Gradient-EM Bayesian Meta-learning

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Abstract

Bayesian meta-learning enables robust and fast adaptation to new tasks with uncertainty assessment. The key idea behind Bayesian meta-learning is empirical Bayes inference of hierarchical model. In this work, we extend this framework to include a variety of existing methods, before proposing our variant based on gradient-EM algorithm. Our method improves computational efficiency by avoiding back-propagation computation in the meta-update step, which is exhausting for deep neural networks. Furthermore, it provides flexibility to the inner-update optimization procedure by decoupling it from meta-update. Experiments on sinusoidal regression, few-shot image classification, and policy-based reinforcement learning show that our method not only achieves better accuracy with less computation cost, but is also more robust to uncertainty.

1 Introduction

Meta-learning, also known as learning to learn, has gained tremendous attention in both academia and industry, especially with applications to few-shot learning Finn et al. [2017]. The nature of multi-task setting in meta-learning is that these tasks share similarities, such that learning from sufficiently many tasks helps mastering new tasks faster. This feature is referred to as fast adaptation.

The early fast meta-learning algorithm was gradient-based and deterministic, which may cause overfitting on both inner-level and meta-level Mishra et al. [2017]. With growing interests in prediction uncertainty evaluation and overfitting control, later studies explored probabilistic meta-learning methods Grant et al. [2018a], Yoon et al. [2018], Finn et al. [2018]. It has been agreed that Bayesian inference is one of the most convenient choices because of its Occam’s Razor property MacKay and Mac Kay [2003] that automatically prevents overfitting, which happens in deep neural network (DNN) very often. It also provides reliable predictive uncertainty because of its probabilistic nature. This makes Bayesian methods important to DNN, which as Guo et al. [2017] shows, unlike shallow neural networks, are usually poorly calibrated on predictive uncertainty.

The theoretical foundation of Bayesian meta-learning is hierarchical Bayes (HB) Good [1980] or empirical Bayes (EB) Robbins and Monro [1985] which restricts the learning of meta-parameters to point estimates. For simplicity we focus on EB in this paper, we can always extend to HB by adding a hyper-prior to the learning of meta-parameters like Ravi and Beatson [2018]. A common solution of EB is a bi-level iterative optimization procedure Ravi and Beatson [2018], Lindstrom and Bates [1988], where the “inner-update” refers to adaptation to a given task, and the “meta-update” is the meta-training objective. We extend the original optimization framework for train/val split in the inner-update procedure to mitigate in-task overfitting which is important for NN based ML. We also hypothesize a mechanism of how EB framework achieves fast-adaptation(few inner-update gradient steps) under Gaussian parameterization, along with empirical evidences. What’s more, we successfully adapt this EB framework to RL both theoretically and empirically which has not been done before.

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We show that many important previous works in (Bayesian) meta-learning Ravi and Beatson [2018], Finn et al. [2018], Yoon et al. [2018], Finn et al. [2017], Nichol et al. [2018] can be included in this extended framework. However, in previous works, the meta-update step requires backpropagation through the inner optimization process Rajeswaran et al. [2019] which imposes large computation and memory burden as the increase of inner-update gradient steps. This puts limits on possible applications, especially those require many inner-update gradient steps or involves large dataset(See Appendix for our examples). Motivated by the above observations, we propose a gradient-based Bayesian algorithm inspired by Gradient-EM algorithm. By designing a new way to compute gradient of meta loss in Bayesian MAML by utilizing the gradient information of prior distribution, we come up with an algorithm that decouples meta-update and inner-update and thus avoids the computation and memory burden of previous methods, making it scalable to a large number of inner-update gradient steps. In addition, it enables large flexibility on the choice of inner-update optimization method because it only requires the value of the result of the inner-update optimization, instead of the optimization process (for example in experiments we use Adam in classifications and Trust Region Policy Optimization in RL). The separability of meta-update and inner-update also makes it a potentially useful scheme for distributed learning and private learning.

In experiments, we show our method can quickly learn the knowledge and uncertainty of a novel task with less computation burden in sinusoidal regression, image classifications benchmarks and reinforcement learning.

2 Problem Formulation and Framework

2.1 General Meta Learning Setting

We set up the K-shot meta-learning framework upon reinforcement learning(RL) with episode length $H$ as in Finn et al. [2017], where supervised learning is a special case with $H = 1$. With a decision rule(policy) $f$ we can sample rollout data $D = \{x_t, a_t, r_t\}_{t=1}^{H}$ from the task environment. A decision rule (policy) $f$ can be evaluated on $D$ with loss function $\ell(D, f)$. We assume each task $\tau$ to be i.i.d. sampled from the task space $\mathcal{T}$, following some task distribution $P(\tau)$. During meta-training phase, we collect $K$ samples rollout of current policy $f$ and another $K$ samples rollout after 1 policy gradient training of $f$ ($f$ is not needed in generating samples in supervised learning). We denote this $2K$ samples as $D_{\tau}^\text{meta-train}, \tau \in \mathcal{T}_{\text{meta-train}}$. At meta-testing phase, for a randomly sampled task $\tau$, $K$ samples are first provided as $D_{\tau}^\text{meta-test}$. We are then required to return $f_\tau$ based on $\{D_{\tau}^\text{meta-train}\}_{\tau \in \mathcal{T}_{\text{meta-train}}} \cup D_{\tau}^\text{meta-test}$ to evaluate its expected loss $l_\tau = E_{D_{\tau} \sim \tau} \ell(D_{\tau}, f_\tau)$ on more samples generated from that task. The objective is to come up with an algorithm that produces a decision rule $f_\tau$ that minimize the expected test loss over all tasks $E_{\tau \sim P(\tau)} l_\tau$.

![Figure 1: (a) Minimal A* (b) Graphical Model](image)

2.2 Extended Empirical Bayes Meta-Learning Framework

We consider parameterized decision rule $f_\theta$ and construct a corresponding generative model $\tau(\theta)$:

$$\log P(D|\theta) = -\mathcal{L}(D, f_\theta)$$

(We leave the detail of this construction in RL to Appendix). For each task $\tau$, denote the best policy parameter as well as the best fitted underlying generative model parameter to be $\theta_\tau = \arg \min_{\theta} E_{D_{\tau} \sim \tau} \mathcal{L}(D_{\tau}, f_\theta) = \arg \max_{\theta} E_{D_{\tau} \sim \tau} \log P(D_{\tau}|\theta)$. In general such maximum is not unique, which is discussed in Section 2.3. With $\theta_\tau$ uniquely defined, we have a distribution $P(\theta_\tau)$ induced by $P(\tau)$ (change of variable).(See Figure 1(b) for a summary of the generative model) Under perfect
approximation, the ground-truth generator matches our generative model: \( P(D_\tau | \tau) = P(D_\tau | \theta_\tau) \), resulting in the following proposition:

**Theorem 1.** Suppose data generator is represented by the hierarchical model \( P(D_\tau | \theta) \) and \( P(\theta) \), and define \( L(Q; D) = \log E_{Q \sim Q} P(D | \theta) \) for distribution \( Q \) over \( \theta \). Let \( (D^g_\tau, D^{eval}_\tau) \) be independent samples from task \( \tau \), and consider \( Q \) determined by \( D^g_\tau \) via \( Q = g(D^g_\tau) \). Then

\[
P(\theta_\tau | D^g_\tau; P(\theta_\tau)) = \arg \max_g E_\tau L(g(D^g_\tau), D^{eval}_\tau)
\]  

Two observations are made here. First, this theorem guarantees best decision rule we can come up with during meta-testing: evaluating posterior \( P(\theta_\tau | D^g_\tau) \) using prior \( P(\theta_\tau) \). Second, this theorem suggests an estimation method for \( P(\theta_\tau) \) during meta-training: \( \arg \max_{\theta} \sum_{\tau} L(P(\theta_\tau | D^g_\tau) ; D^{eval}_\tau) \). We prove in Appendix that this estimator is not only asymptotic consistent but also with good asymptotic normality which means it quickly converge to true value with small variance as number of tasks increases. We further parameterize \( P(\theta_\tau) \) by \( P(\theta_\tau; \Theta) \) (in hierarchical modeling this is called hyper-prior), and introduce short notation \( L(\Theta, D^g_\tau; D^{eval}_\tau) = L(P(\theta_\tau | D^g_\tau; \Theta) ; D^{eval}_\tau) \), then the optimization in meta-training can be written as \( \arg \max_{\Theta} \sum_{\tau} L(\Theta, D^g_\tau; D^{eval}_\tau) \). This is an extension of the popular MLE approach in empirical Bayes, where (marginal) log-likelihood \( L(\Theta; D_\tau) \) is the special case of \( |D^g_\tau| = 0 \). For clarity we denote \( L[1] = L(\Theta; D^{eval}_\tau) \) and \( L[2] = L(\Theta, D^g_\tau; D^{eval}_\tau) \), \( L[i] = E_{\tau} L[1] \). There is a bias/variance trade-off between \( L[1] \) and \( L[2] \). Using \( L[2] \) as the meta loss function improves in-task overfitting problem while \( L[1] \) extracts more information from the data. A detailed discussion is presented in Appendix.

An stochastic gradient descent (SGD) approach to meta-training is provided in Algorithm 1: at iteration \( t \), gradient \( \nabla_{\Theta} L[i] \) for each task in the \( t \)-th meta-training batch is computed by subroutine Meta-Gradient, then gradient ascent is performed. A variational inference (VI) approach to meta-testing is shown in Algorithm 2, where posterior \( P(\theta_\tau | D^g_\tau, \Theta) \) is estimated with fixed \( \Theta \). Detailed discussion of these subroutines are presented in Session 3.

### 2.3 non-uniqueness and fast-adaptation

For neural networks \( f_\theta \), there exists many local optimums that achieves equally good performance for each task. We observe from empirical study [Appendix] that the key to fast-adaptation for gradient-based algorithm is to find a small neighbouring zone \( A^* \) where most tasks have at least one best parameter inside it(Figure 1(a)). The intuition is that when \( \{ \theta_\tau \} \) are close enough they can be learned within a few gradient steps starting from any points within that neighbouring zone(our experiment shows that a perturbation of initial points within that area would still have good performance at meta-test). The existence of this small neighbouring zone \( A^* \) depends on the parametric model \( f_\theta \) and the task distribution \( P(\tau) \). We further demonstrate [Appendix] its existence with Gaussian parameterization of \( P(\theta_\tau; \Theta) \) for uni-modal task distribution like sinusoidal functions and neural networks. Even if we fail to find a single small neighbouring zone \( A^* \) (e.g. multi-modal task distribution like mixture of sinusoidal, linear and quadratic functions), solution may be provided by extension to mixture Gaussian Grant et al. [2018b], Rasmussen [2000]. In this work we focus on the uni-modal situation and leave the extension to future work.
Algorithm Meta-train()
1 randomly initialize \( \Theta \)
2 \( t = 0 \)
3 while not done do
4 Sample batch of tasks \( \mathcal{T}_t \sim P(\tau) \)
5 for each task \( \tau \sim \mathcal{T}_t \) do
6 Compute \( \nabla_{\Theta} L^{[t]} \) by Subroutine Meta-Gradient(\( \Theta^{(t)}, \{ D^\tau_t, D^\tau_{\text{val}} \} \))
7 end
8 \( \Theta^{(t+1)} = \Theta^{(t)} - \beta \sum_{\tau \in \mathcal{T}_t} \nabla_{\Theta} L^{[t]} \)
9 \( t = t + 1 \)
end

Algorithm 1: Extended Empirical Bayes Meta-learning Framework

Algorithm Meta-test()
1 Require: learned \( \Theta, D^\tau_f \) from new task \( \tau \)
2 Compute posterior \( \lambda_\tau = \text{VI}(\Theta, D^\tau_f) \)
3 Sample \( \theta_\tau \sim P(\theta_\tau | \lambda_\tau) \)
4 return \( f(\tau; \theta_\tau) \) for evaluation

Subroutine VI(\( \Theta, D^\tau \))
1 Initialize \( \lambda_\tau \) at \( \Theta \)
2 while not done do
3 Sample \( \bar{\epsilon} \) from \( \epsilon \sim p(\epsilon) \)
4 \( \lambda_\tau \leftarrow \lambda_\tau + \alpha \nabla_{\lambda_\tau} [\log P(D^\tau | g(\lambda_\tau, \bar{\epsilon})) - KL(P(\lambda_\tau | \Theta) || P(\theta_\tau | \Theta))] \)
5 return \( \lambda_\tau \)

Algorithm 2: VI: reparameterize \( \theta_\tau \sim P(\theta_\tau | \lambda_\tau) \) using a differentiable transformation \( g(\lambda_\tau, \epsilon) \) of an auxiliary noise variable \( \epsilon \) such that \( \theta_\tau = g(\lambda_\tau, \epsilon) \) with \( \epsilon \sim p(\epsilon) \) (Kingma and Welling 2013)

3 Method
In this section, we first introduce the gradient-based variational inference subroutine VI related to a variety of existing methods, then present the proposed subroutine Meta-Gradient inspired by Gradient-EM algorithm and compare it with the mostly used existing methods for this subroutine.

3.1 Variational Inference
Notice that this framework requires computing posterior on complex models such as neural networks. We approximate the posterior with the same parametric distribution \( P(\theta; \lambda_\tau) \) as we approximate the prior \( P(\theta; \lambda) \) and use Variational Inference to compute the parameters, as has been done in previous work Ravi and Beatson [2018]. Let \( P(\theta; \lambda_\tau(D^\tau; \Theta)) \) be the approximation of the posterior \( P(D^\tau; \theta; \Theta) \) by minimizing their KL distance. Since

\[
L(\Theta; D^\tau) = \log P(D^\tau; \Theta) = KL[P(\theta; \lambda_\tau) \parallel P(\theta | D^\tau; \Theta)] + E_{P(\theta; \lambda_\tau)}[\log P(D^\tau | \Theta) - \log P(\theta; \lambda_\tau)]
\]

(2)

is constant in terms of \( \lambda_\tau \), we have \( \lambda_\tau(D^\tau; \Theta) = \arg \min_{\lambda_\tau} KL[P(\theta; \lambda_\tau) \parallel P(\theta | D^\tau; \Theta)] = \arg \max_{\lambda_\tau} E_{P(\theta; \lambda_\tau)}[\log P(D^\tau | \Theta) - KL[P(\lambda_\tau) \parallel p(D^\tau; \Theta)]] \) via mini-batch gradient descent. Ravi and Beatson [2018]. The gradient of KL-divergence terms are analytically calculated in Gaussian case whereas the gradient of expectations can be computed by monte-carlo reparameterization along with some variance reduction tricks Kingma et al. [2015], Zhang et al. [2018]. Due to the above analysis in Section 2.3, only a few gradient steps are needed for this process with well learned \( \Theta \) by our framework. We summarize the subroutine VI in Algorithm 2.

A special case worth mentioning is when we use delta function for the posterior approximation \( P(\theta; \lambda_\tau) = \delta_{\mu_\lambda}(\theta) \), we have \( \lambda_\tau(D^\tau; \Theta) = \arg \max_{\mu_\lambda} \log P(D^\tau | \Theta) - \parallel \mu_\lambda - \mu_{\Theta} \parallel^2 / (2\Sigma_{\Theta}^{-2}) \), which is actually the inner-update step of iMAML Rajeswaran et al. [2019], MAML Finn et al. [2017], and reptile Nichol et al. [2018] (if we replace the l2 regularization term with choosing \( \mu_{\Theta} \) as initial point for gradient based optimization: \( \mu_{\lambda_\tau}(\mu_{\Theta}) = \mu_{\Theta} - \nabla_{\theta} \log P(D^\tau; \Theta)_{\theta=\mu_{\Theta}} \)).

3.2 Meta-Gradient
The essential part of this meta-learning framework is to compute the gradient \( \nabla_{\Theta} L^{[t]} \). We reduce this problem to compute \( \nabla_{\Theta} L(\Theta; D^\tau) = \nabla_{\Theta} \log P(D^\tau; \Theta) \) given \( D^\tau \) and \( \Theta \). For \( L^{[1]} \), this is direct. For \( L^{[2]} \), we have two approaches. In the first approach we compute \( \lambda_\tau(D^\tau; \Theta) \) as stated above, then \( \nabla_{\Theta} L^{[2]} = \nabla_{\Theta} L(\Theta; D^\tau_f, D^\tau_{\text{val}}) = \nabla_{\Theta} L(\lambda_\tau(D^\tau_f; \Theta); D^\tau_{\text{val}}) = \nabla_{\Theta} L(\Theta; D^\tau_{\text{val}})_{\Theta=\lambda_\tau(D^\tau_f; \Theta)} \), where \( \nabla_{\Theta} L(\lambda_\tau(D^\tau_f; \Theta)) \) can be computed by auto-gradient (if \( \lambda_\tau(D^\tau_f; \Theta) \) is computed by gradient based algorithms). This approach is widely used in previous work such as Finn
et al. [2017], Finn et al. [2018], Yoon et al. [2018], Grant et al. [2018a]. The second approach we proposed is implemented in subroutine Meta-Gradient: GEM-BML+ below. We utilize a property \(L(\Theta; D_T^r; D_T^{val}) = L(\Theta; D_T^r \cup D_T^{val}) - L(\Theta; D_T^r)\) (proof in [Appendix]) such that \(\nabla_\Theta L^{[1]} = \nabla_\Theta L(\Theta; D_T^r \cup D_T^{val}) - \nabla_\Theta L(\Theta; D_T^r)\) can be expressed by the difference of two \(L[1]\) terms.

We propose an efficient way to compute \(\nabla_\Theta L(\Theta; D_T)\) through gradient of the complete log likelihood. This is guaranteed by the following Gradient-EM Theorem inspired by the observation in Salakhutdinov et al. [2003].

**Theorem 2.** \(\nabla_\Theta L(\Theta; D) = E_{\theta \sim P(\theta|D; \Theta)} \nabla_\Theta \log[P(D; \theta; \Theta)]\)

Proof.

\[
\nabla_\Theta L(\Theta; D) = \frac{\partial}{\partial \Theta} \log P(D; \Theta) \\
= \frac{1}{P(D(\Theta))} \frac{\partial}{\partial \Theta} \int P(D, \theta|\Theta) d\theta \\
= \int \frac{P(D, \theta|\Theta)}{P(D(\Theta))} \frac{\partial}{\partial \Theta} \log P(D, \theta|\Theta) d\theta \\
= \int P(\theta|D, \Theta) \frac{\partial}{\partial \Theta} \log P(D, \theta|\Theta) d\theta \\
= E_{\theta \sim P(\theta|D; \Theta)} \nabla_\Theta \log[P(D; \theta; \Theta)] \\
\]

Under hierarchical modeling structure, we have \(\nabla_\Theta \log P(D_T^r, \theta_T(\Theta) = \nabla_\Theta \log[P(D_T^r|\theta_T) \ast P(\theta_T; \Theta)] = \nabla_\Theta \log[P(\theta_T; \Theta)]\). Using Theorem 1 we have \(\nabla_\Theta L(\Theta; D_T) = E_{\theta_T \sim P(\theta_T|D_T; \Theta)} \nabla_\Theta \log[P(\theta_T; \Theta)]\). Using VI to compute the approximate posterior parameter \(\lambda_T(\Theta)\) we get the GEM estimator \(\hat{g} = E_{\theta_T \sim P(\theta_T; \lambda_T(\Theta))} \nabla_\Theta \log[P(\theta_T; \Theta)]\) which can be calculated analytically in Gaussian case as we show in Appendix. This gives us two Meta-Gradient subroutines GEM-BML and GEM-BML+ for \(\nabla_\Theta L^{[1]}\) and \(\nabla_\Theta L^{[2]}\) respectively. We name Algorithm 1 with these two subroutines as our algorithms GEM-BML and GEM-BML+.

1 Subroutine

| Meta-Gradient: GEM-BML(\(\Theta, \{D_T^r, D_T^{val}\}\)) | Meta-Gradient: GEM-BML+(\(\Theta, \{D_T^r, D_T^{val}\}\)) |
|---|---|
| Compute posterior \(\lambda_T^r = \text{VI}(\Theta, D_T^r)\) | Compute posterior \(\lambda_T^r = \text{VI}(\Theta, D_T^r)\) |
| Compute posterior \(\lambda_T^{val} = \text{VI}(\lambda_T^r, D_T^{val})\) | Compute posterior \(\lambda_T^{val} = \text{VI}(\lambda_T^r, D_T^{val})\) |
| return \(\hat{g} = E_{\theta_T \sim P(\theta_T; \lambda_T^{val})} \nabla_\Theta \log[P(\theta_T; \Theta)]\) | return \(\hat{g} = E_{\theta_T \sim P(\theta_T; \lambda_T^{val})} \nabla_\Theta \log[P(\theta_T; \Theta)] - E_{\theta_T \sim P(\theta_T; \lambda_T^r)} \nabla_\Theta \log[P(\theta_T; \Theta)]\) |

As comparison, one of the most widely used method to optimize \(L[1]\) in Bayesian meta-learning is optimizing ELBO Ravi and Beatson [2018](see Appendix for other existing methods and comparing analysis). Here we show it is actually another way to estimate \(\nabla_\Theta L(\Theta; D_T)\). According to equation (2), when VI approximation error \(KL[P(\theta_T; \lambda_T(D_T; \Theta)) \parallel P(\theta_T|D_T; \Theta)]\) is small enough, we have \(L(\Theta; D_T) \simeq E_{P(\theta_T, \lambda_T(D_T; \Theta))} [\log P(D_T|\theta_T) \ast \log P(\theta_T; \lambda_T(D_T; \Theta))] = [E_{P(\theta_T, \lambda_T(D_T; \Theta))} \log P(D_T|\theta_T)] - KL[P(\theta_T; \lambda_T(D_T; \Theta)) \parallel P(\theta_T|D_T; \Theta)] = \frac{\partial}{\partial \Theta} \text{ELBO}^{(\tau)}(\lambda_T(D_T; \Theta))\). So the gradient can be computed by \(\nabla_\Theta L(\Theta; D_T) \simeq \nabla_\Theta \text{ELBO}^{(\tau)}(\lambda_T(D_T; \Theta); \Theta) = \frac{\partial}{\partial \Theta} \text{ELBO}^{(\tau)}(\lambda_T(D_T; \Theta))|_{\lambda_T = \lambda_T(\Theta)} \ast \nabla_\Theta \lambda_T(\Theta) + \frac{\partial}{\partial \Theta} \text{ELBO}^{(\tau)}(\lambda_T(D_T; \Theta); \Theta)\). The first partial gradient term can be computed by the same method in Section 3.1 and the second one can be calculated analytically in Gaussian case.

In fact, Gradient-EM can also be reviewed as an co-ordinate descent algorithm to optimize ELBO as a variant of EM as we show in Appendix. Comparing to ELBO gradient, Gradient-EM avoids the backProps computation of \(\nabla_\Theta \lambda_T(D_T; \Theta)\) which gives it a series of advantages as we specify in Section 4.2. Both GEM and ELBO gradient has estimation error arise from the discrepancy of estimated posterior by VI and the true posterior. We show empirical results in Appendix that GEM has stably lower estimation error than ELBO gradient. We also show in Appendix that our method has a theoretical bound of estimation error in terms of the VI discrepancy \(\| \hat{g} - \nabla_\Theta L(\Theta; D_T) \| \leq M \sqrt{D_K L(\Theta; D_T; \Theta) \parallel P(\theta; \lambda_T(D_T; \Theta))}\) where \(M\) is a bounded constant.
4 Analysis

We compare Gradient-EM (our method) with ELBO-gradient over two loss functions \(L[1]\), \(L[2]\), summarized in Table 1. It turns out each element of this matrix is related to a related work/our method. Here we only show how MAML and Reptile can be fit into this Bayes frame, while further details are left to [Appendix]. To see this, consider using fixed variance parameters for both prior \(P(\theta; \mu_\Theta, \Sigma_\Theta = C_0)\) and posterior \(P(\theta; \mu_{\lambda_r}, \Sigma_{\lambda_r} = C_r)\) and let \(C_r \to 0\) so posterior becomes delta distribution \(\delta_{\mu_{\lambda_r}}(\theta_r)\). We can compute \(\mu_{\lambda_r}(\mu_\Theta)\) by gradient descent from \(\mu_\Theta\). MAML uses \(L[2]\) as meta-loss function. Under delta distribution posterior \(L[2]_r = \log f(D_r|\theta_r)\delta_{\mu_{\lambda_r}}(\mu_\Theta) = \log P(D_r|\mu_{\lambda_r}(\mu_\Theta))\) \(= f(D_r; \mu_{\lambda_r}(\mu_\Theta))\). Then \(\nabla_{\mu_\Theta} L[2]_r = \nabla_{\mu_\Theta} f(D_r; \mu_{\lambda_r}(\mu_\Theta))\) can be directly computed through back-propagation in neural networks. One the other hand, Reptile uses \(L[1]\) as meta-loss function. Using GEM-gradient \(\hat{g}, \nabla_{\Theta} L_r[1] = E_{\delta_{\mu_{\lambda_r}}(\mu_\Theta)}(\theta_r)\nabla_{\Theta} \log[P(\theta_r; \mu_\Theta, \Sigma_\Theta = C_0)] = \nabla_{\mu_\Theta} \frac{[\mu_{\Theta} - \mu_{\lambda_r}(\mu_\Theta)]^2}{2\Sigma_\Theta}\) which is the Reptile gradient. In this sense, Gradient-EM is the Bayesian version of Reptile. Also notice that, if we let \(C_0 \to 0\) and so the prior becomes delta, then \(\nabla_{\mu_\Theta} L[2]_r = \nabla_{\mu_\Theta} \log f(D_r|\theta_r)\delta_{\mu_{\lambda_r}}(\theta_r) = \nabla_{\mu_\Theta} \log P(D_r|\mu_\Theta) = \nabla_{\mu_\Theta} f(D_r; \mu_\Theta)\). This corresponds to "pre-train" which simply train a model to fit data of all tasks combined. Previous work has shown empirically that this method doesn’t perform well [Finn et al. 2017]. Here we can provide a theoretical explanation. We show in Appendix that \(\arg\max_{\mu_\Theta} L[1](\mu_\Theta, \Sigma_\Theta = C_0)\) is a biased estimator when \(C_0 \to 0\) while unbiased in Reptile where \(C_0 \to \infty\).

| ELBO gradient | Amortized BML Ravi and Beatson (2018) | Related to PMAML Finn et al. (2018) |
|---------------|---------------------------------|----------------------------------|
| \(L[1]\) = \(E_{\tau \in T} L(\Theta, D^m_r \cup D^m_{\text{val}})\) | \(L[2]\) = \(E_{\tau \in T} L(\lambda_r(D^m_r, \Theta), D^m_{\text{val}})\) |

**Table 1:** Matrix of related works

Observe that all methods in the above matrix requires to compute the posterior parameters \(\lambda_r(D_r; \Theta)\) first and use it to compute the sampled meta-loss function gradient \(\nabla_{\Theta} L[2]_r\). Following the convention of Finn et al. [2017], we define the step of computing \(\lambda_r(D_r; \Theta)\) as inner-update and the step of computing \(\nabla_{\Theta} L[2]_r\) as meta-update. Notice that both the \(L[2] = \int_{\Theta} L(\lambda_r(D^m_r, \Theta), D^m_{\text{val}})\) column and the ELBO-gradient row involves the computation of \(\nabla_{\Theta} \lambda_r(D_r; \Theta)\). This means the inner-update computation of these three methods(highlighted in colour) has to compute backpropagation through the inner optimization process which leads to a number of burden and limitation while our method avoids this computation and thus provides a number of advantages as mentioned in Introduction. Also notice that, if assuming independence between neural network layers, the meta-update of our algorithm (Line 4 of Subroutine GEM-BML()) can be computed among different neural network layers in parallel, which may largely reduce the computation time in deep neural networks. We summarize a detailed analysis of our advantages to [Appendix].

5 Experiment

5.1 Regression

The purpose of this experiment is to test our methods on fast adaptation ability and robustness to meta-level uncertainty.

We compare our model GEM-BML and GEM-BML+ with MAML Finn et al. [2017], Reptile Nichol et al. [2018] and Amortized BML Ravi and Beatson [2018] on the same sinusoidal function regression problem. We first apply the default setting in Finn et al. [2017] then apply a more challenging setting which contains more uncertainty as proposed in Yoon et al. [2018] to demonstrate the robustness to meta-level uncertainty. Data of each task is generated from \(y = A \sin(wx + b) + \epsilon\) with amplitude \(A\), frequency \(w\), and phase \(b\) as task parameter and observation noise \(\epsilon\). Task parameters are sampled from uniform distributions \(A \in [0.1, 5.0], b \in [0.0, 2\pi], w \in [0.5, 2.0]\) and observation noise follows \(\epsilon \sim N(0, (0.01A)^2)\). \(x\) ranges from \([-5.0, 5.0]\). For each task, \(K = 10\) observations \((x_i, y_i)\) pairs are given. The underlying network architecture(2 hidden layers of size 40 with RELU activation) is the same as Finn et al. [2017] to make a fair comparison. Since our model is a probabilistic model, we use the expectations of model weights in the inference phase for evaluations.
In Figure 2 (a), we plot the mean squared error (MSE) performance on test tasks during meta-test process under both settings. Under default setting, our methods show similar fast-adaptation ability as previous methods. The challenging setting result shows that Bayesian methods GEM-BML(+) and Amortized BML can still extract information in high uncertainty environment while non-Bayesian models MAML and Reptile fail to learn. We also observe that our model provides a stable meta-train learning curve and continues to improve with more gradient steps without overfitting. This demonstrates the robustness of Bayesian methods resulted from its probabilistic nature and the ability to control overfitting.

5.2 Classification

The purpose of this experiment aims to answer the following questions: (1) Does our model save computation time and memory requirement by avoiding meta-update backProp as we claimed? (2) Can our methods be scaled to few-shot image classification benchmarks and achieve good accuracy and predictive uncertainty?

To study (1), we turn to Mini-ImageNet Ravi and Larochelle [2016] dataset on 1-shot,5-class. We compare GEM-BML+(GEM-BML is even less expensive) with MAML and its first order variants fOMAML, Reptile, iMAML, Amortized BML and BMAML in Fig 2(b). Just like other first-order meta-learning algorithms and iMAML which decouples the inner-update and meta-update, the memory usage of GEM-BML(+) is independent of the number of inner-update gradient steps since the inner-update computation other than final step results need not to be stored. On the other hand, MAML-like algorithms (MAML, Amoritized BML) need memory growing linearly with inner-update gradient steps. It is also similar for compute time, MAML-like algorithms requires expensive backProp over the inner-update optimization in meta-update, where the compute cost grows at a

Table 2: Few-shot classification on Omniglot dataset. The ± shows 95% confidence intervals over different testing tasks. All results to compare are from original literature.

| Omniglot  | 1-shot, 5-class | 5-shot, 5-class | 1-shot, 20-class | 5-shot, 20-class |
|-----------|-----------------|-----------------|-----------------|-----------------|
| MAML      | 98.7 ± 0.4 %    | 99.9 ± 0.1 %    | 98.8 ± 0.3 %    | 98.9 ± 0.2 %    |
| Reptile   | 97.68 ± 0.04 %  | 99.48 ± 0.06 %  | 89.43 ± 0.14 %  | 97.12 ± 0.32 %  |
| fOMAML    | 97.50 ± 0.26 %  | 99.74 ± 0.11 %  | 96.18 ± 0.36 %  | 99.14 ± 0.1 %   |
| GEM-BML+(Ours) | 99.23 ± 0.42 % | 99.64 ± 0.08 %  | 98.24 ± 0.35 %  | 98.94 ± 0.25 %  |

Table 3: Accuracy and Predictive Uncertainty Measurement of Few-shot classification on the MiniImagenet dataset. Small ECE and MCE indicate a model is better calibrated.
faster rate than GEM-BML(+), foMAML, Reptile and iMAML (which has a relatively high base 
compute cost because of Hessian computation).

To study (2) we applied our method to N-class image classification on the Omniglot dataset and 
MiniImagenet dataset which are popular few-shot learning benchmarks(Vinyals et al. [2016], Santoro 
et al. [2016], Ravi and Larochelle [2016]). Notice that the purpose of this experiment is not to 
compete with state-of-the-art on this benchmark but to provide an apples-to-apples comparison 
with prior works within our extended Empirical Bayes framework. So for a fair comparison, we 
use the identical backbone convolutional architectureFinn et al. [2017] as these prior works. Note 
however that this backbone architecture can be replaced with other ones and lead to better results 
for all algorithms Chen et al. [2019], Kim et al. [2018]. We leave to the future work to improve 
our method with better backbone architectures to challenge the state-of-the-art of this benchmark. 
The inner-update is computed using Adam to demonstrate the flexibility of our methods in choosing 
inner-update optimizer. The results in Table 2 shows that our methods performs as good as the the 
best prior methods within our extended Empirical Bayes framework.

Predictive uncertainty is the probability associated with the predicted class label which indicates how 
likely the predictions to be correct. To measure the predictive uncertainty of the models, we use two 
quantitative metrics ECE and MCE (Naeini et al. [2015], Guo et al. [2017]) to MiniImagenet dataset. 
Smaller ECE and MCE indicate a better-calibrated model. A perfectly calibrated model achieves 
0 for both metrics. The results of ECE and MCE for our models and previous works are shown in 
Table 3. We can see that our model is slightly better calibrated compared to the state-of-art bayesian 
meta-learning model Amortized BML and well outperform non-Bayesian models. This shows our 
model can learn a good prior and make good probability predictions as an advantage of Bayesian 
model.

5.3 Reinforcement learning

We test and compare the models on the same 2D Navigation and MuJoCo continuous control tasks as 
are used in Finn et al. [2017]. See Appendix for detailed descriptions on experiment settings and 
hyper-parameters.

For a fair comparison, we use the same policy network architecture as Finn et al. [2017] with two 
hidden layers each with 100 ReLU units. At meta-train, we collect $K$ samples rollout of current 
policy and another $K$ samples rollout after 1 policy gradient update as Finn et al. [2017]. At meta-test, 
we compare adaptation to a new task with up to 3 gradient updates, each with 40 samples. We 
compare to two baseline models: MAML and reptile.

MAML uses TRPO in meta-update to boost performance while our meta-update is data-free as 
specified in the above sections. For inner-updates, due to our model’s flexibility of choosing inner-
update optimizer, we can either use vanilla policy gradient (REINFORCE) (Williams, 1992) or a 
specially designed TRPO proposed by Finn et al. [2017]. We find that TRPO inner-update performs 
better in 2d navigation while vanilla policy gradient tend to be better in MuJoCo continuous control 
tasks. We hypothesis that the reasons could be in complex task setting the task distribution variance 
tend to be higher($A^*$ is larger in Figure 1 (a)). While TRPO limits the step size of each inner-update 
which makes the task parameters hard to be attained within a few gradient steps.

As shown in Fig 3, GEM-BML+ outperforms MAML while reptile and GEM-BML has less superior 
performance. This shows $L^{[2]}$ variant is necessary in RL which has high in-task variance and easily 
overfitted. Previous work Nichol et al. [2018] show it is hard to adapt algorithms to RL with the 
advantage of data-free meta-update(reptile like algorithm). But with our $L^{[2]}$ variant we can adapt 
to RL while preserving this advantage. Our results show that for RL, the key to adaptation is $L^{[2]}$ 
variant.

In Appendix, we also provide the results on multi-arm bandit task, where we observe similar 
superiority of our methods which demonstrate the advantage of Bayesian methods in exploration.

6 Related Works

Hierarchical Bayes(HB) and Empirical Bayes(EB) have been decently studied Heskes [1998] in the 
past to utilize statistical connections between related tasks. Since then, deep neural network(DNN)
caught enormous attention and efforts of measuring the uncertainty of DNN also started ongoing in which Bayesian and sampling method are widely applied. Blundell et al. [2015] The research trend of multi-task learning and transfer learning also changed to the fine-tuning framework for DNN after then. Model Agnostic Meta-learning (MAML) Finn et al. [2017] emerged in such a motivation to find good initial parameters that can be fast adapted to new tasks in a few gradient steps. Recently, Bayesian models have a big comeback because of their probabilistic nature in uncertainty measure and automatic overfitting preventing. Wilson et al. [2007] applied HBM to multi-task reinforcement learning. Grant et al. [2018a] related MAML to Hierarchical Bayesian model and proposed a Laplace approximation method to capture isotopic Gaussian uncertainty of the model parameters. Yoon et al. [2018] used Stein Variational Gradient Descent (SVDG) to obtain posterior samples and proposed a Chaser Loss in order to prevent meta-level overfitting. Finn et al. [2018] also proposed a gradient-based method to obtain a fixed measure of prior and posterior uncertainty. Ravi and Beatson [2018] proposed a MAML-like variational inference method for amortized Bayesian meta-learning. All of the methods above can not make inner-update and meta-update separable thus largely limit the flexibility of the optimization process of inner-update. Rajeswaran et al. [2019] propose an implicit gradients method for MAML which can make inner-update and meta-update separable with the cost of computation on second order derivatives and solving a quadratic optimization problem in each inner-update step.

7 Conclusion

Inspired by Gradient-EM algorithm we have proposed GEM-BML(+) Algorithm for Bayesian Meta-learning. Our method is based on a theoretical insight of the Gradient-EM Theorem and the Bayesian formulation of multi-task meta-learning. This method avoids backProp in meta-update and decouples the meta-update and inner-update. We have tested our method on sinusoidal regression, few-shot image classifications and reinforcement learning to demonstrate the advantage of our method. For future work, we consider to apply our method to start-of-art image classification backbone and extending our work to nonparametric Gaussian approximation to handle multimodal and dynamic task-distribution situations.

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Appendix

A. Proofs

A.1. Theorem 1 (Section 2.2)

Theorem 1. Suppose data generator is represented by the hierarchical model \( P(D|\theta_\tau) \) and \( P(\theta_\tau) \), and define \( L(Q; D) = \log E_{\theta \sim Q} P(D|\theta) \) for distribution \( Q \) over \( \theta \). Let \( D^\tau_{tr}, D^\tau_{eval} \) be independent samples from task \( \tau \), and consider \( Q \) determined by \( D^\tau_{tr} \) via \( Q = g(D^\tau_{tr}) \). Then

\[
P(\theta_\tau|D^\tau_{tr}, P(\theta_\tau)) = \arg \max_g E_{\tau} L(g(D^\tau_{tr}); D^\tau_{eval})
\]

(1)

Proof. For any distribution \( Q \), observe that \( E_{\theta \sim Q} P(D|\theta) \) is a distribution over data \( D \). For clarity of the proof, we denote \( E_{\theta \sim g(D^\tau_{tr})} P(D|\theta) \) by conditional distribution \( P_g(D|D^\tau_{tr}) \). Denote \( P(D^\tau_{eval}|D^\tau_{tr}) = P(D^\tau_{eval}|D^\tau_{tr}; \Theta^*) \) where subscript \( \star \) denotes the underlying truth. Then,

\[
E_{\tau} L(g(D^\tau_{tr}); D^\tau_{eval}) = E_{\tau} \log E_{\theta \sim g(D^\tau_{tr})} P(D^\tau_{eval}|\theta)
\]

(2)

\[
= E_{D^\tau_{tr}} \left[ E_{D^\tau_{eval}|D^\tau_{tr}} \log P_g(D^\tau_{eval}|D^\tau_{tr}) \right]
\]

(3)

The cross entropy term achieves maximum as \( P_g(D^\tau_{eval}|D^\tau_{tr}) = P(D^\tau_{eval}|D^\tau_{tr}) \), that is,

\[
\int P(D^\tau_{eval}|\theta) Q(\theta)d\theta = \int P(D^\tau_{eval}|\theta) P(\theta|D^\tau_{tr})d\theta
\]

(4)

Equation holds when \( Q(\theta) = P(\theta|D^\tau_{tr}) \), the posterior distribution of \( \theta \) given \( D^\tau_{tr} \). In other words, we have \( g(D^\tau_{tr}) = P(\theta_\tau|D^\tau_{tr}, P(\theta_\tau)) \), generating posterior from \( D^\tau_{tr} \). Lastly, to finish the proof, note that this (point-wise) maximum is feasible, because \( g \) is a function of \( D^\tau_{tr} \) and the cross entropy terms is inside the expectation/integral over \( D^\tau_{tr} \).

As suggested in article, if we parameterize the prior as \( P(\theta_\tau; \Theta) \), then this theorem motivates an estimator \( \hat{\Theta} \) for meta-training by empirical risk minimization ("training in the same way as testing", more explanation below):

\[
\hat{\Theta} = \arg \max_\Theta \sum_\tau \left( P(\theta_\tau|D^\tau_{tr}, \Theta); D^\tau_{eval} \right)
\]

(5)

A.2. Asymptotic consistency and normality of \( L^{[2]} \) estimator (Section 2.2)

Similar to MLE \( (L^{[1]} \) case), this is also an M-estimator, thus under some regularity conditions \([\text{Van der Vaart, A. (1998). Asymptotic Statistics. Cambridge University Press.}]\) we can establish asymptotic normality for \( \hat{\Theta} \):

\[
\sqrt{n}(\hat{\Theta}_n - \Theta^*) \rightarrow_d \mathcal{N}(0, R^{-1}S^{-1})
\]

(6)

where \( n \) is the number of tasks in meta-training set, and

\[
R = E_{\tau} \left( \frac{\partial^2}{\partial \Theta \partial \Theta^T} L \left( P(\theta_\tau|D^\tau_{tr}, \Theta); D^\tau_{eval} \right) \bigg| \Theta^* \right)
\]

(7)

\[
S = E_{\tau} \left[ \left( \frac{\partial}{\partial \Theta} L \left( P(\theta_\tau|D^\tau_{tr}, \Theta); D^\tau_{eval} \right) \bigg| \Theta^* \right) \left( \frac{\partial}{\partial \Theta} L \left( P(\theta_\tau|D^\tau_{tr}, \Theta); D^\tau_{eval} \right) \bigg| \Theta^* \right)^T \right]
\]

(8)
As comparison, in the MLE case, \( S = -R = I(\Theta^*) \) is Fisher information, thus the asymptotic variance is given by \( I(\Theta^*)^{-1} \), which is also the Cramer-Rao lower bound. For our \( L^{[2]} \) case, first we use the Corollary: \( L(\theta, D^{|tr}, \Theta; D^{|eval}) = L(\Theta; D^{|tr}, D^{|eval}) - L(\Theta; D^{|tr}) \). Then, with some calculation we obtain

\[
R^{-1}SR^{-1} = \frac{m}{m-k}I(\Theta^*)^{-1}
\]

where \( |D^{|tr}| = k \) and \( |D^{|eval}| = m-k \). This suggests that the asymptotic variance of \( L^{[2]} \) is larger than that of \( L^{[1]} \) (lower efficiency) unless \( k = 0 \) (validation set only, where \( L^{[2]} \) degenerates to \( L^{[1]} \)). This is expected, because \( L^{[2]} \) “wasted” some sample on its cross-validation formulation. Intuitively, the variance (or CI) can be described by the curvature of the MLE maximum. Note that from \( L^{[2]} = L(\Theta; D^{|tr}, D^{|eval}) - L(\Theta; D^{|tr}) \), part of the curvature is cancelled out by the existence of second term, resulting in a larger variance of \( \hat{\Theta} \).

### A.3. Bound of GEM gradient estimation error (Section 2.2)

We show a general proposition in VI (or other measure approximation methods). Define

\[
g(x) = E_{Z \sim P} f(x, Z) \tag{10}
g(x) = E_{Z \sim Q} f(x, Z) \tag{11}
\]

To make \( \tilde{g}(x) \approx g(x) \), we let \( Q \approx P \), in the sense that \( D_{KL}(Q||P) \) is minimized over \( Q \). Then

\[
\|g(x) - \tilde{g}(x)\| \leq E_{Z \sim P} \left[ f(x, Z) \left( 1 - \frac{q(Z)}{p(Z)} \right) \right] \tag{12}
\leq E_{Z \sim P} \left[ \|f(x, Z)\| \cdot 1 - \frac{q(Z)}{p(Z)} \right] \tag{13}
\leq \left[ E_{Z \sim P} \|f(x, Z)\|^{2} \right]^\frac{1}{2} \cdot \left[ E_{Z \sim P} \left( 1 - \frac{q(Z)}{p(Z)} \right)^{2} \right]^\frac{1}{2} \tag{14}
\leq M \cdot E_{Z \sim P} \left| 1 - \frac{q(Z)}{p(Z)} \right| \tag{15}
= M \cdot \int |p(z) - q(z)| \, dz \tag{16}
= 2M \cdot D_{TV}(P, Q) \tag{17}
\leq \sqrt{2}M \cdot \sqrt{D_{KL}(Q||P)} \tag{18}
\]

where \( M = \left[ E_{Z \sim P} \|f(x, Z)\|^2 \right]^{\frac{1}{2}} \). In our discussion of gradient approximation, we let \( x = \Theta, z = \theta, f(x, z) = \nabla_{\theta} \log p(\theta|\Theta), \) and \( p(z) = p(\theta|D, \Theta) \). Then \( M = \left[ E_{\theta \sim p(\theta|D, \Theta)} \| \nabla_{\theta} \log p(\theta|\Theta) \|^2 \right]^{\frac{1}{2}} \).
B. Theory

B.1. generative model of RL (Section 2.2)

Using the relation between posterior and ELBO we have \( P(\theta | D; \Theta) = \arg \max_{g} E_{\theta \sim g} \log P(D | \theta) - D_{KL}(g | \Theta) = \arg \min_{\phi} \mathcal{L}(D, f_{\phi}) + D_{KL}(g | \Theta) \). In RL, \( D \) is trajectories \( \{x_{t}, a_{t}, r_{t}\}_{t=1}^{H} \). In policy gradient, \( \pi(a| x) = f_{\theta}(x)(a) \), so \( \mathcal{L}(D, f_{\phi}) = \sum \pi(a_{t}| x_{t}) \pi(r_{t}) = \sum f_{\theta}(x_{t})(a_{t}) \pi(r_{t}) \). The posterior tends to find distribution of \( \theta \) that maximize the expected loss function under regularization of a KL-distance to the prior. For a given environment, when data is infinitely sufficient \( P(\theta | D; \Theta) \rightarrow P(\theta | D; \Theta) \). Theorem 1 holds for any distribution in \( P \). There are \( \prod_{t} n_{\tau} \) choices of sets and the same number of distributions \( P(\tau) \) denoted as \( P \). Theorem 1 holds for any distribution in \( P \) which means we can use any of them as prior to come up with optimal decision rules at meta-testing.

However, it’s not easy to model an arbitrary prior distribution with effective and efficient Bayesian inference. The common feasible Bayesian Inference method for neural networks is gradient based variational inference with Gaussian parametric approximation. This method only works well for distributions that are uni-modal with small variance or multi-modal and each with small variance (which can be modeled by mixture Gaussian) for two reasons. First, the smaller the variance of the distribution the lower the approximate error of Gaussian (property of Gaussian approximation). Second, prior \( P(\theta) \) also serves as initial points in the fast-adaptation Bayesian inference procedure. This requires \( P(\tau) \) to be compact enough such that each task posterior can be attained within a few variational inference gradient steps.

For single cluster of tasks, we show empirical evidences in Appendix C that there exist such kind of a distribution. In another word, there exist a small neighbouring area \( \mathcal{A}^{'} \) where most tasks have at least one best parameter inside it as shown in Figure 1(a). Some other works about multi-modal meta-learning also provide evidences for the feasibility of applying mixture Gaussian to multi-cluster tasks situation which our methods can be adapted to (Grant et al., 2018b; Rasmussen, 2000). In this work we focus on the uni-modal situation and leave the multi-modal situation to future work. So in this work, we use Gaussian \( P(\theta | D; \Theta) \) in the above framework. By doing so \( P(\theta | D; \Theta) \) will converge to the best fit of the smallest variance distribution in \( P \) because Gaussian fits the smallest variance distribution best.

Proof.

\[
L(\Theta, D_{tr}^{\tau}; D_{val}^{\tau}) = \log P(D_{val}^{\tau}|\Theta, D_{tr}^{\tau})
\]

\[
= \log \int P(D_{val}^{\tau}|\theta_{\tau}) \ast P(\theta_{\tau}|\Theta, D_{tr}^{\tau}) d\theta_{\tau}
\]

\[
= \log \int \frac{P(D_{val}^{\tau}|\theta_{\tau}) P(\theta_{\tau}|\Theta)}{P(D_{tr}^{\tau}|\Theta)} d\theta_{\tau}
\]

\[
= \log \frac{P(D_{val}^{\tau}|\Theta)}{P(D_{tr}^{\tau}|\Theta)}
\]

\[
= L(\Theta; D_{tr}^{\tau} \cup D_{val}^{\tau}) - L(\Theta; D_{tr}^{\tau})
\]
Appendix

B.3. co-ordinate descent (Section 3.2)

Following the ELBO property mentioned in Section 3.2 we have

\[
\max_\Theta L(\Theta; D) \simeq \max_\Theta \mathbb{E}_{P(\theta; \lambda(D; \Theta))}[\log P(D; \Theta) - \log P(\Theta; \lambda^*(\Theta))]
\]

\[
= \max_\Theta \mathbb{E}_{P(\theta; \lambda(D; \Theta))}[\log P(D; \Theta) + \log P(\Theta) - \log P(\Theta; \lambda^*(\Theta))]
\]

\[
= \max_\Theta \mathbb{E}_{P(\theta; \lambda(D; \Theta))}[\log P(D; \Theta) - KL(P(\Theta; \lambda^*(\Theta)) \parallel P(\Theta))]
\]

\[
= \max_\Theta ELBO(\tau) (\lambda^*(\Theta), \Theta)
\]

\[
= \max_\Theta \mathbb{E}_{P(\theta; \lambda)} P(D; \Theta) - KL(P(\Theta; \lambda) \parallel P(\Theta))
\]

Now we can show that algorithm GEM-BML is a stochastic co-ordinate descent algorithm to optimize ELBO and thus optimize \( L^{[1]} = E_L(L(\Theta; D)) \). For each iteration we sample a batch of tasks \( \tau \) and optimize over \( \lambda \) and \( \Theta \) alternately. At inner-update, we fix \( \Theta \) and maximize (20) in terms of \( \lambda \), \( \lambda \leftarrow \arg \max \lambda \) \( ELBO(\tau) (\lambda, \Theta) \) which corresponds to the posterior computation in Line 2.3 of Subroutine GEM-BML. At meta-update, we fix \( \lambda \) and improve (20) in terms of \( \Theta \), \( \Theta \leftarrow \Theta - \beta \nabla_{\Theta} KL(P(\Theta; \lambda) \parallel P(\Theta)) = \Theta - \beta \mathbb{E}_{\theta \sim P(\theta; \lambda)} \nabla_{\Theta} \log [P(\theta; \Theta)] \) which corresponds to the \( \Theta \) update in Line 4 of Subroutine GEM-BML and Line 10 of Algorithm 1.

B.4. recasting related works to our framework (Section 4)

For simplicity, we first set up some notations as follows:

- \( \Theta \): stop gradient
- \( D_2 = D^{val} \)
- \( D_1 = D^{tr} \)
- \( \lambda_2(\Theta) \): trained posterior given \( D_2 \cup D_1 \)
- \( \lambda_1(\Theta) \): trained posterior given \( D_1 \)
- \( L_i(\Theta) \): \( \mathbb{E}_{P(\theta; \Theta)} P(D_i|\Theta) \)
- \( L_i^{pos}(\Theta); \Theta = \mathbb{E}_{P(\theta_1; \Theta)} P(D_i|\Theta) \) the gradients of which are estimated by LRP or Flipout (Kingma et al., 2015; Zhang et al., 2018).

Recall that \( L(\Theta; D) \simeq ELBO(\tau) (\lambda(D; \Theta); \Theta) = [\mathbb{E}_{P(\theta; \lambda(D; \Theta))} \log P(D; \Theta)] - KL[P(\Theta; \lambda(D; \Theta)) \parallel P(\Theta)] \). Apply ELBO gradient estimator to \( L^{[1]} = L(\Theta; D) \) we get \( \nabla_{\Theta} [L^{pos}(\Theta) - KL(\lambda_1(\Theta), \Theta)] \) which is the meta-gradient of Amortized BML. In the original work they have a variant of \( \nabla_{\Theta} [L^{pos}(\Theta) - KL(\lambda_1(\Theta), \Theta)] \) to improve the generalization. Apply ELBO gradient estimator to \( L^{[2]} = L(\lambda(D; \Theta); D_2) \) (simply replace \( \Theta \) of \( \lambda(D; \Theta) \)) we get \( \nabla_{\Theta} [L^{pos}(\Theta) - KL(\lambda_2(\Theta), \lambda_1(\Theta))] \) which corresponds to the meta-gradient of PMAML.

Apply GEM gradient estimator \( \hat{g} = \mathbb{E}_{\theta \sim P(\theta; \lambda(D; \Theta))} \nabla_{\Theta} \log [P(\theta; \Theta)] \) to \( L^{[1]} \) and \( L^{[2]} \) as the above procedure we get GEM-BML: \( \nabla_{\Theta} [KL(\text{sg}(\lambda_1(\Theta)), \Theta), KL(\text{sg}(\lambda_2(\Theta)), \Theta)] \) and KL-Chaser Loss: \( \nabla_{\Theta} [KL(\text{sg}(\lambda_2(\Theta)), \lambda_1(\Theta))] \). The Chaser Loss meta-gradient in BMAML is \( \nabla_{\Theta} [\parallel \text{sg}(\lambda_2(\Theta)) - \lambda_1(\Theta) \parallel^2] \) which is similar to KL-Chaser Loss but replace the KL loss with \( l_2 \) loss.

B.5. Advantages of our methods (Section 4)

Observe that all methods in the above matrix requires to compute the posterior parameters \( \lambda(D; \Theta) \) first and use it to compute the sampled meta-loss function gradient \( \nabla_{\Theta} L^{[i]} \). Following the convention of (Finn et al., 2017), we define the step of computing \( \lambda(D; \Theta) \) as inner-update and the step of computing \( \nabla_{\Theta} L^{[i]} \) as meta-update. Notice that both the \( L^{[2]} = E_{\tau \in L}(\lambda(\tau; D^{tr}; \Theta)) \) column and the ELBO-gradient involves the computation of \( \nabla_{\Theta} \lambda(D; \Theta) \). This means the inner-update computation of these three methods (highlighted in colour) has to be built in Tensors in order to compute the gradients by auto-grad. This tensor building and backProps procedure has several drawbacks. First, this procedure is time-consuming, if using SGD for inner-update, the computation time grows rapidly as the number of inner-update gradient steps increase as we show in Experiment (Figure 2), which limits the number of maximum steps. Empirical evidence is
Appendix

C.2. Necessity of many inner-update steps example (Section 1)

This example is based on the same sinusoidal function regression problem in Section 5.1 with a slightly easier setting than the challenging one. All the settings are the same as described in Section 5.1 except the noise parameter $A = 0$ and $\omega \in [0.5, 1.0]$. We plot in Figure 2 the meta-test result for MAML with number of inner-update equals to 1, 2, 3. We can see clearly that in this case multiply inner-update steps is necessary and important for MAML to work. We observe similar

provided in C.2 where multiple inner-update gradient steps are necessary for this framework of methods to work. Second, this procedure limits the choice of optimization method in inner-update. The only optimization method so far that can be trivially written in Tensors is SGD. However, in many situations SGD is not enough or sub-optimal for this framework to work. We show policy-gradient RL examples in Experiment where Trust Region optimization instead of SGD in inner-update is necessary and supervise learning examples where ADAM optimizer works better than SGD. Our method, on the other way, avoids the computation of $\nabla_\theta \lambda_r(D_\tau; \Theta)$ and thus avoids the drawbacks mentioned above. Since it only requires the value of inner-update result $\lambda_r(D_\tau; \Theta)$ instead of the Tensor of optimization process, the meta-update and inner-update can be decoupled. For inner-update, it has much more degree of freedom in choosing optimization methods to compute the value of $\lambda_r(D_\tau; \Theta)$ without the burden of building Tensors on optimization process as mentioned above. For meta-update, it avoids back-propagation computations and does not involve with data explicitly since it only requires the value of $\lambda_r(D_\tau; \Theta)$ to compute meta-gradient (Line 4 of Subroutine GEM-BML and GEM-BML+). This gives our method more potential for distributed computing and privacy sensitive situations. Also notice that, if assuming independence between neural network layers, the GEM-gradient can be computed among different neural network layers in parallel, which may largely reduce the computation time in deep neural networks.

B.6. Other methods to compute Meta-Gradient (Section 3.2)

There are several other methods of Subroutine Meta-Gradient in previous works. (Grant et al., 2018a) uses Gaussian $P(\theta|\Theta)$ and approximate $P(D_\tau|\theta)$ with Gaussian by applying Laplace approximation which uses a second-order Taylor expansion of $P(D_\tau|\theta)$. However, there are evidences show that for neural network $P(D_\tau|\theta)$ can be highly asymmetric. Approximate it with symmetric distribution such as Gaussian may cause a series of problem. (Yoon et al., 2018) proposes to use M particles $\Theta = \{\theta^m\}_{m=1}^M$ to represent $\theta \sim P(\theta|\Theta)$ and compute gradients on them $\nabla_\theta L(\Theta; D_\tau) = \nabla_{\{\theta^m\}_{m=1}^M} \log [\frac{1}{M} \sum_{m=1}^M P(D_\tau|\theta^m)]$. This methods requires $O(M^2)$ times more computation in each gradient iteration.

B.7. Gaussian case solution (Section 3.2)

Under Gaussian approximation, we assume the prior and approximate posteriors to be $P(\theta_r|\Theta) \sim N(\mu_{\theta_r}, \Lambda_{\theta_r}^{-1})$ and $q(\theta_r; \lambda_{\theta_r}^\tau) \sim N(\mu_{\theta_r}^{tr\tau\text{val}}, \Lambda_{\theta_r}^{tr\tau\text{val}})$, $q(\theta_r; \lambda_{\theta_r}^\tau) \sim N(\mu_{\theta_r}^{tr\tau\text{val}}, \Lambda_{\theta_r}^{tr\tau\text{val}})$. Then the meta-gradient of GEM-BML+ $\nabla_\Theta L(\Theta, D^{tr\tau}; D^{val\tau})$ has close form solution given as follows.

$$
\frac{\partial L(\Theta, D^{tr\tau}; D^{val\tau})}{\partial \mu_{\theta_r}} = \sum_{\tau \in T} (\mu_{\theta_r}^{tr\tau\text{val}} - \mu_{\theta_r}^{tr\tau})^T \Lambda_{\theta_r}^{-1}
$$

$$
\frac{\partial L(\Theta, D^{tr\tau}; D^{val\tau})}{\partial \Lambda_{\theta_r}^{-1}} = \sum_{\tau \in T} -\frac{1}{2} (\Lambda_{\theta_r}^{tr\tau\text{val}} - \Lambda_{\theta_r}^{tr\tau})
$$

$$
- \frac{1}{2} (\Lambda_{\theta_r}^{tr\tau\text{val}} - \mu_{\theta_r}^{tr\tau}) (\mu_{\theta_r}^{tr\tau\text{val}} + \mu_{\theta_r}^{tr\tau} - 2\mu_{\theta_r})^T
$$

(21)

C. Experiment

C.1. Meta-Gradient estimation error (Section 3.2)

To study the question of meta-gradient accuracy, we considers a synthetic linear regression example. This provides an analytical expression for the true meta-gradient $\nabla_\Theta L(\Theta; D_\tau)$, allowing us to compute the estimation error of different Meta-Gradient subroutines. We plot in Figure 1 the estimation error of repeated random runs. We find that both GEM and ELBO-gradient asymptotically match the exact meta-gradient, but GEM computes a better approximation in finite iterations with more stability.

C.2. Necessity of many inner-update steps example (Section 1)

This example is based on the same sinusoidal function regression problem in Section 5.1 with a slightly easier setting than the challenging one. All the settings are the same as described in Section 5.1 except the noise parameter $A = 0$ and $\omega \in [0.5, 1.0]$. We plot in Figure 2 the meta-test result for MAML with number of inner-update equals to 1, 2, 3. We can see clearly that in this case multiply inner-update steps is necessary and important for MAML to work. We observe similar
Appendix

Figure 1. Meta-Gradient estimation error

Figure 2. Necessity of many inner-update steps example

phenomena for other methods under our extended EB framework.

C.3. A* (Section 2.3)

We use MAML for this experiment on sinusoidal function regression with the default setting and image classification on Omniglot 1-shot, 5-class. Let $\Theta$ be a well learned initial point (delta prior) by the meta-train process. At meta-test, denote $\theta_i$ as the adapted parameter (delta posterior) from $\Theta$ on a new task $i$. We have verified that MAML works on the two settings we use for this experiment in the sense that $L(D_i; \theta_i) \ll L(D_i; \Theta)$. Now we provide evidence that the area enclosed by $\{\theta_i\}, i \sim P(\tau)$ is a small neighboring area $A^*$ that any point within it is a good initial point with good meta-test behaviour. To be specific, we randomly choose any point within the convex combination of $\{\theta_i\}, i \in T_{meta-test}$ as initial point $\Theta$, then use it as initial point for meta-test on new tasks. We plot in Figure 3 the meta-test result of some random runs and the average of 100 random runs. We can see that the original trained initial point does have the best performance but other random initial points within $A^*$ also have good performance. We also observe that random initial points within $A^*$ has lower error before adaptation while losing some fast adaptation ability. This is consistent with our intuition that MAML tends to find a point in the center of $A^*$ which has the best few-step reach-out ability to all task parameters within $A^*$. While a random initial points within $A^*$ may be close to some of the task parameters and a little bit more far away from other task parameters.
C.4. Experiment Details

We summarize the hyperparameters in Table 1, 2 and 3, in which Meta-batch size is the number of tasks used in one meta-update iteration. All experiments were conducted on a single NVIDIA (Tesla P40) GPU.

C.4.1. Regression

All comparing models are trained using the same network architecture and initialized with the same parameters. For all models, the negative log likelihood $-\log P(D_{\tau}|\theta_{\tau})$ is the mean squared error between the predicted and true y value and the same for loss functions in all other models.

| Meta-update Learning Rate | 0.001 |
|----------------------------|--------|
| Inner-update Learning Rate | 0.001  |
| Inner Gradient steps at meta-train | 1 |
| Inner Gradient steps at meta-test | 10 |
| Meta-batch Size | 5 |

*Table 1. Hyperparameters for sinusoidal regressions.*

C.4.2. Classification

The set up of N-way classification is as follows: select N unseen classes, provide the model with 1 or 5 different instances of each of the N classes, and evaluate the models ability to classify new instances within the N classes. For Omniglot, 1200 characters are selected for training, and the remaining are used for testing, irrespective of the alphabet. Each of the characters is augmented with rotations by multiples of 90 degrees (Santoro et al., 2016). Our Bayesian Neural Network follows the same architecture as the embedding function used by (Finn et al., 2017), which has 4 modules with $3 \times 3$ convolutions and 64 filters, followed by batch normalization (Ioffe & Szegedy, 2015), a ReLU non-linearity, and $2 \times 2$ max-pooling. The Omniglot images are downsampled to $28 \times 28$, so the dimensionality of the last hidden layer is 64. The last layer is fed into a softmax (Vinyals et al., 2016). For Omniglot, we used strided convolutions instead of max-pooling. For MiniImagenet, we used 32 filters per layer to reduce overfitting. For all models, the negative log likelihood $-\log P(D_{\tau}|\theta_{\tau})$ is the cross-entropy error between the predicted and true class.

C.4.3. Reinforcement Learning

In 2D Navigation, the point agent is trained to move to different goal positions in 2D, randomly chosen for each task within a unit square. The observation is its current position, and actions are velocity clipped to be in the range $[-0.1, 0.1]$. The reward is the negative squared distance to the goal. Additional hyperparameter settings for this problem and the following RL problems are in Appendix. For MuJoCo continuous control, we perform goal velocity and goal direction two kinds of task on half cheetah (our available current infrastructure is limited to perform experiment on more advanced environment...
Appendix

|                           | Omniglot,5-class | Omniglot,5-class | miniImageNet |
|---------------------------|------------------|------------------|--------------|
| Meta-update Learning Rate | 0.001            | 0.001            | 0.001        |
| Inner-update Learning Rate| 0.01             | 0.01             | 0.001        |
| Inner Gradient steps at meta-train | 1       | 5                | 5            |
| Inner Gradient steps at meta-test | 10      | 10               | 10           |
| Meta-batch Size           | 32               | 16               | 4            |

Table 2. Hyperparameters for few-shot image classifications.

like 3D ant, we leave it to future work). In the goal velocity task, the agent receives higher rewards as its current velocity approaches the goal velocity of the task. In the goal direction task, the reward is the magnitude of the velocity in either the forward or backward direction. The goal velocity is sampled uniformly at random from \([0, 2.0]\) for the cheetah.

|                           | 2D navigation | half-cheetah, goal velocity | half-cheetah, forward/backward |
|---------------------------|----------------|-----------------------------|-------------------------------|
| Meta-update Learning Rate | 0.001          | 0.001                       | 0.001                         |
| Inner-update Learning Rate| 0.1            | 0.1                         | 0.1                           |
| Inner Gradient steps at meta-train | 1         | 1                            | 1                             |
| Inner Gradient steps at meta-test | 3         | 3                            | 3                             |
| Meta-batch Size           | 20             | 40                           | 40                            |

Table 3. Hyperparameters for reinforcement learning.

D. Erratum

Figure 1(b): green line represents "change of variable" and red line represents "generate". 

\( D^{val} \) and \( D^{val} \) is the same
Algorithm 2 is Algorithm 1
\[ L^{[1]} = E_{\tau} L^{[1]} \]

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