Bayesian Meta-Learning

CS 330
Logistics

Homework 2 due next Wednesday.

Project proposal due in two weeks.

Poster presentation: Tues 12/3 at 1:30 pm.
Disclaimers

Bayesian meta-learning is an active area of research
(like most of the class content)

More questions than answers.

This lecture covers some of the most advanced topics of the course.

So ask questions!
Recap from last time.

**Computation graph perspective**

**Black-box**

\[ y_{ts}^{\text{ts}} = f_\theta(D_{i}^{\text{tr}}, x_{ts}) \]

**Optimization-based**

\[ y_{ts}^{\text{ts}} = f_{\text{MAML}}(D_{i}^{\text{tr}}, x_{ts}) = f_{\phi_i}(x_{ts}) \]

where \( \phi_i = \theta - \alpha \nabla_\theta \mathcal{L}(\theta, D_{i}^{\text{tr}}) \)

**Non-parametric**

\[ y_{ts}^{\text{ts}} = f_{\text{PN}}(D_{i}^{\text{tr}}, x_{ts}) = \text{softmax}(-d(f_\theta(x_{ts}), c_n)) \]

where \( c_n = \frac{1}{K} \sum_{(x,y) \in D_{i}^{\text{tr}}} \mathbb{1}(y=n)f_\theta(x) \)
Recap from last time.

*Algorithmic properties perspective*

**Expressive power**

the ability for \( f \) to represent a range of learning procedures

*Why?*

scalability, applicability to a range of domains

**Consistency**

learned learning procedure will solve task with enough data

*Why?*

reduce reliance on meta-training tasks,

good OOD task performance

These properties are important for most applications!
Recap from last time.

**Algorithmic properties perspective**

- **Expressive power**
  - the ability for $f$ to represent a range of learning procedures
  - *Why?* scalability, applicability to a range of domains

- **Consistency**
  - learned learning procedure will solve task with enough data
  - *Why?* reduce reliance on meta-training tasks, good OOD task performance

- **Uncertainty awareness**
  - ability to reason about ambiguity during learning
  - *Why?* active learning, calibrated uncertainty, RL principled Bayesian approaches

*this lecture*
Plan for Today

Why be Bayesian?
Bayesian meta-learning approaches
How to evaluate Bayesians.
**Multi-Task & Meta-Learning Principles**

Training and testing must match.
Tasks must share “structure.”

What does “structure” mean? statistical dependence on shared latent information $\theta$

If you condition on that information,
- task parameters become independent
  i.e. $\phi_{i_1} \perp \phi_{i_2} | \theta$
  and are not otherwise independent $\phi_{i_1} \not\perp \phi_{i_2}$
- hence, you have a lower entropy
  i.e. $\mathcal{H}(p(\phi_i | \theta)) < \mathcal{H}(p(\phi_i))$

**Thought exercise #1:** If you can identify $\theta$ (i.e. with meta-learning), when should learning $\phi_i$ be faster than learning from scratch?

**Thought exercise #2:** what if $\mathcal{H}(p(\phi_i | \theta)) = 0$?
Training and testing must match.
Tasks must share “structure.”

What does “structure” mean?

- statistical dependence on shared latent information \( \theta \)

What information might \( \theta \) contain...

...in the toy sinusoid problem?

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

...in the machine translation example?

- \( \theta \) corresponds to the family of all language pairs

Note that \( \theta \) is narrower than the space of all possible functions.

Thought exercise #3: What if you meta-learn without a lot of tasks?

“meta-overfitting”
Recall parametric approaches: Use deterministic \( p(\phi_i | D_{i}^{\text{tr}}, \theta) \) (i.e. a point estimate)

**Why/when is this a problem?**

Few-shot learning problems may be *ambiguous*. (even with prior)

Can we learn to *generate hypotheses* about the underlying function? i.e. sample from \( p(\phi_i | D_{i}^{\text{tr}}, \theta) \)

**Important for:**

- safety-critical few-shot learning (e.g. medical imaging)
- learning to *actively learn*
- learning to *explore* in meta-RL

**Active learning w/ meta-learning:** Woodward & Finn ’16, Konyushkova et al. ’17, Bachman et al. ’17
Plan for Today

Why be Bayesian?

**Bayesian meta-learning approaches**

How to evaluate Bayesians.
\[ y^{ts} = f_\theta (D^{tr}_i, x^{ts}) \]

**Black-box**

**Optimization-based**

\[ y^{ts} = f_{\text{MAML}} (D^{tr}_i, x^{ts}) \]
\[ = f_{\phi_i} (x^{ts}) \]
where \( \phi_i = \theta - \alpha \nabla \theta L(\theta, D^{tr}_i) \)

**Non-parametric**

\[ y^{ts} = f_{\text{PN}} (D^{tr}_i, x^{ts}) \]
\[ = \text{softmax} (-d(f_\theta(x^{ts}), c_n)) \]
where \( c_n = \frac{1}{K} \sum_{(x,y) \in D^{tr}_i} \mathbb{1}(y = n) f_\theta(x) \)

**Version 0:** Let \( f \) output the parameters of a distribution over \( y^{ts} \).

For example:
- probability values of discrete **categorical distribution**
- mean and variance of a **Gaussian**
- means, variances, and mixture weights of a **mixture of Gaussians**
- for multi-dimensional \( y^{ts} \): parameters of a **sequence of distributions** (i.e. autoregressive model)

Then, optimize with maximum likelihood.
Version 0: Let $f$ output the parameters of a distribution over $y^{ts}$.

For example:
- probability values of discrete categorical distribution
- mean and variance of a Gaussian
- means, variances, and mixture weights of a mixture of Gaussians
- for multi-dimensional $y^{ts}$: parameters of a sequence of distributions (i.e. autoregressive model)

Then, optimize with maximum likelihood.

Pros:
+ simple
+ can combine with variety of methods

Cons:
- can’t reason about uncertainty over the underlying function [to determine how uncertainty across datapoints relate]
- limited class of distributions over $y^{ts}$ can be expressed
- tends to produce poorly-calibrated uncertainty estimates

Thought exercise #4: Can you do the same maximum likelihood training for $\phi$?
The Bayesian Deep Learning Toolbox

*a broad one-slide overview*

(CS 236 provides a thorough treatment)

**Goal:** represent distributions with neural networks

- **Latent variable models + variational inference** (Kingma & Welling ‘13, Rezende et al. ‘14):
  - approximate likelihood of latent variable model with variational lower bound
- **Bayesian ensembles** (Lakshminarayanan et al. ‘17):
  - particle-based representation: train separate models on bootstraps of the data
- **Bayesian neural networks** (Blundell et al. ‘15):
  - explicit distribution over the space of network parameters
- **Normalizing Flows** (Dinh et al. ‘16):
  - invertible function from latent distribution to data distribution
- **Energy-based models & GANs** (LeCun et al. ‘06, Goodfellow et al. ‘14):
  - estimate unnormalized density

We’ll see how we can leverage the first two. The others could be useful in developing new methods.
Background: The Variational Lower Bound

Observed variable $x$, latent variable $z$

\[ \log p(x) \geq \mathbb{E}_{q(z|x)} \left[ \log p(x, z) \right] + \mathcal{H}(q(z | x)) \]

Can also be written as:

\[ = \mathbb{E}_{q(z|x)} \left[ \log p(x | z) \right] - D_{KL} \left( q(z | x) \| p(z) \right) \]

$p$: model $p(x | z)$ represented w/ neural net,
$p(z)$ represented as $\mathcal{N}(0, I)$
model parameters $\theta$,
variational parameters $\phi$

$q(z | x)$: inference network, variational distribution

Problem: need to backprop through sampling
i.e. compute derivative of $\mathbb{E}_q$ w.r.t. $q$

Reparametrization trick
For Gaussian $q(z | x)$:
\[ q(z | x) = \mu_q + \sigma_q \epsilon \]
where $\epsilon \sim \mathcal{N}(0, I)$

Can we use amortized variational inference for meta-learning?
Bayesian black-box meta-learning
with standard, deep variational inference

\[ D_{tr} \xrightarrow{\text{neural net}} q(\phi_i | D_{tr}) \phi_i \xrightarrow{y_{ts}} \]

**Standard VAE:**

Observed variable \( x \), latent variable \( z \)

ELBO: \( \mathbb{E}_{q(z|x)} \left[ \log p(x | z) \right] - D_{KL} \left( q(z | x) \| p(z) \right) \)

\( p \): model, represented by a neural net

\( q \): inference network, variational distribution

**Meta-learning:**

Observed variable \( \mathcal{D} \), latent variable \( \phi \)

\( \max \mathbb{E}_{q(\phi)} \left[ \log p(\mathcal{D} | \phi) \right] - D_{KL} \left( q(\phi) \| p(\phi) \right) \)

Final objective (for completeness): \( \max_\theta \mathbb{E}_{\mathcal{T}_i} \left[ \mathbb{E}_{q(\phi_i | D_{tr}, \theta)} \left[ \log p \left( y_{ts}^{i | x_{ts}^{i}}, \phi_i \right) \right] - D_{KL} \left( q \left( \phi_i | D_{tr}, \theta \right) \| p(\phi | \theta) \right) \right] \)

What should \( q \) condition on?

\[
\begin{align*}
\max_\phi \mathbb{E}_{\mathcal{D}_{tr}} \left[ \log p(\mathcal{D} | \phi) \right] & - D_{KL} \left( q(\phi | \mathcal{D}_{tr}) \| p(\phi) \right) \\
\max_\phi \mathbb{E}_{\mathcal{D}_{tr}} \left[ \log p \left( y_{ts} | x_{ts}, \phi \right) \right] & - D_{KL} \left( q \left( \phi | \mathcal{D}_{tr} \right) \| p(\phi) \right)
\end{align*}
\]

What about the meta-parameters \( \theta \)?

\[
\begin{align*}
\max_\theta \mathbb{E}_{\mathcal{D}_{tr}, \theta} \left[ \log p \left( y_{ts} | x_{ts}, \phi \right) \right] & - D_{KL} \left( q \left( \phi | \mathcal{D}_{tr}, \theta \right) \| p(\phi | \theta) \right) \\
\text{Can also condition on } \theta \text{ here}
\end{align*}
\]
Bayesian black-box meta-learning
with standard, deep variational inference

\[
\max_{\theta} \mathbb{E}_{\mathcal{D}_i^{tr}} \left[ \mathbb{E}_{q(\phi_i | \mathcal{D}_i^{tr}, \theta)} \left[ \log p(y_{ts}^{i} | x_{ts}^{i}, \phi_i) \right] - D_{KL} \left( q(\phi_i | \mathcal{D}_i^{tr}, \theta) \parallel p(\phi_i | \theta) \right) \right]
\]

Pros:
+ can represent non-Gaussian distributions over \( y_{ts}^{i} \)
+ produces distribution over functions

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

Not always restricting: e.g. if \( p(y_{ts}^{i} | x_{ts}^{i}, \phi_i, \theta) \) is also conditioned on \( \theta \).
What about Bayesian optimization-based meta-learning?

Recall: *Recasting Gradient-Based Meta-Learning as Hierarchical Bayes* (Grant et al. ’18)

**Task-specific parameters**

**Meta-parameters**

\[
\begin{align*}
\theta & \rightarrow \phi_i \rightarrow X_{in} \rightarrow N \rightarrow T_i \\
\text{max} \log \prod_i p(D_i | \theta) & = \log \prod_i \int p(D_i | \phi_i) p(\phi_i | \theta) d\phi_i \quad \text{(empirical Bayes)} \\
& \approx \log \prod_i p(D_i | \hat{\phi}_i) p(\hat{\phi}_i | \theta)
\end{align*}
\]

How to compute MAP estimate?

**Gradient descent with early stopping = MAP inference** under **Gaussian prior** with mean at initial parameters [Santos ’96]

(exact in linear case, approximate in nonlinear case)

Provides a Bayesian interpretation of MAML.

But, we can’t sample from \( p(\phi_i | \theta, D_i^{tr}) \)!
What about Bayesian optimization-based meta-learning?

Recall: Bayesian black-box meta-learning
with standard, deep variational inference

\[
\max_\theta \mathbb{E}_{\mathcal{F}_i} \left[ \mathbb{E}_{q(\phi_i|\mathcal{D}_i^{tr}, \theta)} \left[ \log p(y_i^{ts}|x_i^{ts}, \phi_i) \right] - D_{KL} \left( q(\phi_i|\mathcal{D}_i^{tr}, \theta) \| p(\phi_i|\theta) \right) \right]
\]

\( q \): an arbitrary function

\( q \) can include a gradient operator!

Amortized Bayesian Meta-Learning
(Ravi & Beatson ’19)

\( q \) corresponds to SGD on the mean & variance of neural network weights \((\mu_{\phi}, \sigma^2_{\phi})\), w.r.t. \( \mathcal{D}_i^{tr} \)

Pro: Running gradient descent at test time.

Con: \( p(\phi_i|\theta) \) modeled as a Gaussian.

Can we model non-Gaussian posterior?
What about Bayesian optimization-based meta-learning?

Can we use ensembles?

Kim et al. Bayesian MAML ’18

Ensemble of MAMLs (EMAML)

Train M independent MAML models.

Won’t work well if ensemble members are too similar.

Can we model non-Gaussian posterior over all parameters?

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)

Stein Variational Gradient (BMAML)

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

\[
\phi(\theta_t) = \frac{1}{M} \sum_{j=1}^{M} \left[ k(\theta_t^j, \theta_t) \nabla_{\theta_t^j} \log p(\theta_t^j) + \nabla_{\theta_t^j} k(\theta_t^j, \theta_t) \right]
\]

Optimize for distribution of M particles to produce high likelihood.

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

Note: Can also use ensembles w/ black-box, non-parametric methods!
What about Bayesian *optimization-based* meta-learning?

Sample parameter vectors with a procedure like **Hamiltonian Monte Carlo**?

Finn*, Xu*, Levine. Probabilistic MAML ‘18

**Intuition:** Learn a prior where a random kick can put us in different modes

\[ \mathcal{L}(\phi, \mathcal{D}_{\text{train}}) \]

\[ \phi \leftarrow \theta + \epsilon \]

\[ \phi \leftarrow \phi + \alpha \nabla_{\phi} \mathcal{L}(\phi, \mathcal{D}_{\text{train}}) \]
What about Bayesian **optimization-based** meta-learning?

Sample parameter vectors with a procedure like **Hamiltonian Monte Carlo**?

Finn*, Xu*, Levine. Probabilistic MAML ‘18

\[ \theta \sim p(\theta) = \mathcal{N}(\mu_\theta, \Sigma_\theta) \quad \phi_i \sim p(\phi_i|\theta) \]

(not single parameter vector anymore)

Goal: sample \( \phi_i \sim p(\phi_i|x^{\text{train}}_i, y^{\text{train}}_i, x^{\text{test}}_i) \)

\[
p(\phi_i|x^{\text{train}}_i, y^{\text{train}}_i) \propto \int p(\theta)p(\phi_i|\theta)p(y^{\text{train}}_i|x^{\text{train}}_i, \phi_i)d\theta
\]

⇒ this is completely intractable!

what if we knew \( p(\phi_i|\theta, x^{\text{train}}_i, y^{\text{train}}_i) \)?

⇒ now sampling is easy! just use ancestral sampling!

**key idea:** \( p(\phi_i|\theta, x^{\text{train}}_i, y^{\text{train}}_i) \approx \delta(\hat{\phi}_i) \)

this is extremely crude

but extremely convenient!

\[
\hat{\phi}_i \approx \theta + \alpha \nabla_\theta \log p(y^{\text{train}}_i|x^{\text{train}}_i, \theta)
\]

(Santos ’92, Grant et al. ICLR ’18)

Training can be done with **amortized variational inference**.
What about Bayesian **optimization-based** meta-learning?

Sample parameter vectors with a procedure like **Hamiltonian Monte Carlo**?

Finn*, Xu*, Levine. Probabilistic MAML ‘18

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

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

\[
\hat{\phi}_i \approx \theta + \alpha \nabla_\theta \log p(y_i^{\text{train}} | x_i^{\text{train}}, \theta)
\]

What does ancestral sampling look like?

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

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

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

**Con:** More complex training procedure.
Methods Summary

**Version 0:** $f$ outputs a distribution over $y^{ts}$.

**Pros:** simple, can combine with variety of methods

**Cons:** can’t reason about uncertainty over the underlying function, limited class of distributions over $y^{ts}$ can be expressed

**Black box approaches:** Use latent variable models + amortized variational inference

**Optimization-based approaches:**

- **Amortized inference**
  - **Pro:** Simple.
  - **Con:** $p(\phi_i | \theta)$ modeled as a Gaussian.

- **Ensembles**
  - **Pros:** Simple, tends to work well, non-Gaussian distributions.
  - **Con:** maintain M model instances. (or do inference on last layer only)

- **Hybrid inference**
  - **Pros:** Non-Gaussian posterior, simple at test time, only one model instance.
  - **Con:** More complex training procedure.
Plan for Today

Why be Bayesian?
Bayesian meta-learning approaches

How to evaluate Bayesians.
How to evaluate a Bayesian meta-learner?

Use the standard benchmarks?
(i.e. MiniImagenet accuracy)

+ standardized
+ real images
+ good check that the approach didn’t break anything
  - metrics like accuracy don't evaluate uncertainty
  - tasks may not exhibit ambiguity
  - uncertainty may not be useful on this dataset!

What are better problems & metrics?
It depends on the problem you care about!
Qualitative Evaluation on Toy Problems with Ambiguity
(Finn*, Xu*, Levine, NeurIPS ’18)

Ambiguous regression:

Ambiguous classification:
Evaluation on Ambiguous Generation Tasks
(Gordon et al., ICLR ’19)

Table 2: View reconstruction test results.
Accuracy, Mode Coverage, & Likelihood on Ambiguous Tasks
(Finn*, Xu*, Levine, NeurIPS ’18)

### Ambiguous celebA (5-shot)

<table>
<thead>
<tr>
<th>Method</th>
<th>Accuracy</th>
<th>Coverage (max=3)</th>
<th>Average NLL</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAML</td>
<td>89.00 ± 1.78%</td>
<td>1.00 ± 0.0</td>
<td>0.73 ± 0.06</td>
</tr>
<tr>
<td>MAML + noise</td>
<td>84.3 ± 1.60 %</td>
<td>1.89 ± 0.04</td>
<td>0.68 ± 0.05</td>
</tr>
<tr>
<td>PLATIPUS (ours) (KL weight = 0.05)</td>
<td>88.34 ± 1.06 %</td>
<td>1.59 ± 0.03</td>
<td>0.67 ± 0.05</td>
</tr>
<tr>
<td>PLATIPUS (ours) (KL weight = 0.15)</td>
<td>87.8 ± 1.03 %</td>
<td>1.94 ± 0.04</td>
<td>0.56 ± 0.04</td>
</tr>
</tbody>
</table>
Reliability Diagrams & Accuracy

(Ravi & Beatson, ICLR ’19)

\[ \text{miniImageNet: 1-shot, 5-class} \]

- MAML
  - ECE: 0.0471
  - MCE: 0.1104
- Probabilistic MAML
  - ECE: 0.0472
  - MCE: 0.0856
- Ravi & Beatson
  - ECE: 0.0124
  - MCE: 0.0257

<table>
<thead>
<tr>
<th>miniImageNet</th>
<th>1-shot, 5-class</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAML (ours)</td>
<td>47.0 ± 0.59</td>
</tr>
<tr>
<td>Prob. MAML (ours)</td>
<td>47.8 ± 0.61</td>
</tr>
<tr>
<td>Our Model</td>
<td>45.0 ± 0.60</td>
</tr>
</tbody>
</table>
Both experiments:
- Sequentially choose datapoint with **maximum predictive entropy** to be labeled
- or choose datapoint at random (MAML)
Algorithmic properties perspective

Expressive power
the ability for $f$ to represent a range of learning procedures
Why? scalability, applicability to a range of domains

Consistency
learned learning procedure will solve task with enough data
Why? reduce reliance on meta-training tasks, good OOD task performance

Uncertainty awareness
ability to reason about ambiguity during learning
Why? active learning, calibrated uncertainty, RL principled Bayesian approaches
Next Time

Wednesday:
Meta-learning for unsupervised, semi-supervised, weakly-supervised, active learning

Next Monday:
Start of reinforcement learning!

Reminders

Homework 2 due next Wednesday.

Project proposal due in two weeks.

Poster presentation: Tues 12/3 at 1:30 pm.