Meta-Learning to Improve Pre-Training

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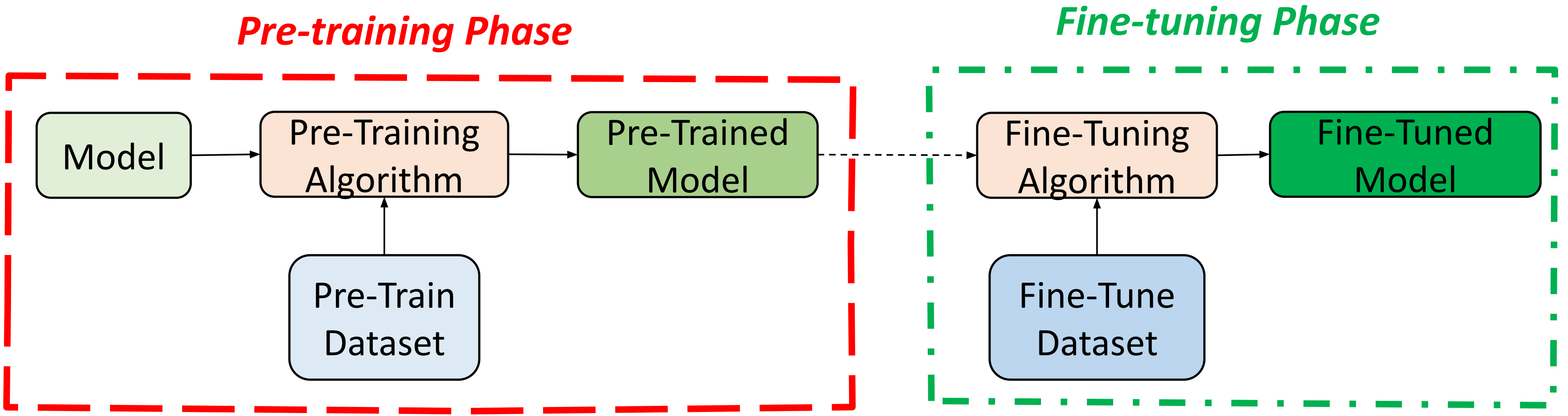
Matthew McDermott, David Duvenaud

Pre-training (PT) followed by Fine-tuning (FT):
An important neural network training paradigm...



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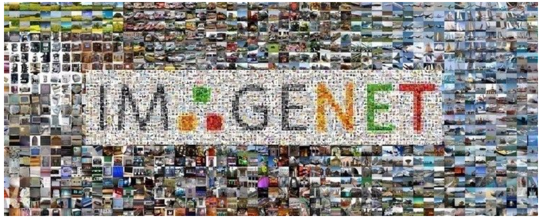
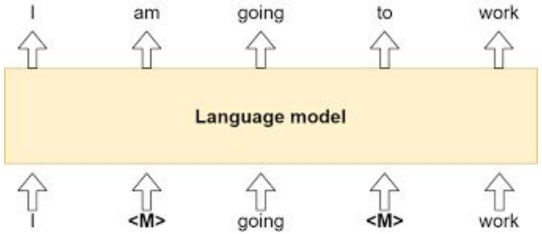
Examples include:



- Supervised PT on ImageNet
- (Masked) language modelling for NLP
- Self-supervised PT: SimCLR, BYOL, …



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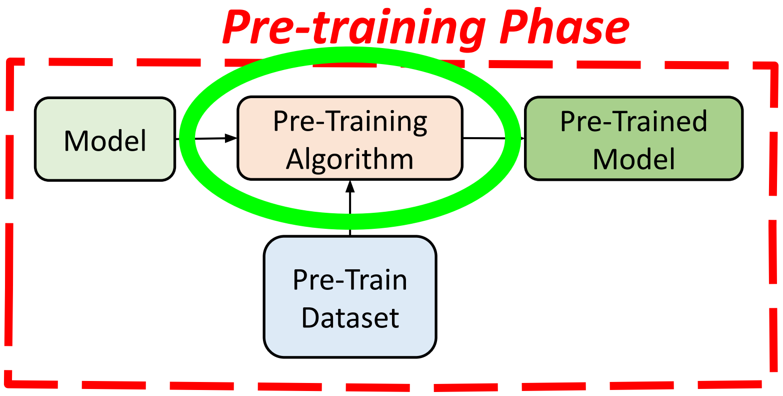
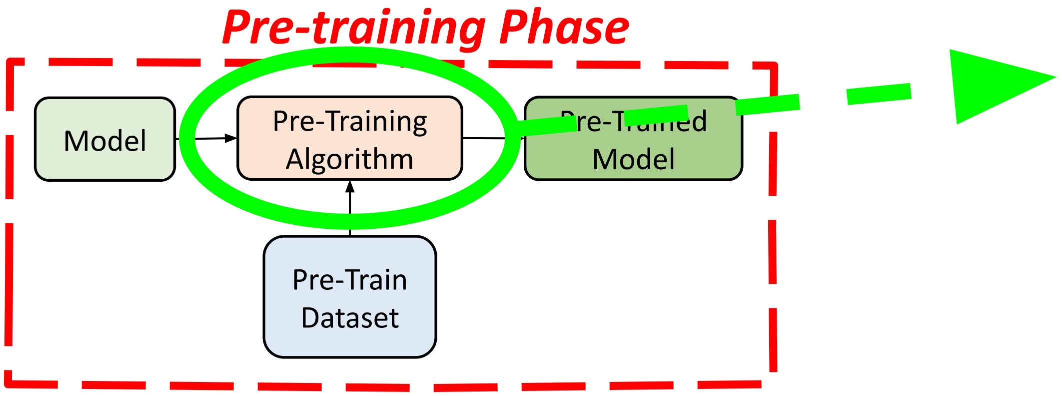


… but introduces many complex design choices (meta-parameters), especially during pre-training (PT)



Meta-parameters may include:

- Task weights for multitask PT
- Sampling strategies
- Augmentation strategies for self-supervised PT
- Noise models for PT
- …

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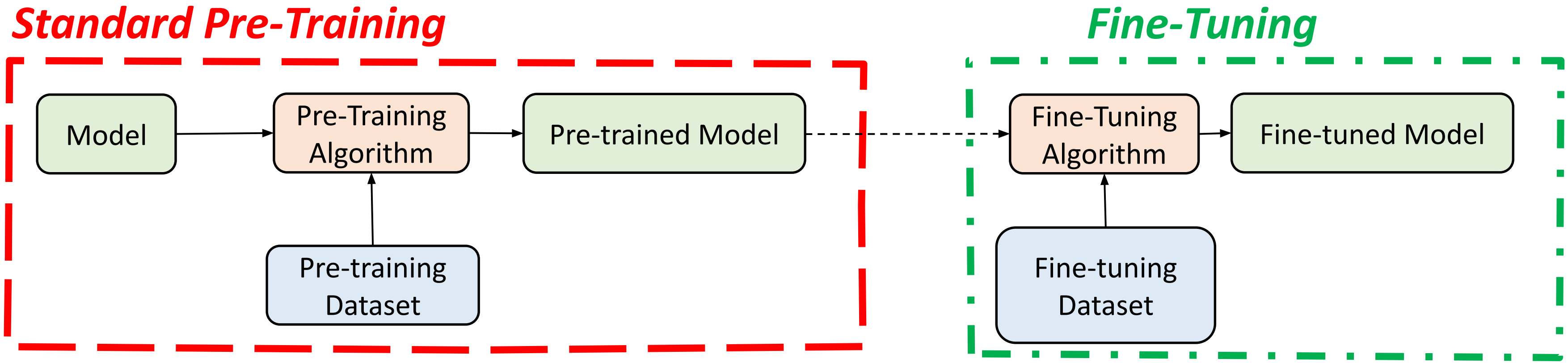
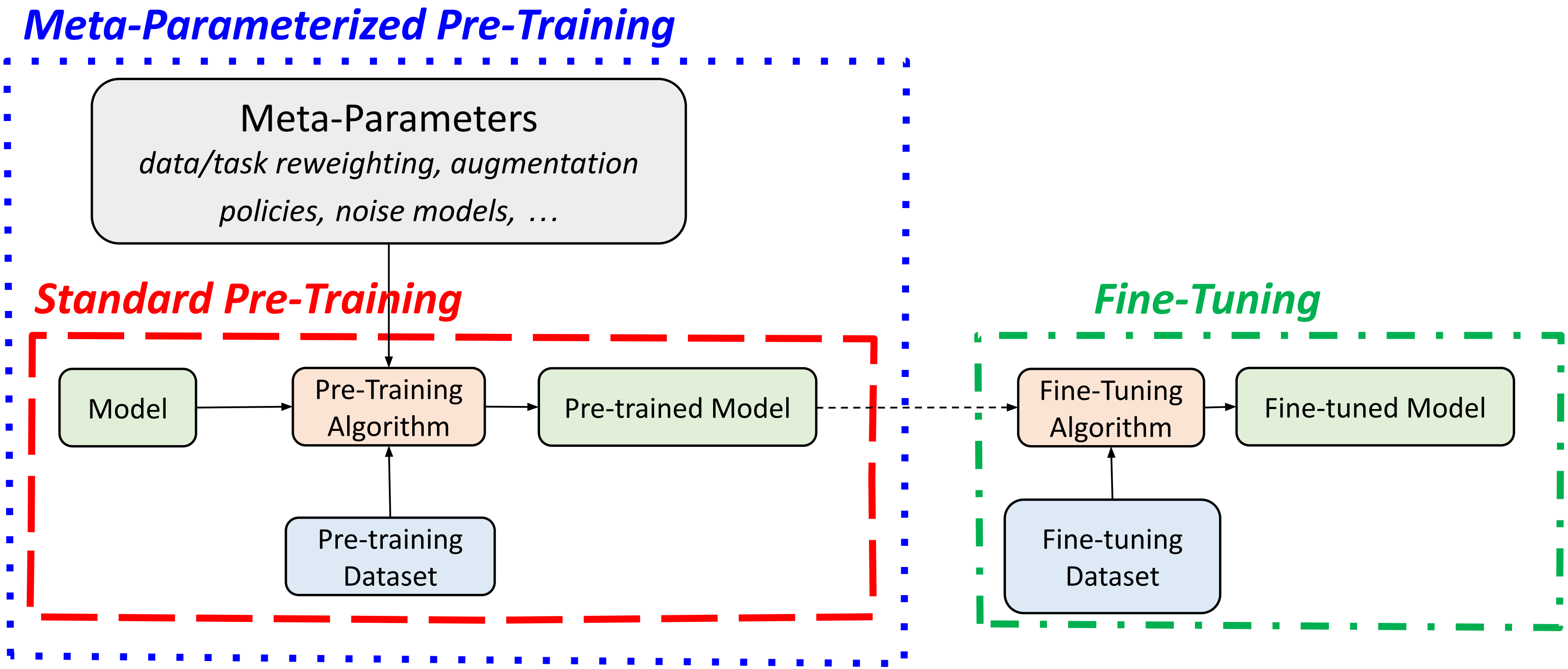
- Gradient based
  - How to efficiently obtain gradients through two optimization stages (PT and FT)?

This work: An efficient and scalable algorithm to optimize these meta-parameters

Standard Pre-Training (PT)



Meta-Parameterized Pre-Training (PT)



More formally...

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Result: Pre-trained parameters: θ^*_{PT}

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Informally: $$\frac{\partial L_{\mathrm{FT}}}{\partial \phi} = \frac{\partial L_{\mathrm{FT}}}{\partial \theta^*_{\mathrm{FT}}} \times \frac{\partial \mathrm{Alg}_{\mathrm{FT}}}{\partial \theta^*_{\mathrm{PT}}} \times \frac{\partial \mathrm{Alg}_{\mathrm{PT}}}{\partial \phi}$$

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Need to differentiate through two optimization problems!

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Key insight: Approximate gradient by combining backpropagation through training and implicit differentiation

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$$\frac{\partial L_{\mathrm{FT}}}{\partial \phi} = \underbrace{\overbrace{\boxed{\frac{\partial L_{\mathrm{FT}}}{\partial \theta^{*}_{\mathrm{FT}}}}}^{\text{FT Loss Gradient}}}_{\substack{\text{Easy to compute:} \\ \text{Use direct backprop}}} \times \underbrace{\overbrace{\boxed{\frac{\partial \mathrm{Alg}_{\mathrm{FT}}}{\partial \theta^{*}_{\mathrm{PT}}}}}^{\text{FT Best Response Jacobian}}}_{\substack{\text{Harder to compute:} \\ \text{Use (Truncated) Backprop} \\ \text{through training}}} \times \underbrace{\overbrace{\boxed{\frac{\partial \mathrm{Alg}_{\mathrm{PT}}}{\partial \phi}}}^{\text{PT Best Response Jacobian}}}_{\substack{\text{Harder to compute:} \\ \text{Use Implicit differentiation}}}$$

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In practice, learn meta-parameters and network parameters online for efficiency

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- Perform meta-parameter update: $\phi \leftarrow \phi - \eta \frac{\partial L_{\mathrm{FT}}}{\partial \phi}$

Experimental evaluation

Synthetic Experiments:
Can our algorithm learn optimal meta-parameters?

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Yes! In two synthetic MNIST domains, the algorithm finds optimal meta-parameters.

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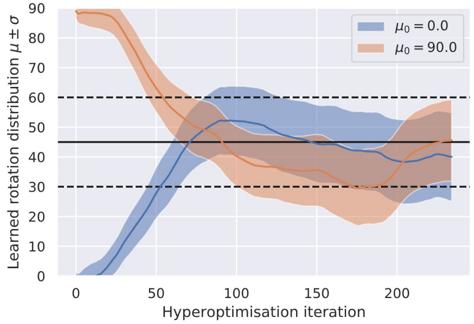
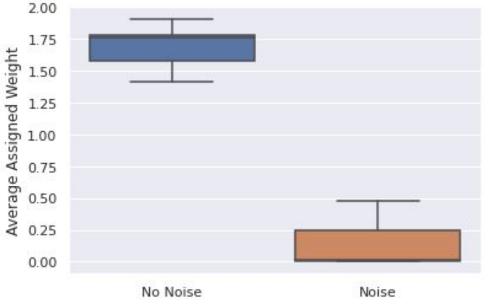
- PT augmentations:
  learns the optimal augmentation distribution



- PT example importance weighting with noisy labels:
  downweights noisy label examples



Real-world experimental evaluation

Study two settings:

1) Optimizing task weights for multi-task PT with GNNs

2) Optimizing data augmentation pipeline for self-supervised learning with electrocardiogram signals

Focus on 1) in this talk

Multitask Pre-training with GNNs

- **Task:** Given input Protein-Protein Interaction graph, predict the presence of several biological functions [1]

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- **PT:** Input graphs (*x*) together with 5000 binary attributes (*y*)
  FT: Input graphs (*x*) together with 40 (distinct) binary attributes (*y*)

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- **PT:** Input graphs (*x*) together with 5000 binary attributes (*y*)
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- **Meta-parameters:** 5000-dimensional vector representing a weight for each task in PT, used to weight PT loss.

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Multitask Pre-training with GNNs

- **Baselines:**
  - No PT
  - Supervised PT: weights set to 1
  - CoTrain: PT jointly on all labels
  - CoTrain + PCGrad [1]: Like above, but apply PCGrad to reduce conflicting gradient updates among tasks

[1] Gradient Surgery for Multi-Task Learning, Yu et al., NeurIPS 2020

Multitask Pre-training with GNNs

- **Results:**

Method	Average AUC across tasks
No PT	66.6 ± 0.7
Graph Supervised PT	74.7 ± 0.1
CoTrain	70.2 ± 0.3
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Meta-Parameterized PT	$\mathbf{78.6 \pm 0.1}$

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- Additional experimental settings and baselines in paper
  - Testing generalization to new tasks
  - Further studies on sample efficiency
  - Other meta-parameter learning baselines

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- **This work:**
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- **Experimental evaluation**: our algorithm can effectively optimize these meta-parameters, and improves performance in two-real world domains