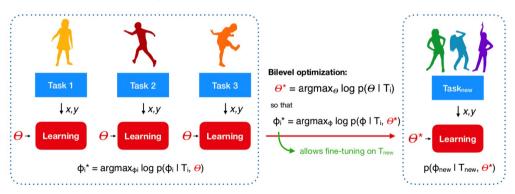
AutoML: Meta-Learning Gradient-based meta-learning

Bernd Bischl Frank Hutter Lars Kotthoff Marius Lindauer <u>Joaquin Vanschoren</u>

Gradient-based meta-learning

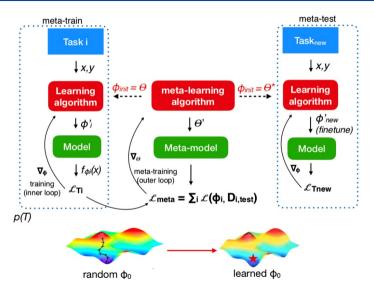
parameterize some aspect of the learner that we want to learn as meta-parameters θ meta-learn θ across tasks



 $\Theta(Prior)$, could encode an initialization ϕ , the hyperparameters λ , the optimizer,...

Learned θ^* should learn T_{new} from small amount of data, yet generalize to a large number of tasks

Gradient-based methods: learning ϕ_{init}



- θ (prior): model initialization ϕ_{init}
 - learn representation suitable for many tasks (e.g. pretrained CNN)
 - · maximize rapid learning
- Each task i yields task-adapted φ_i
 - Update algorithm u

$$\varphi_i = u(\varTheta, D_i, train)$$

• Finetune Θ^* on T_{new} (in few steps)

$$\phi'_{new} = u(\Theta^*, D_{new,train})$$

Can be seen as bilevel optimization:

$$\Theta^* = \operatorname{argmin}_{\Theta} \sum_{i} \mathcal{L}_{i}(\phi_{i}, D_{i, test})$$

$$\varphi_i = u(\varTheta, D_{i,train})$$

Meta-training

• Current initialization Θ , model f_{Θ}

derivative of test-set loss

 On i tasks, perform k SGD steps to find evaluate , then $rac{ extstyle e$

$$\phi_i = \theta - \alpha \, \nabla_\theta \mathcal{L}_i(f_{\phi_i^*})$$

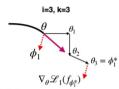
- Update task-specific parameters:
- Update Θ to minimize sum of per-task losses, repeat $\theta \leftarrow \theta \beta \nabla_{\theta} \sum_{i} \mathscr{L}_{i}(f_{\phi})$ α_{i}, β_{i} learning rates

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \boldsymbol{\beta} \, \nabla_{\boldsymbol{\theta}} \sum_{i} \mathcal{L}_{i} (f(\boldsymbol{\theta} - \boldsymbol{\alpha} \, \nabla_{\boldsymbol{\theta}} \mathcal{L}_{i}(f_{\boldsymbol{\phi}_{i}^{*}})))$$

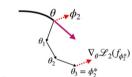
meta-gradient: $second-order\ gradient + backpropagate$ compute how changes in θ affect the gradient at new θ

Meta-testing

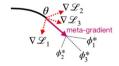
- · Training data of new task Dtrain
- θ^* : pre-trained parameters
- Finetune: $\phi = \theta^* \alpha \nabla_{\theta} \mathcal{L}(f_{\theta})$



£Task 1



 \mathcal{L} Task 2



Meta-training

- Current initialization θ , model f_{θ}
 - On i tasks, perform k SGD steps to find , then $\nabla_{\theta}\mathscr{L}_{i}(f_{\phi_{i}^{*}})$

$$\phi_i = \theta - \alpha \nabla_{\theta} \mathcal{L}_i(f_{\phi_i^*})$$

- Update task-specific parameters:
- Update Θ to minimize sum of per-task losses, repeat $\theta \leftarrow \theta \beta \nabla_{\theta} \sum_{i} \mathscr{L}_{i}(f_{\theta_{i}})$ α_{i}, β_{i} : learning rates

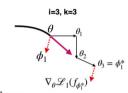
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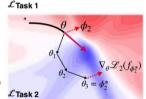
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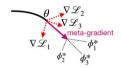
derivative of test-set loss

Meta-testing

- Training data of new task D_{train}
- Θ^* : pre-trained parameters
- Finetune: $\phi = \theta^* \alpha \nabla_{\theta} \mathcal{L}(f_{\theta})$







Meta-training

- Current initialization θ , model f_{θ}
 - On i tasks, perform k SGD steps to find , then $\nabla_{\theta} \mathcal{L}_{i}(f_{\phi_{i}^{*}})$ evaluate
 - $\phi_i = \theta \alpha \nabla_{\theta} \mathcal{L}_i(f_{\phi_i^*})$ Update task-specific parameters:
- Update Θ to minimize sum of per-task losses, repeat $\theta \leftarrow \theta \beta \nabla_{\theta} \sum_{i} \mathscr{L}_{i}(f_{db})$ α , β : learning rates

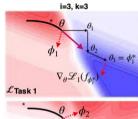
$$\theta \leftarrow \theta - \beta \nabla_{\theta} \sum_{i} \mathcal{L}_{i}(f(\theta - \alpha \nabla_{\theta} \mathcal{L}_{i}(f_{\phi_{i}^{*}})))$$

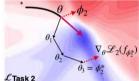
meta-gradient: $\underline{second-order\ gradient}$ + backpropagate compute how changes in θ affect the gradient at new θ

derivative of test-set loss

Meta-testing

- Training data of new task D_{train}
- θ^* : pre-trained parameters
- Finetune: $\phi = \theta^* \alpha \nabla_{\theta} \mathcal{L}(f_{\theta})$



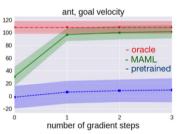




Example of reinforcement learning:

• Goal: reach certain velocity in certain direction





Other gradient-based techniques

- Changing update rule yield different variants:
 - MAML ^{1,6}

$$\theta \leftarrow \theta - \beta \nabla_{\theta} \sum_{i} \mathcal{L}_{i}(f_{\phi_{i}})$$

$$\phi_{i} = \theta - \alpha \nabla_{\theta} \mathcal{L}_{i}(f_{\phi_{i}^{*}})$$

$$\bullet \text{ MetaSGD }^{2}$$

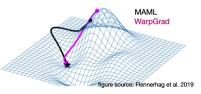
$$\phi_{i} = \theta - \alpha diag(w) \nabla_{\theta} \mathcal{L}_{i}(f_{\phi_{i}^{*}}) \text{ w: weight per parameter}$$

$$\phi_{i} = \theta - \alpha \nabla_{\theta} \mathcal{L}_{i}(f_{\phi_{i}^{*}}, w) \text{ All use second-order gradients,}$$

$$\phi_{i} = \theta - \alpha B(\theta, w) \nabla_{\theta} \mathcal{L}_{i}(f_{\phi_{i}^{*}})$$

$$\bullet \text{ Thet }^{3}$$

- Meta curvature ${}^4\phi_i=\theta-\alpha P(\theta,\phi_i)\nabla_{\!\theta}\mathcal{L}_i(f_{\phi_i^*})$
- Online MAML (Follow the Meta Leader) ⁷
 - WarpGrad ⁵
 - Minimizes regret
 - · Robust, but computation costs grow over time

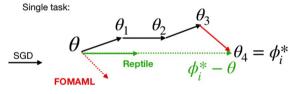


Scalability

- Backpropagating derivates of ϕ_i wrt θ is compute + memory intensive (for large models)
- First order approximations of MAML:
 - First order MAML¹ uses only the last inner gradient update:

 Pentile 2: iterate over tasks, update Θ in direction of θ .

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 - Reptile ²: iterate over tasks, update θ in direction of



FOMAML meta-gradient:



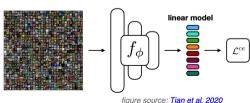
Generalizability

- ¹ Finn et al. 2018
- ² Raghu et al. 2020 ³ Tian et al. 2020
- ⁴ Stadie et al. 2019
- MAML is more resilient to overfitting than many other meta-learning techniques
- Effectiveness seems mainly due to feature reuse (finding θ) ²
 - Fine-tuning only the last layer equally good



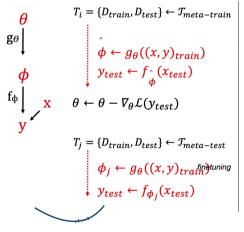
- On few-shot learning benchmarks, a good embedding outperforms most meta-learning
 - Learn representation on <u>entire</u> meta-dataset (merged into single task)
 - Train a linear classifier on embedded few-shot D_{train}, predict D_{test}

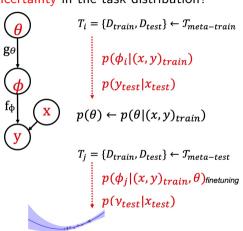
- For meta-RL, also learn how to explore (how to sample new environments)
 - E-MAML: add exploration to metaobjective (allows longer term goals)



Bayesian meta-learning

Can meta-learning reason about uncertainty in the task distribution?





Fully Bayesian meta-learning

- Use approximation methods to represent uncertainty over
 - Sampling technique + variational inference: PLATIPUS 1, BMAML 2, ABML 3
 - Laplace approximation: LLAMA 4
 - Variational approximation of posterior:
 - Neural Statistician ⁵, Neural Processes ⁶
- What if our tasks are not IID?
- Impose additional structure, e.g. with task-specific variable z ⁷

mini-ImageNet with filters for non-homogeneous tasks:



(a) plain



(b) blur

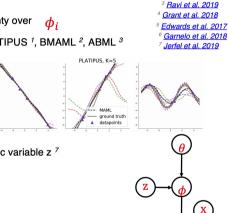






(d) pencil

Figure source: Jerfel et al. 2019

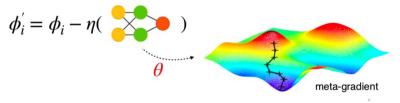


¹ Finn et al. 2019 ² Kim et al. 2018

Meta-learning optimizers

Our brains probably don't do backprop, instead:

- weights: networks that continuously modify the weights of another network
- Gradient based: parameterize the update rule using a neural network
 - ▶ Learn meta-parameters across tasks, by gradient descent



Represent update rule as an LSTM, hierarchical RNN

Meta-learning optimizers

- Meta-learned (RNN) optimizers 'rediscover' momentum, gradient clipping, learning rate schedules, learning rate adaptation,...
- RL-based optimizers: represent updates as a policy, learn using guided policy search
- Combined with MAML:
 - learn per-parameter learning rates
 - learn precondition matrix (to 'warp' the loss surface)
- Black-box optimizers: meta-learned with an RNN, or with user-defined priors
- Speed up backpropagation by meta-learning sparsity and weight sharing

