]$

<https://proceedings.neurips.cc/paper/2018/file/e1021d43911ca2c1845910d84f40a6...paper.pdf>

# Bayesian ensembles

- Bayesian MAML with Chaser loss

---

**Algorithm 3** Bayesian Meta-Learning with Chaser Loss (BMAML)

---

```
1: Initialize  $\Theta_0$ 
2: for  $t = 0, \dots$  until converge do
3:   Sample a mini-batch of tasks  $\mathcal{T}_t$  from  $p(\mathcal{T})$ 
4:   for each task  $\tau \in \mathcal{T}_t$  do
5:     Compute chaser  $\Theta_\tau^n(\Theta_0) = \text{SVGD}_n(\Theta_0; \mathcal{D}_\tau^{\text{tr}}, \alpha)$ 
6:     Compute leader  $\Theta_\tau^{n+s}(\Theta_0) = \text{SVGD}_s(\Theta_\tau^n(\Theta_0); \mathcal{D}_\tau^{\text{tr}} \cup \mathcal{D}_\tau^{\text{val}}, \alpha)$ 
7:   end for
8:    $\Theta_0 \leftarrow \Theta_0 - \beta \nabla_{\Theta_0} \sum_{\tau \in \mathcal{T}_t} d_s(\Theta_\tau^n(\Theta_0) \parallel \text{stopgrad}(\Theta_\tau^{n+s}(\Theta_0)))$ 
9: end for
```

---

- Chaser loss

$$\mathcal{L}_{\text{BMAML}}(\Theta_0) = \sum_{\tau \in \mathcal{T}_t} d_s(\Theta_\tau^n \parallel \Theta_\tau^{n+s}) = \sum_{\tau \in \mathcal{T}_t} \sum_{m=1}^M \|\theta_\tau^{n,m} - \theta_\tau^{n+s,m}\|_2^2$$

$$\begin{aligned} \delta(\phi_i^*) & p(\phi_i \mid \mathcal{D}_i^{\text{tr}}, \theta^*) \\ \delta(\theta^*) & p(\theta \mid \mathcal{D}_{\text{meta-train}}) \end{aligned}$$

# Bayesian ensembles

- Bayesian MAML with Chaser loss

---

**Algorithm 3** Bayesian Meta-Learning with Chaser Loss (BMAML)

---

```
1: Initialize  $\Theta_0$ 
2: for  $t = 0, \dots$  until converge do
3:   Sample a mini-batch of tasks  $\mathcal{T}_t$  from  $p(\mathcal{T})$ 
4:   for each task  $\tau \in \mathcal{T}_t$  do
5:     Compute chaser  $\Theta_\tau^n(\Theta_0) = \text{SVGD}_n(\Theta_0; \mathcal{D}_\tau^{\text{tr}}, \alpha)$ 
6:     Compute leader  $\Theta_\tau^{n+s}(\Theta_0) = \text{SVGD}_s(\Theta_\tau^n(\Theta_0); \mathcal{D}_\tau^{\text{tr}} \cup \mathcal{D}_\tau^{\text{val}}, \alpha)$ 
7:   end for
8:    $\Theta_0 \leftarrow \Theta_0 - \beta \nabla_{\Theta_0} \sum_{\tau \in \mathcal{T}_t} d_s(\Theta_\tau^n(\Theta_0) \parallel \text{stopgrad}(\Theta_\tau^{n+s}(\Theta_0)))$ 
9: end for
```

---

- Chaser loss

$$\mathcal{L}_{\text{BMAML}}(\Theta_0) = \sum_{\tau \in \mathcal{T}_t} d_s(\Theta_\tau^n \parallel \Theta_\tau^{n+s}) = \sum_{\tau \in \mathcal{T}_t} \sum_{m=1}^M \|\theta_\tau^{n,m} - \theta_\tau^{n+s,m}\|_2^2$$

**Pros:** Simple, tends to work well,  
non-Gaussian distributions.

**Con:** Need to maintain M model instances.  
(or do gradient-based inference on **last layer only**)

$\delta(\phi_i^*)$	X	$p(\phi_i \mid \mathcal{D}_i^{\text{tr}}, \theta^*)$	✓
$\delta(\theta^*)$	X	$p(\theta \mid \mathcal{D}_{\text{meta-train}})$	✓

[http://cs330.stanford.edu/fall2020/slides/cs330\\_bayesian\\_meta\\_learning\\_2020.pdf](http://cs330.stanford.edu/fall2020/slides/cs330_bayesian_meta_learning_2020.pdf)

<https://proceedings.neurips.cc/paper/2018/file/e1021d43911ca2c1845910d84f40ac/paper.pdf>

# Outline

- Introduction
  - Why Bayesian meta-learning?
  - The evidence lower bound (ELBO)
- Bayesian meta-learning approaches based on
  - Amortized variational inference
    - Black-box
    - Optimization
  - Bayesian ensembles
  - Bayesian neural networks
- Bayesian meta-learning evaluation
  - Qualitative visualization
  - Quantitative evaluation
  - Active-learning evaluation



# Bayesian neural networks

- Key idea: explicit distribution over the space of network parameters
  - Monte Carlo dropout in neural networks can be used to perform variational inference to make it Bayesian
- model parameter is sampled by dropping different neurons

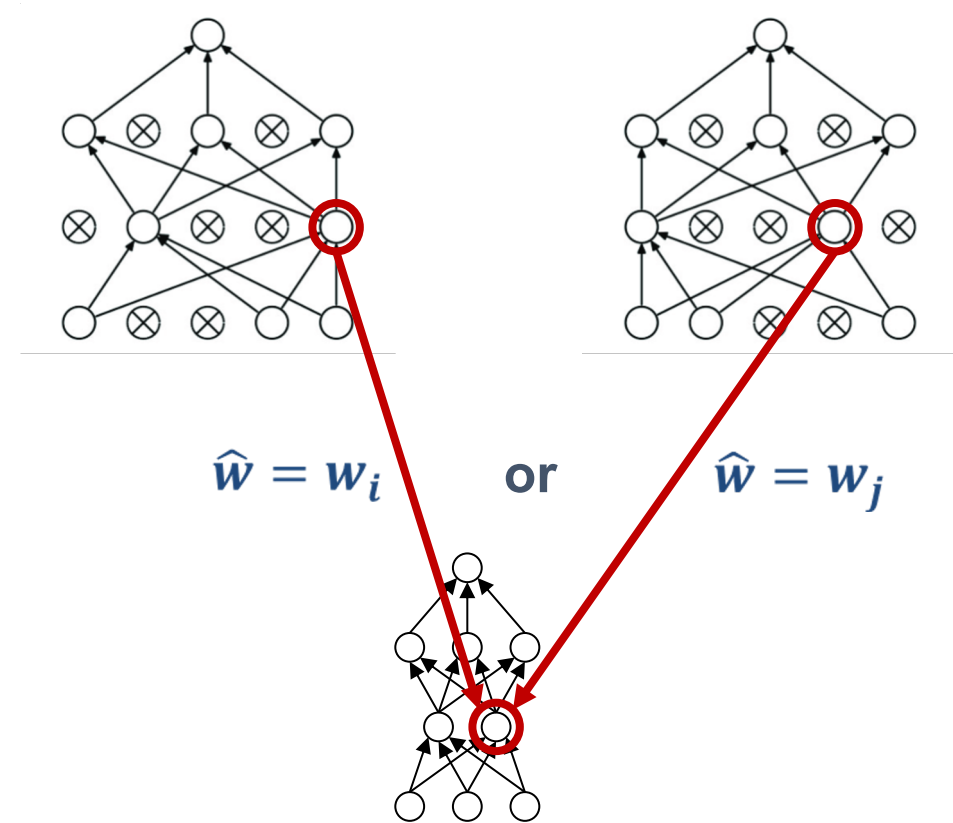
$q(\omega)$  :

$$\mathbf{W}_i = \mathbf{M}_i \cdot \text{diag}([z_{i,j}]_{j=1}^{K_i})$$

$$z_{i,j} \sim \text{Bernoulli}(p_i) \text{ for } i = 1, \dots, L, j = 1, \dots, K_{i-1}$$

Easiest way to get a distribution approximating the posterior distribution

$$q(\omega) \xrightarrow{\text{Approx.}} p(\omega | \mathcal{D}^{\text{tr}})$$



<https://arxiv.org/pdf/1506.02142.pdf>  
<https://www.hvnguyen.com/bayesian-neural-network-learning/>

# Bayesian neural networks

Combine the SGD with Bayesian neural networks (AGILE)

$$q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) \rightarrow p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta)$$

1. Initial learner's parameter with  $\theta$
2. Calculate the inner loop loss on  $\mathcal{D}_i^{\text{tr}}$  using model with dropout parametrized by  $\phi_i$
3. Update parameter  $\phi_i$  using SGD
4. Go back to step 2 for more gradient descent steps

Loss function:

- Inner loop loss for optimizing  $\phi_i$ :  $\lambda_i = \arg \max_{\lambda_i} \log p(\mathcal{D}_i^{\text{tr}} | \phi_i) + \log p(\phi_i | \theta)$ ,  $\lambda_i = M_i$  is a set of complete parameter (no dropout)

- Outer loop loss for optimizing  $\theta$ :
$$\begin{aligned}\theta^* &= \arg \max_{\theta \in \Theta} \prod_{i=1}^M p(\mathcal{D}_i^{\text{te}} | \mathcal{D}_i^{\text{tr}}, \theta) \\ &= \arg \max_{\theta \in \Theta} \prod_{i=1}^M \left( \int p(\mathcal{D}_i^{\text{te}} | \phi_i) p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta) d\phi_i \right) \\ &\approx \arg \max_{\theta \in \Theta} \prod_{i=1}^M \left( \frac{1}{T} \sum_{t=1}^T p(y_i^{\text{te}} | x_i^{\text{te}}, \phi_i^t) \right), \quad \text{where } \phi_i^t \sim q(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta).\end{aligned}$$

# Bayesian neural networks

Combine the SGD with Bayesian neural networks (AGILE)

- Dropout as well during test

$$p(\mathbf{y}^{\text{te}} | \mathbf{x}^{\text{te}}, \mathcal{D}^{\text{tr}}, \theta) = \int p(\mathbf{y}^{\text{te}} | \mathbf{x}^{\text{te}}, \phi) q(\phi | \mathcal{D}^{\text{tr}}, \theta) d\phi$$
$$\approx \frac{1}{T} \sum_{t=1}^T p(y^{\text{te}} | x^{\text{te}}, \phi^t), \quad \text{where } \phi^t \sim q(\phi | \mathcal{D}^{\text{tr}}, \theta)$$

Not the complete parameter set  $\mathbf{M}$

**Pros:** Simple, only one model instance

**Cons:** Can only model Gaussian distribution (Bayesian neural network), need to finetune the hyperparameter dropout rate

$\delta(\phi_i^*)$	X	$p(\phi_i   \mathcal{D}_i^{\text{tr}}, \theta^*)$	✓
$\delta(\theta^*)$	✓	$p(\theta   \mathcal{D}_{\text{meta-train}})$	X



# Bayesian meta-learning approaches summary

- **Latent variable models + variational inference**

approximate likelihood of latent variable model with variational lower bound

**Approximating**

$$p(\phi_i | \mathcal{D}_i^{\text{tr}}, \theta^*)$$

**Pros:**

- + can represent non-Gaussian distributions over  $y^{\text{ts}}$
- + produces distribution over functions

**Cons:**

- Can only represent Gaussian distributions  $p(\phi_i | \theta)$

$$p(\theta | \mathcal{D}_{\text{meta-train}})$$

**Pros:** Non-Gaussian posterior, simple at test time, only one model instance.

**Con:** More complex training procedure.

- **Bayesian ensembles**

particle-based representation: train separate models on bootstraps of the data

**Pros:** Simple, tends to work well, non-Gaussian distributions.

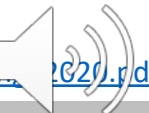
**Con:** Need to maintain M model instances. (or do gradient-based inference on last layer only)

- **Bayesian neural networks**

explicit distribution over the space of network parameters

**Pros:** Simple, only one model instance

**Cons:** Can only model Gaussian distribution (Bayesian neural network), need to finetune the hyperparameter dropout rate





# Outline

- Introduction
  - Why Bayesian meta-learning?
  - The evidence lower bound (ELBO)
- Bayesian meta-learning approaches based on
  - Amortized variational inference
    - Black-box
    - Optimization
  - Bayesian ensembles
  - Bayesian neural networks
- Bayesian meta-learning evaluation
  - Qualitative visualization
  - Quantitative evaluation
  - Active-learning evaluation

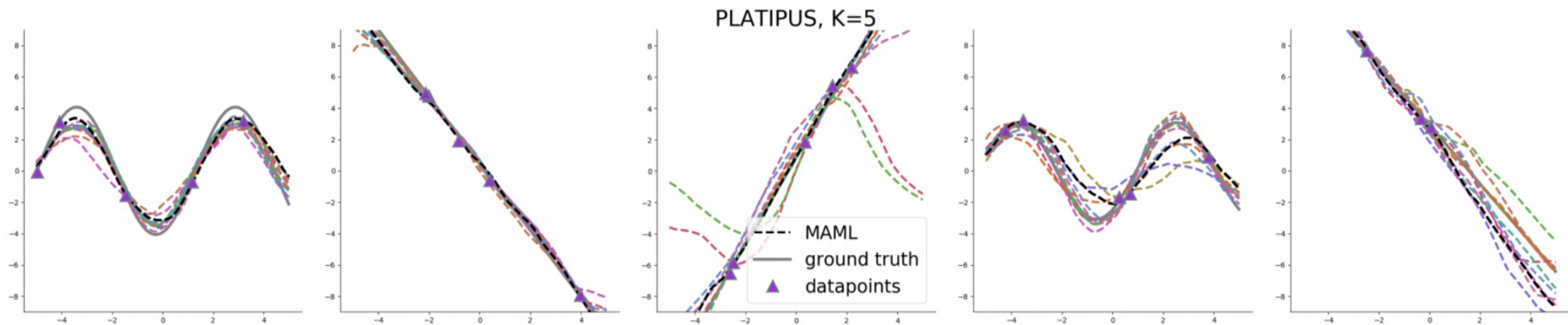


# Qualitative visualization

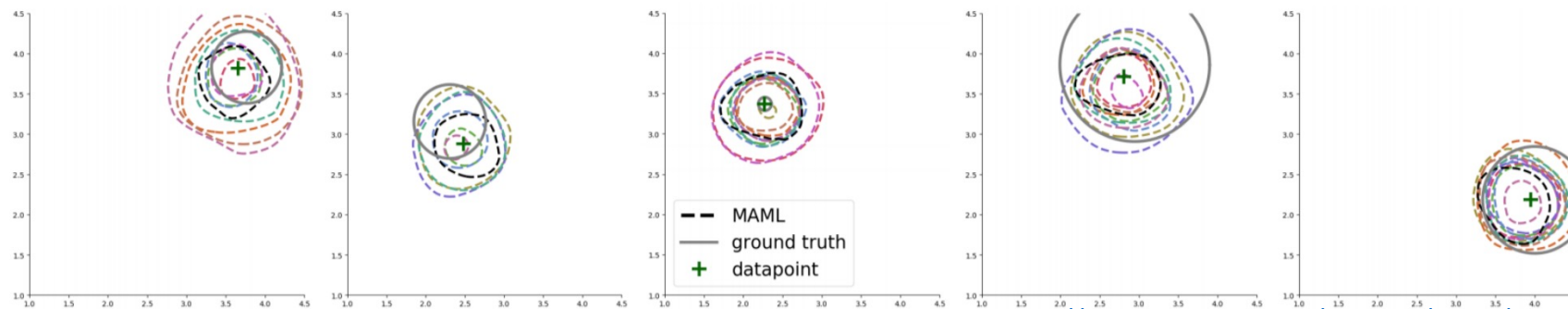
## Qualitative Evaluation on Toy Problems with Ambiguity

(Finn\*, Xu\*, Levine, NeurIPS '18)

Ambiguous regression:



Ambiguous classification:

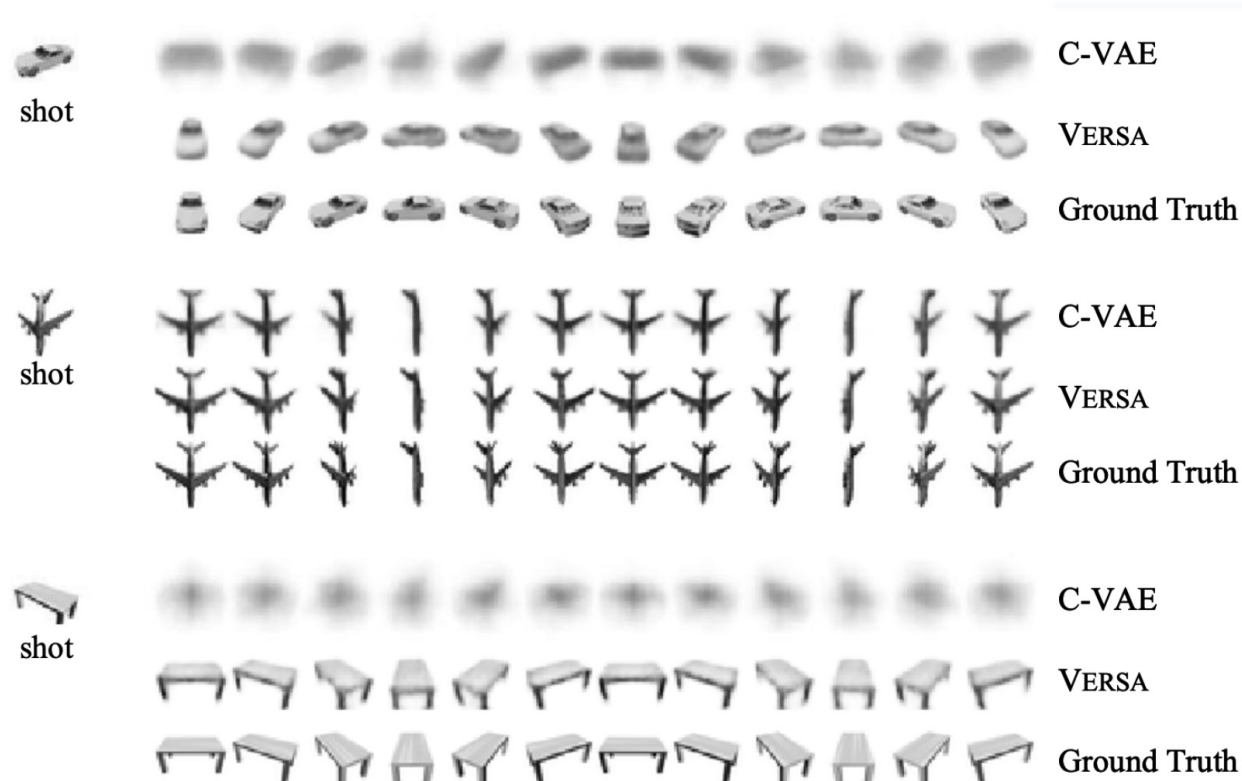


[http://cs330.stanford.edu/fall2020/slides/cs330\\_bayesian\\_meta\\_learning\\_020.pdf](http://cs330.stanford.edu/fall2020/slides/cs330_bayesian_meta_learning_020.pdf)

# Quantitative evaluation

## Evaluation on Ambiguous Generation Tasks

(Gordon et al., ICLR '19)



Model	MSE	SSIM
C-VAE 1-shot	0.0269	0.5705
VERSA 1-shot	0.0108	0.7893
VERSA 5-shot	0.0069	0.8483

**Table 2:** View reconstruction test results.

# Quantitative evaluation

## Accuracy, Mode Coverage, & Likelihood on Ambiguous Tasks

(Finn\*, Xu\*, Levine, NeurIPS '18)



- (a)
- ✓ Mouth Open
  - ✓ Wearing Hat
  - ✓ Young
- (b)
- ✓ Mouth Open
  - ✗ Wearing Hat
  - ✓ Young
- (c)
- ✓ Mouth Open
  - ✗ Wearing Hat
  - ✓ Young

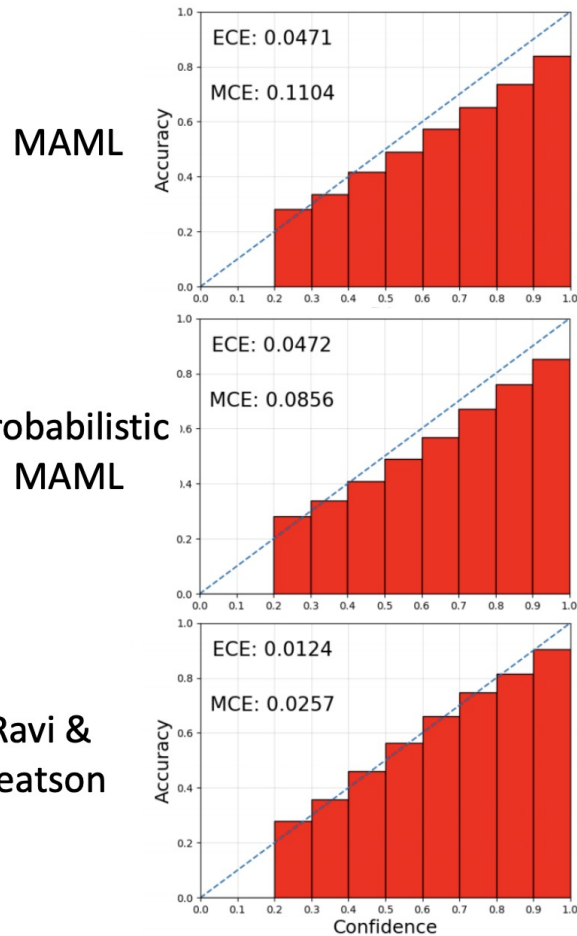
Ambiguous celebA (5-shot)			
	Accuracy	Coverage (max=3)	Average NLL
MAML	<b>89.00 ± 1.78%</b>	1.00 ± 0.0	0.73 ± 0.06
MAML + noise	84.3 ± 1.60 %	1.89 ± 0.04	0.68 ± 0.05
<b>PLATIPUS (ours) (KL weight = 0.05)</b>	<b>88.34 ± 1.06 %</b>	1.59 ± 0.03	0.67 ± 0.05
<b>PLATIPUS (ours) (KL weight = 0.15)</b>	<b>87.8 ± 1.03 %</b>	<b>1.94 ± 0.04</b>	<b>0.56 ± 0.04</b>

# Quantitative evaluation

## Reliability Diagrams & Accuracy

(Ravi & Beatson, ICLR '19)

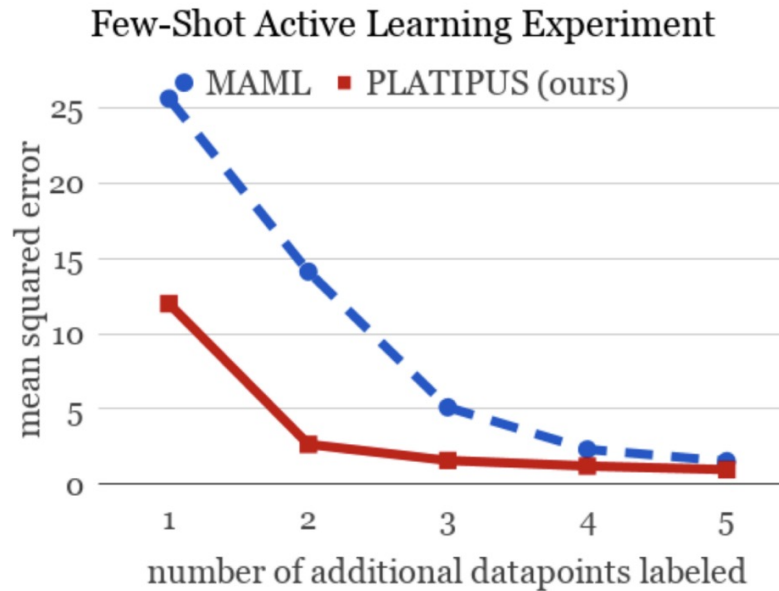
*miniImageNet*: 1-shot, 5-class



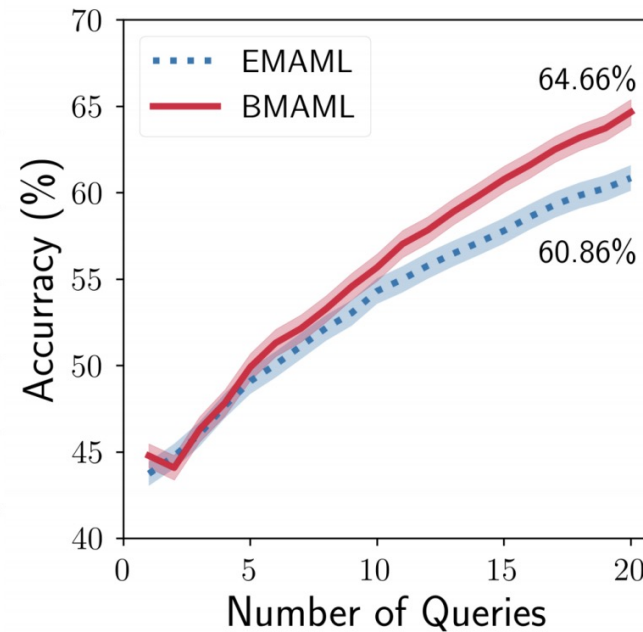
<i>miniImageNet</i>	1-shot, 5-class
MAML (ours)	47.0 $\pm$ 0.59
Prob. MAML (ours)	47.8 $\pm$ 0.61
Our Model	45.0 $\pm$ 0.60

# Active-learning evaluation

Finn\*, Xu\*, Levine, NeurIPS '18  
Sinusoid Regression



Kim et al. NeurIPS '18  
MinilmageNet



Both experiments:

- Sequentially choose datapoint with **maximum predictive entropy** to be labeled
- or choose datapoint at random (MAML)

# Take away

- Uncertainty is important when study meta-learning as few annotated samples are provided for each tasks
- Uncertainty can exist in either meta parameter or learner's parameter or both
- There are several tools to make the meta learning algorithm Bayesian:
  - Latent variable models + variational inference
  - Bayesian ensembles
  - Bayesian neural networks
- Learn different ways to evaluate the Bayesian meta learning algorithm



