Graph Representation Learning for Multi-Task Settings: a Meta-Learning Approach

Davide Buffelli  
Department of Information Engineering  
University of Padova  
Padova, Italy  
DAVIDE.BUFFELLI@UNIPD.IT

Fabio Vandin  
Department of Information Engineering  
University of Padova  
Padova, Italy  
FABIO.VANDIN@UNIPD.IT

Abstract

Graph Neural Networks (GNNs) have become the state-of-the-art method for many applications on graph structured data. GNNs are a framework for graph representation learning, where a model learns to generate low dimensional node embeddings that encapsulate structural and feature-related information. GNNs are usually trained in an end-to-end fashion, leading to highly specialized node embeddings. While this approach achieves great results in the single-task setting, generating node embeddings that can be used to perform multiple tasks (with performance comparable to single-task models) is still an open problem. We propose a novel training strategy for graph representation learning, based on meta-learning, which allows the training of a GNN model capable of producing multi-task node embeddings. Our method avoids the difficulties arising when learning to perform multiple tasks concurrently by, instead, learning to quickly (i.e. with a few steps of gradient descent) adapt to multiple tasks singularly. We show that the embeddings produced by a model trained with our method can be used to perform multiple tasks with comparable or, surprisingly, even higher performance than both single-task and multi-task end-to-end models.

Keywords: Graph Representation Learning, Graph Neural Networks, Multi-Task Learning, Meta-Learning, Graph Embedding

1. Introduction

Graph Neural Networks (GNNs) are deep learning models for graph structured data, and have become one of the main topics of the deep learning research community. The high interest in GNNs is due, in part, to their great empirical performance on many graph-related tasks. Three tasks in particular, with many practical applications, have received the most attention: graph classification, node classification, and link prediction.

GNNs are centered around the concept of node representation learning, and typically follow the same architectural pattern with an encoder-decoder structure (Hamilton et al., 2017; Chami et al., 2020; Wu et al., 2020). The encoder produces node embeddings (low-dimensional vectors capturing relevant structural and feature-related information about each node), while the decoder uses the embeddings to carry out the desired downstream task. The model is then trained in an end-to-end manner, leading to highly specialized node...
embeddings. While this approach can achieve state-of-the-art performance, it also affects the generality and reusability of the embeddings. In fact, taking the node embeddings generated by an encoder trained for a given task, and using them to train a decoder for a different task leads to substantial performance loss, as shown in Figure 1.

The low transferability of node embeddings requires the use of one specialized encoder and one specialized decoder for each considered task. However, many practical machine learning applications operate in resource-constrained environments where being able to share part of the model architecture between tasks is of great importance. Furthermore, the training signal from multiple related tasks may lead to higher generalization. Nevertheless, making sure tasks do not negatively interfere with each other is not trivial (Standley et al., 2020). The problem of learning models that perform multiple tasks is an open area of research known as Multi-Task Learning (MTL) (Vandenhende et al., 2020).

MTL on graphs has not received much attention. In fact, the straightforward application to GNNs of the classical MTL procedure (that is, training a multi-head model by performing multiple tasks concurrently on each graph, and updating the parameters with some form of gradient descent to minimize the sum of the single-task losses) leads to a significant performance loss with respect to single-task models, as we show in Section 5. Therefore, until now, no single model capable of performing the three most common graph-related tasks (with performance comparable to single-task models) has been proposed. Thus, we propose a novel training procedure for multi-task representation learning, based on optimization-based meta-learning (Finn et al., 2017), that learns a GNN encoder producing node embeddings that generalize across multiple tasks.

Our proposed meta-learning procedure trains a GNN encoder that produces task-generalizing node embeddings by training an encoder-decoder model without aiming at a setting of the parameters that can perform multiple tasks concurrently (like a classical method would do), or to a setting that allows fast multi-task adaptation, but to a setting that can easily be adapted to perform each of the tasks singularly. In fact, our procedure aims at a

Figure 1: Performance drop when transferring node embeddings on the ENZYMES dataset to perform the following tasks: (a) Node Classification (NC), (b) Graph Classification (GC), and (c) Link Prediction (LP). “x -> y” indicates that the embeddings obtained from a model trained on task x are used to train a network for task y.
setting of the parameters where a few steps of gradient descent on a given task lead to good performance on that task, hence removing the burden of directly learning to solve multiple tasks concurrently. At the end of the training procedure, the decoder is discarded, and the encoder can be used to generate embeddings for new graphs.

We summarize our contributions as follows:

• We propose a novel method for training a deep learning model that generates representations that generalize to multiple tasks. We apply it to the challenging setting of graph MTL, and show that a GNN trained with our method produces node embeddings leading to higher downstream performance with respect to classical end-to-end training procedures. Our method is based on meta-learning and is model-agnostic and task-agnostic, which makes it easily applicable to a wide range of multi-task domains.

• To the best of our knowledge, we are the first to propose a GNN model generating a single set of node embeddings that can be used to perform the three most common graph-related tasks (i.e., graph classification, node classification, and link prediction). In particular, our embeddings lead to comparable or higher performance with respect to end-to-end single-task models even when used as input to a simple linear classifier.

• We show that the episodic training strategy at the base of our proposed meta-learning procedure leads to a model that generates node embeddings more effective for downstream tasks, even in single-task settings. This unexpected finding is of interest in itself, and may provides fruitful directions for future research.

2. Related Work

GNNs, MTL, and meta-learning are very active areas of research. We highlight works that are at the intersection of these subjects, and point the interested reader to comprehensive reviews of each field. To the best of our knowledge there is no work using meta-learning to train a model for graph MTL, or proposing a GNN performing graph classification, node classification, and link prediction concurrently.

Graph Neural Networks. GNNs have a long history (Scarselli et al., 2009), but in the past few years the field has grown exponentially (Chami et al., 2020; Wu et al., 2020). The first popular GNN approaches were based on filters in the graph spectral domain (Bronstein et al., 2017), and presented many challenges including high computational complexity. Defferrard et al. (2016) introduced ChebNet, which uses Chebyshev polynomials to produce localized and efficient filters in the graph spectral domain. Graph Convolutional Networks (Kipf and Welling, 2017) then introduced a localized first-order approximation of spectral graph convolutions which was then extended to include attention mechanisms (Veličković et al., 2018). Recently, Xu et al. (2019) provided theoretical ground for the expressivity of GNNs.

Multi-Task Learning. Works at the intersection of MTL and GNNs have mostly focused on multi-head architectures. These models are composed of a series of GNN layers followed by multiple heads (i.e., independent neural network layers) that perform the desired downstream tasks. In this category, Montanari et al. (2019) propose a model for the prediction of physico-chemical properties. Holtz et al. (2019) and Xie et al. (2020) propose
multi-task models for concurrently performing node and graph classification. Finally, Avelar et al. (2019) introduce a multi-head GNN for learning multiple graph centrality measures, and Li and Ji (2019) propose a MTL method for the extraction of multiple biomedical relations. Other related work includes (Haonan et al., 2019) which introduces a model that can be trained for several tasks singularly, hence, unlike the previously mentioned approaches and our proposed method, it can not perform multiple tasks concurrently. There are also some works that use GNNs as a tool for MTL: Liu et al. (2019b) use GNNs to allow communication between tasks, while Zhang et al. (2018) use GNNs to estimate the test error of a MTL model. We further mention the work by Wang et al. (2020) which considers the task of generating “general” node embeddings, however their method is not based on GNNs, does not consider node attributes (unlike our method), and is not focused on the three most common graph related tasks. In summary, the current literature on graph MTL has focused on multi-head architectures that are trained end-to-end for specific tasks, and hence ignoring the graph representation learning scenario, which involves the learning of node/graph embeddings that can be used for several downstream tasks. In this work we tackle the latter problem, and propose a method to learn a GNN generating node embeddings that can be used to perform the three most common graph related tasks.

Training multi-task models is challenging (Standley et al., 2020), as some losses may dominate over others, or gradients for different tasks may point in opposite directions. Some methods have been proposed to counteract these issues (Kendall et al., 2018; Chen et al., 2018), but they are not always effective and it is not clear how one should choose which method to apply (Vandenhende et al., 2020). For an exhaustive review of deep MTL techniques we refer the reader to Vandenhende et al. (2020).

Meta-Learning. Meta-Learning consists in learning to learn. Many methods have been proposed (see the review by Hospedales et al. (2020)), specially in the area of few-shot learning. Garcia and Bruna (2018) frame the few-shot learning problem with a partially observed graphical model and use GNNs as an inference algorithm. Liu et al. (2019a) use GNNs to propagate messages between class prototypes and improve existing few-shot learning methods, while Suo et al. (2020) use GNNs to introduce domain-knowledge in the form of graphs. There are also several works that use meta-learning to train GNNs in few-shot learning scenarios with applications to node classification (Zhou et al., 2019; Yao et al., 2020), edge labelling (Kim et al., 2019), link prediction (Alet et al., 2019; Bose et al., 2019), and graph regression (Nguyen et al., 2020). Finally, other combinations of meta-learning and GNNs involve adversarial attacks (Zügner and Günnemann, 2019) and active learning (Madhawa and Murata, 2020). In contrast to previous work, we propose a novel meta-learning procedure that is applied only at training time, for training a GNN model that can generate node embeddings, which can be used for multiple downstream tasks.

3. Preliminaries

In this section we briefly introduce GNNs (Section 3.1) and optimization-based meta-learning techniques (Section 3.2), which are at the core of our proposed method.
3.1 Graph Neural Networks

Many popular state-of-the-art GNN models follow the message-passing paradigm (Gilmer et al., 2017), which we now briefly describe. We represent a graph $G = (A, X)$ with an adjacency matrix $A \in \{0, 1\}^{n \times n}$, such that $A_{ij} = 1$ if and only if there is an edge between the $i$-th vertex and the $j$-th vertex, and a node feature matrix $X \in \mathbb{R}^{n \times d}$, where the $v$-th row $X_v$ represents the $d$ dimensional feature vector of node $v$. Let $H^{(l)} \in \mathbb{R}^{n \times d}$ be the matrix containing the node representations at layer $\ell$. A message passing layer updates the representation of every node $v$ as follows:

$$msg_{v}^{(l)} = \text{AGGREGATE}((H_u^{(l)} \forall u \in N_v))$$

$$H_v^{(l+1)} = \text{UPDATE}(H_v^{(l)}, msg_v^{(l)})$$

where $H^{(0)} = X$, $N_v$ is the set of neighbours of node $v$, AGGREGATE is a permutation invariant function, and UPDATE is usually a neural network. After $L$ message-passing layers, the final node embeddings $H^{(L)}$ are the representations used to perform a given task (e.g., they are the input to a neural component that performs the given task), and the network is trained end-to-end.

3.2 Model-Agnostic Meta-Learning and ANIL

MAML (Model-Agnostic Meta-Learning) is an optimization-based meta-learning strategy proposed by Finn et al. (2017). Let $f_\theta$ be a deep learning model, where $\theta$ represents its parameters. Let $p(\mathcal{E})$ be a distribution over episodes\(^1\), where an episode $\mathcal{E}_i \sim p(\mathcal{E})$ is defined as a tuple containing a loss function $\mathcal{L}_{\mathcal{E}_i}(\cdot)$, a support set $\mathcal{S}_{\mathcal{E}_i}$, and a target set $\mathcal{T}_{\mathcal{E}_i}$: $\mathcal{E}_i = (\mathcal{L}_{\mathcal{E}_i}(\cdot), \mathcal{S}_{\mathcal{E}_i}, \mathcal{T}_{\mathcal{E}_i})$, where support and target sets are simply sets of labelled examples. MAML’s goal is to find a value of $\theta$ that can quickly, i.e. in a few steps of gradient descent, be adapted to new episodes. This is done with a nested loop optimization procedure: an inner loop adapts the parameters to the support set of an episode by performing some steps of gradient descent, and an outer loop updates the initial parameters aiming at a setting that allows fast adaptation. Formally, by defining $\theta_i(t)$ as the parameters after $t$ adaptation steps on the support set of episode $\mathcal{E}_i$, we can express the computations in the inner loop as

$$\theta_i(t) = \theta_i(t-1) - \alpha \nabla_{\theta_i(t-1)} \mathcal{L}_{\mathcal{E}_i}(f_{\theta_i(t-1)}; \mathcal{S}_{\mathcal{E}_i})$$

where $\theta_i(0) = \theta$, $\mathcal{L}(f_{\theta_i(t-1)}; \mathcal{S}_{\mathcal{E}_i})$ indicates the loss over the support set $\mathcal{S}_{\mathcal{E}_i}$ of the model $f_{\theta_i(t-1)}$ with parameters $\theta_i(t-1)$, and $\alpha$ is the learning rate. The meta-objective that the outer loop tries to minimize is defined as $\mathcal{L}_{\text{meta}} = \sum_{\mathcal{E}_i \sim p(\mathcal{E})} \mathcal{L}_{\mathcal{E}_i}(f_{\theta_i(t)}; \mathcal{T}_{\mathcal{E}_i})$, which leads to the following parameter update\(^2\) performed in the outer loop:

$$\theta = \theta - \beta \nabla_{\theta} \mathcal{L}_{\text{meta}} = \theta - \beta \nabla_{\theta} \sum_{\mathcal{E}_i \sim p(\mathcal{E})} \mathcal{L}_{\mathcal{E}_i}(f_{\theta_i(t)}; \mathcal{T}_{\mathcal{E}_i}).$$

---

1. The meta-learning literature usually derives episodes from tasks (i.e., tuples containing a dataset and a loss function). We focus on episodes to avoid using the term task for both a MTL task, and a meta-learning task.
2. We limit ourselves to one step of gradient descent for clarity, but any optimization strategy could be used.
Raghu et al. (2020) showed that feature reuse is the dominant factor in MAML: in the adaptation loop, only the last layer(s) in the network are updated, while the first layer(s) remain almost unchanged. The authors then propose ANIL (Almost No Inner Loop) where they split the parameters in two sets: one that is used for adaptation in the inner loop, and one that is only updated in the outer loop. This simplification leads to computational improvements while maintaining performance.

4. SAME: Single-Task Adaptation for Multi-Task Embeddings

Our novel training technique for multi-task representation learning is based on meta-learning, and builds on three insights:

(i) optimization-based meta-learning is implicitly learning robust representations. The findings by Raghu et al. (2020) suggest that, in a model trained with MAML, the first layers learn features that are reusable across episodes, while the last layers are set up for fast adaptation. MAML is then implicitly learning a model with two components: an encoder (the first layers), focusing on learning reusable representations that generalize across episodes, and a decoder (the last layers) that can be quickly adapted for different episodes.

(ii) meta-learning episodes can be designed to encourage generalization. If we design support and target sets to mimic the training and validation sets of a classical training procedure, then the meta-learning procedure is effectively optimizing for generalization.

(iii) meta-learning can learn to quickly adapt to multiple tasks singularly, without having to learn to solve multiple tasks concurrently. We can design the meta-learning procedure so that, for each considered task, the inner loop adapts the parameters to a task-specific support set, and tests the adaptation on a task-specific target set. The outer loop then updates the parameters to allow this fast multiple single-task adaptation. This procedure is effectively searching for a parameter setting that can be easily adapted to obtain good single-task performance on multiple tasks singularly, without learning to solve multiple tasks concurrently. The procedure differs from classical multi-task learning methods (which aim at solving multiple tasks concurrently), and has a completely different scope from conventional meta-learning methods (which may be seen as special cases of our method). In particular we use meta-learning only at training time, and do not perform any adaptation at test time. (We provide a broader discussion in Section 4.4.)

Based on (ii) and (iii), we develop a meta-learning procedure where the inner loop adapts to multiple tasks singularly, each time with the goal of single-task generalization. Using an encoder-decoder architecture, (i) suggests that this procedure leads to an encoder that learns features that are reusable across episodes. Moreover, in each episode, the learner is adapting to multiple tasks, hence the encoder is learning features that generalize across multiple tasks. After training a model with our meta-learning strategy, the decoder is discarded, and only the encoder is kept and used to generate representations that generalize across multiple tasks (hence there is no adaptation performed at test time).

In the rest of this section, we formally present our novel meta-learning procedure for training multi-task graph representation learning models. There are three aspects that we need to define: (1) Episode Design: how is an an episode composed, (2) Model Ar-

3. We provide an additional analysis on the differences with traditional methods in Appendix C
Figure 2: **Main ingredients of our method SAME.** (a) Schematic representation of a *multi-task episode*. For each task, support and target set are designed to be as the training and validation sets for single-task training. (b) Scheme of iSAME: both the backbone GNN and the task-specific output layers are adapted (one at a time) in the inner loop of our meta-learning procedure. (c) Scheme of eSAME: only the task-specific output layers are adapted (one at a time) in the inner loop of our meta-learning procedure. Both in iSAME and eSAME, after training the model with our proposed meta-learning procedure, only the backbone GCN is kept, and is used to generate embeddings that can be used for multiple downstream tasks.

**Architecture Design:** what is the architecture of our model, (3) **Meta-Training Design:** how, and which, parameters are adapted/updated.

### 4.1 Episode Design

In our case, an episode becomes a *multi-task episode* (Figure 2 (a)). To formally introduce the concept, let us consider the case where the tasks are graph classification (GC), node classification (NC), and link prediction (LP). We define a *multi-task episode* \( \mathcal{E}_i^{(m)} \sim p(\mathcal{E}^{(m)}) \) as a tuple

\[
\mathcal{E}_i^{(m)} = (\mathcal{L}_{\mathcal{E}_i}^{(m)}, \mathcal{S}_{\mathcal{E}_i}^{(m)}, \mathcal{T}_{\mathcal{E}_i}^{(m)})
\]

\[
\mathcal{L}_{\mathcal{E}_i}^{(m)} = \lambda^{(GC)} \mathcal{L}_{\mathcal{E}_i}^{(GC)} + \lambda^{(NC)} \mathcal{L}_{\mathcal{E}_i}^{(NC)} + \lambda^{(LP)} \mathcal{L}_{\mathcal{E}_i}^{(LP)}
\]

\[
\mathcal{S}_{\mathcal{E}_i}^{(m)} = \{\mathcal{S}_{\mathcal{E}_i}^{(GC)}, \mathcal{S}_{\mathcal{E}_i}^{(NC)}, \mathcal{S}_{\mathcal{E}_i}^{(LP)}\},
\]

\[
\mathcal{T}_{\mathcal{E}_i}^{(m)} = \{\mathcal{T}_{\mathcal{E}_i}^{(GC)}, \mathcal{T}_{\mathcal{E}_i}^{(NC)}, \mathcal{T}_{\mathcal{E}_i}^{(LP)}\}
\]

where \( \lambda^{(i)} \) are balancing coefficients. The meta-objective \( \mathcal{L}_{\text{meta}}^{(m)} \) of our method then becomes:

\[
\mathcal{L}_{\text{meta}}^{(m)} = \sum_{\mathcal{E}_i^{(m)} \sim p(\mathcal{E}^{(m)})} \lambda^{(GC)} \mathcal{L}_{\mathcal{E}_i}^{(GC)} + \lambda^{(NC)} \mathcal{L}_{\mathcal{E}_i}^{(NC)} + \lambda^{(LP)} \mathcal{L}_{\mathcal{E}_i}^{(LP)}. \tag{1}
\]

Support and target sets are set up to resemble training and validation sets. This way the outer loop’s objective becomes to maximize the performance on a validation set, *given a training set*, hence pushing towards generalization. In more detail, given a batch of graphs, we divide it in equally sized splits (one per task), and we create support and target sets as follows:
Graph Classification: $S_{\bar{E}_i}^{(GC)}$ and $T_{\bar{E}_i}^{(GC)}$ contain labeled graphs, obtained with a random split.

Node Classification: $S_{\bar{E}_i}^{(NC)}$ and $T_{\bar{E}_i}^{(NC)}$ are composed of the same graphs, with different labelled nodes. We mimic the common semi-supervised setting (Kipf and Welling, 2017) where feature vectors are available for all nodes, and only a small subset of nodes is labelled.

Link Prediction: $S_{\bar{E}_i}^{(LP)}$ and $T_{\bar{E}_i}^{(LP)}$ are composed of the same graphs, with different query edges. In every graph we randomly remove some edges, used as positive examples together with non-removed edges, and randomly sample couples of non-adjacent nodes as negative examples.

Notice how we only need labels for one task for each graph. The full algorithm for the creation of multi-task episodes is provided in Appendix A.

4.2 Model Architecture Design

We use an encoder-decoder model with a multi-head architecture. The backbone (which represents the encoder) is composed of 3 GCN (Kipf and Welling, 2017) layers with ReLU non-linearities and residual connections (He et al., 2016). The decoder is composed of three heads. The node classification head is a single layer neural network with a Softmax activation that is shared across nodes and maps node embeddings to class predictions. In the graph classification head, first a single layer neural network (shared across nodes) performs a linear transformation (followed by a ReLU activation) of the node embeddings. The transformed node embeddings are then averaged and a final single layer neural network with Softmax activation outputs the class predictions. The link prediction head is composed of a single layer neural network with ReLU non-linearity that transforms node embeddings, and a single layer neural network that given concatenation of two embeddings outputs the probability of a link between them. We remark that after training the full model with our proposed meta-learning procedure, only the encoder is kept, and is used to generate node embeddings which can then be fed to any machine learning model for performing multiple downstream tasks.

4.3 Meta-Training Design

We first present our meta-learning training procedure, and successively describe which parameters are adapted/updated in the inner and outer loops.

Meta-Learning Training Procedure. To avoid the problems arising from training a model that performs multiple tasks concurrently, we design a meta-learning procedure where the inner loop adaptation and the meta-objective computation involve a single task at a time. Only the parameter update performed to minimize the meta-objective involves multiple tasks, but, crucially, it does not aim at a setting of parameters that can solve, or quickly adapt to, multiple tasks concurrently, but to a setting that allows multiple fast single-task adaptation.

The pseudocode of our procedure is in Algorithm 1. init is a method that initializes the weights of the GNN. ADAPT performs a few steps of gradient descent on a task-specific
Algorithm 1 Proposed (meta-learning based) training procedure for multi-task representation learning.

| Input: | Model $f_\theta$; Episodes $\mathcal{E} = \{\mathcal{E}_1, ..., \mathcal{E}_n\}$ |
|--------|------------------------------------------------------------------------|
| init($\theta$) | for $\mathcal{E}_i$ in $\mathcal{E}$ do 
| | o_loss $\leftarrow 0$ 
| | for $\tau$ in (GC, NC, LP) do 
| | $\theta^{(\tau)}$ $\leftarrow \theta$ 
| | $\theta^{(\tau)}$ $\leftarrow$ ADAPT($f_\theta$, $S^{(\tau)}_E$, $L^{(\tau)}_E$) 
| | o_loss $\leftarrow$ o_loss + TEST($f_{\theta^{(\tau)}}$, $T^{(\tau)}_E$, $L^{(\tau)}_E$) 
| | end for 
| | $\theta$ $\leftarrow$ UPDATE($\theta$, o_loss, $\theta^{(GC)}$, $\theta^{(NC)}$, $\theta^{(LP)}$) 
| end for |

loss function and support set, TEST computes the value of the meta-objective component on a task-specific loss function and target set, and UPDATE optimizes the parameters by minimizing the meta-objective in Equation 1. Notice the multiple heads of the decoder in our model are never used concurrently.

Parameter Update in Inner/Outer Loop. Let us partition the parameters of our model in four sets: $\theta = [\theta_{GCN}, \theta_{NC}, \theta_{GC}, \theta_{LP}]$ representing the parameters of the backbone ($\theta_{GCN}$), node classification head ($\theta_{NC}$), graph classification head ($\theta_{GC}$), and link prediction head ($\theta_{LP}$). We name our proposed meta-learning strategy SAME (Single-Task Adaptation for Multi-Task Embeddings), and present two variants (Figure 2 (b)-(c)):

**Implicit SAME (iSAME):** all the parameters $\theta$ are used for adaptation. This strategy makes use of the implicit feature-reuse factor of MAML, leading to parameters $\theta_{GCN}$ that are general across multi-task episodes.

**Explicit SAME (eSAME):** only the head parameters $\theta_{NC}, \theta_{GC}, \theta_{LP}$ are used for adaptation. Contrary to the previous, this strategy explicitly aims at learning the parameters $\theta_{GCN}$ to be general across multi-task episodes by only updating them in the outer loop.

Note that the pseudocode in Algorithm 1 is the same for both iSAME and eSAME. The difference between the methods is in which subset of the parameters $\theta$ is updated by the ADAPT function. In more detail, for iSAME the ADAPT function will update the head parameters and the backbone parameters (i.e., $\theta_{GCN}, \theta_{NC}, \theta_{GC}, \theta_{LP}$), while for eSAME only the head parameters ($\theta_{NC}, \theta_{GC}, \theta_{LP}$) will be updated.

4.4 SAME as a General Framework for Optimization-based Meta-Learning

SAME can be seen as a general version of optimization-based meta-learning approaches, with MAML (and ANIL) being a special case of SAME. In particular SAME extends MAML’s procedure as follows: 

1. SAME allows each episode to be composed of multiple tasks. Tasks in the inner loop can differ from tasks in the outer loop. 
2. In SAME each task (both in the inner and in the outer loop) can involve only a subset of the parameters of the model. The subsets can overlap. 
3. In the inner loop of SAME, if the episode is
Table 1: Results for a single-task model trained in a classical supervised manner, a fine-tuned model (trained on all, and fine-tuned on two tasks), and a linear classifier trained on node embeddings generated by a model trained with our proposed strategies (iSAME, eSAME) in a multi-task setting.

| Task | Dataset | GC | NC | LP | ENZYMES | PROTEINS | DHFR | COX2 |
|------|---------|----|----|----|---------|----------|------|------|
|      |         |    |    |    |         |          |      |      |
|      | Classical End-to-End Training | | | | | | | |
| ✓    | 51.6    | 73.3 | 71.5 | 76.7 |
| ✓    | 87.5    | 72.3 | 97.3 | 96.4 |
| ✓    | 75.5    | 85.6 | 98.8 | 98.2 |
|      | Fine-Tuning | | | | | | | |
| ✓    | ✓       | 48.3 | 85.3 | 73.6 | 72.0 | 66.4 | 92.4 | 80.0 | 92.3 |
| ✓    | ✓       | 49.3 | 71.6 | 69.6 | 80.7 | 65.3 | 58.9 | 80.2 | 50.9 |
| ✓    | ✓       | 87.7 | 73.9 | 80.4 | 81.5 | 80.7 | 56.6 | 87.4 | 52.3 |
|      | iSAME (ours) | | | | | | | |
| ✓    | ✓       | 50.1 | 86.1 | 73.1 | 76.6 | 71.6 | 94.8 | 75.2 | 95.4 |
| ✓    | ✓       | 50.7 | 83.1 | 73.4 | 85.2 | 71.6 | 99.2 | 77.5 | 98.9 |
| ✓    | ✓       | 86.3 | 83.4 | 79.4 | 87.7 | 96.5 | 99.3 | 95.5 | 99.0 |
| ✓    | ✓       | 50.0 | 86.5 | 82.3 | 71.4 | 76.6 | 87.3 | 71.2 | 95.5 |
|      | eSAME (ours) | | | | | | | |
| ✓    | ✓       | 51.7 | 86.1 | 71.5 | 79.2 | 70.1 | 95.7 | 75.6 | 95.5 |
| ✓    | ✓       | 51.9 | 80.1 | 71.7 | 85.4 | 70.1 | 99.1 | 77.5 | 98.8 |
| ✓    | ✓       | 86.7 | 82.2 | 80.7 | 86.3 | 96.6 | 99.4 | 95.6 | 99.1 |
| ✓    | ✓       | 51.5 | 86.3 | 81.1 | 71.3 | 79.6 | 86.8 | 70.2 | 95.3 |


composed of multiple tasks, then, starting from the same parameter configuration, multiple separate adaptations are performed. In the outer loop, the meta-objective defines how these multiple adaptations are combined for the update of the parameters.

Finally, there is a crucial difference between SAME and previous meta-learning approaches: SAME is a training strategy for multi-task representation learning. Conventional meta-learning approaches are used as an adaptation strategy, and assume the presence of a support and target set also at test time. On the contrary, after training a model with SAME, an encoder is extracted and used to generate representations of the input that can then be fed to any machine learning model. SAME does not perform any adaptation at test time, and hence does not require the presence of the support and target sets at test time.

5. Experiments

Our goal is to assess the quality of the representations learned by models trained with SAME, and to study the impact of SAME’s underlying components. In more detail, we aim to answer the following questions:

Q1: Do iSAME and eSAME lead to a model generating node embeddings that can be used to perform multiple downstream tasks with comparable (or better) performance than end-to-end single-task models?

Q2: Do iSAME and eSAME extract information that is not captured by classically trained multi-task models?

Q3: Can node embeddings learned by a model trained with iSAME and eSAME be used for multiple tasks with comparable or better performance than classically trained multi-task models?

Q4 (Ablation Study): What are the contributions of the different components of SAME’s meta-learning procedure?

Unless otherwise stated, accuracy (%) is used for NC and GC, while ROC AUC (%) is used for LP. (As a reminder, we use GC to refer to graph classification, NC for node classification, and LP for link prediction.)

Datasets. To perform multiple tasks, we consider datasets with graph labels, node attributes, and node labels from the TUDataset library (Morris et al., 2020): ENZYMES (Schomburg et al., 2004), PROTEINS (Dobson and Doig, 2003), DHFR and COX2 (Sutherland et al., 2003).

Experimental Setup. We perform a 10-fold cross validation, and average results across folds. To ensure a fair comparison, we use the same architecture for all training strategies. We tested loss balancing techniques (e.g. uncertainty weights (Kendall et al., 2018), and gradnorm (Chen et al., 2018)) but found that they were not effective (in fact, Vandenhende et al. (2020) also observe that when the multiple losses are of the same form, e.g. all cross-entropies, then these techniques tend to fail). We also noticed that the losses do not need to be balanced, and we set $\lambda^{(GC)} = \lambda^{(NC)} = \lambda^{(LP)} = 1$ without performing any tuning. For more information we refer to Appendix B, and we provide source code as supplementary material.
Q1: We train a model with our proposed methods, on all multi-task combinations, and use the embeddings produced by the learned encoder as the input for a **linear classifier**. We compare against models with the same task-specific architecture trained in the classical manner on a single task, and with a fine-tuning baseline. The latter is a model that has been trained on all three tasks, and then fine-tuned on two specific tasks. The idea is that the initial training on all tasks should lead the model towards the extraction of features that it would otherwise not consider (by only seeing 2 tasks), and the fine-tuning process should then allow the model to use these features to target the specific tasks of interest. Results are shown in Table 1 (we omit standard deviation for space limitations). We notice that the embeddings produced by the model learned with our procedures in a multi-task setting, followed by a **linear** classifier, achieve performance comparable to, and frequently even better than, end-to-end single-task models. In fact, the **linear** classifier is never outperformed by more than 3%, and in 50% of the cases it actually achieves higher performance. We further notice that the fine-tuning baseline severely struggles, and is almost always outperformed by both single-task models, and our proposed methods. These results indicate that the episodic meta-learning procedure adopted by SAME is extracting features that are otherwise not accessible with standard training techniques.

Q2: We train a multi-task model, and we then train a new simple network (with the same architecture as the heads described in Section 4.2), which we refer to as classifier, on the embeddings generated by the multi-task model to perform a task that was not seen during training. We compare the performance of the classifier on the embeddings generated by a model trained in a classical manner, and with SAME. Intuitively, this tests gives us a way to analyse if the embeddings generated by a model trained with SAME contain “more information” than embeddings generated by a model trained in a classical manner. Results on the ENZYMES dataset are shown in Figure 3, where we notice that embeddings generated by a model trained with SAME lead to at least 10% higher performance. We observe an analogous trend on the other datasets (full results are in Appendix D).

![Figure 3: Results for neural network, trained on the embeddings generated by a multi-task model, performing a task that was not seen by the multi-task model during training. “x, y->z” indicates that x, y are the tasks used for training the multi-task model, and z is the new task.](image-url)
Table 2: $\Delta_m$ (%) results for a classically trained multi-task model (Cl), a fine-tuned model (FT; trained on all three tasks and fine-tuned on two) and a linear classifier trained on the node embeddings generated by a model trained with our meta-learning strategies (iSAME, eSAME) in a multi-task setting.

| Task | Model | Dataset |
|------|-------|---------|
| GC   | NC    | LP      |
| Cl   | ENZYMES | PROTEINS | DHFR | COX2 |
| ✓    | ✓     | ✓       |
| FT   | $-0.1 \pm 0.5$ | $4.0 \pm 1.0$ | $-0.3 \pm 0.2$ | $0.5 \pm 0.1$ |
| SAME | $-4.5 \pm 1.2$ | $0.1 \pm 0.5$ | $-7.4 \pm 1.4$ | $0.1 \pm 0.4$ |
| Cl   | $-2.3 \pm 0.9$ | $2.7 \pm 1.5$ | $-1.2 \pm 0.4$ | $-1.6 \pm 0.2$ |
| eSAME| $-0.8 \pm 0.8$ | $3.2 \pm 1.4$ | $-1.8 \pm 0.3$ | $-1.2 \pm 0.3$ |
| ✓    | ✓     | ✓       |
| FT   | $-25.3 \pm 3.2$ | $-5.3 \pm 1.2$ | $-28.3 \pm 4.3$ | $-21.4 \pm 3.4$ |
| SAME | $-5.1 \pm 1.9$ | $-5.4 \pm 1.5$ | $-24.5 \pm 3.7$ | $-22.6 \pm 3.8$ |
| Cl   | $4.1 \pm 0.5$ | $-0.2 \pm 0.9$ | $0.2 \pm 3.2$ | $0.2 \pm 0.5$ |
| SAME | $3.2 \pm 0.4$ | $-1.2 \pm 1.1$ | $-0.7 \pm 3.4$ | $-0.8 \pm 0.7$ |
| ✓    | ✓     | ✓       |
| FT   | $7.2 \pm 2.7$ | $6.8 \pm 0.9$ | $-29.1 \pm 7.7$ | $-28.2 \pm 4.5$ |
| SAME | $-1.0 \pm 0.3$ | $3.1 \pm 1.2$ | $-28.9 \pm 6.4$ | $-28.3 \pm 4.2$ |
| Cl   | $4.4 \pm 1.1$ | $6.1 \pm 1.0$ | $-0.1 \pm 6.2$ | $-0.6 \pm 2.5$ |
| SAME | $3.9 \pm 1.3$ | $6.1 \pm 1.1$ | $0.1 \pm 6.4$ | $-0.6 \pm 2.6$ |
| ✓    | ✓     | ✓       |
| SAME | $1.6 \pm 1.3$ | $2.9 \pm 0.3$ | $-18.9 \pm 2.3$ | $-16.9 \pm 3.1$ |
| Cl   | $1.5 \pm 1.0$ | $2.2 \pm 0.2$ | $-0.5 \pm 1.4$ | $-0.9 \pm 1.3$ |
| SAME | $1.8 \pm 0.9$ | $2.8 \pm 0.2$ | $-1.0 \pm 1.7$ | $-0.4 \pm 1.2$ |

Q3: We train the same multi-task model, both in the classical supervised manner, and with our proposed approaches, on all multi-task combinations. For our approaches, we then train a linear classifier on top of the node embeddings produced by the learned encoder. We further consider the fine-tuning baseline introduced in Q1. We use the multi-task performance ($\Delta_m$) metric (Maninis et al., 2019), defined as the average per-task drop with respect to the single-task baseline: $\Delta_m = \frac{1}{T} \sum_{i=1}^{T} (M_{m,i} - M_{b,i}) / M_{b,i}$, where $M_{m,i}$ is the value of a task’s metric for the multi-task model, and $M_{b,i}$ is the value for the baseline. Results are shown in Table 2. We first notice that usually multi-task models achieve lower performance than specialized single-task ones. We then highlight that linear classifiers trained on the embeddings generated by a model trained with SAME are not only comparable, but in many cases significantly superior to classically trained multi-task models. In fact, a multi-task model trained in a classical manner is highly sensible to the tasks that are being learned (e.g. GC and LP negatively interfere with each other in every dataset), while our methods seem much less sensible: the former has a worst-case average drop in performance of 29%, while our method has a worst-case average drop of less than 3%. Finally, we also notice that the fine-tuning baseline generally performs worst than classically trained models, confirming that transferring knowledge in multi-task settings is not easy, and more advanced techniques, like our proposed method SAME, are needed.

Q4 (Ablation Study): SAME’s meta-learning procedure has two main ingredients: (1) the design of support and target sets, that is made to encourage generalization by creating the sets as if they were training and validation sets (see Section 4.1), and (2)
Figure 4: Results for a Single-Task GNN model (ST GNN) trained with the classical procedure, and a linear classifier trained on the embeddings generated by a model trained with an ablated “single-task” version of SAME.

the separate multiple single-task adaptations that are performed in the inner loop, which relieve the model from having to learn to solve all the tasks concurrently (see Section 4.3). To better understand the importance and contribution of each component we perform two experiments, for which we summarize results below (the full results can be found in Appendix E).

First, we isolate the contribution of (1) by applying iSAME and eSAME in a single-task setting (i.e., the same single task is performed in both inner and outer loops), with episodes designed following the generalization-encouraging design proposed in Section 4.1 (notice that this is like applying the original MAML and ANIL training procedures, but with our design of support and target sets). In this experiment, for every task, we train a linear classifier on top of the embeddings produced by a model trained with “single-task” iSAME and eSAME, and compare against a network with the same architecture trained in a classical end-to-end manner. We show results in Figure 4. For all three tasks, a linear classifier on the embeddings produced by a model trained with our methods achieves comparable, if not superior, performance to an end-to-end model. In fact, the linear classifier is never outperformed by more than 2%, and it can outperform the classical end-to-end model by up to 12%. We believe this unexpected outcome is particularly interesting, and hints that episodic training procedures can be used to learn better representations.

Second, we investigate the benefits of (2) by removing the separate multiple single-task adaptations of SAME and performing all tasks (i.e., GC, NC, and LP) concurrently both in the inner and outer loop (notice this leads to a simple multi-task version of the conventional training procedure of MAML and ANIL, but with our support and target set design). For this experiment, we evaluate the ablated versions of SAME on the same procedure of Q2 and Q3, and compare against the results of iSAME and eSAME. We notice that the ablated version reaches results that are not significantly different from those of non-ablated iSAME and eSAME (see Appendix E for more details).

From these experiments we conclude that (i) the generalization-encouraging design of support and target sets is what allows SAME to reach performance on multiple tasks that are comparable to specialised single-task models trained in a classical manner, and (ii) the separate multiple single-task adaptations that are performed in the inner loop of iSAME and eSAME allow the models to reach the same performance of a version of SAME where
all tasks are performed concurrently on all graphs, hence increasing the learning efficiency by not requiring labels for each task on every graph.

6. Conclusions

In this work we propose a novel training strategy for representation learning in multi-task settings. Our method overcomes the problems that arise when learning to solve multiple tasks concurrently by optimizing for a parameter setting that can quickly, i.e. with few steps of gradient descent, be adapted for high single-task performance on multiple different tasks. We apply our method to graph representation learning, and find that our training procedure leads to models that generate higher quality node embeddings in the multi-task setting. In fact, we show that a linear classifier trained on the embeddings produced by a model learned with our method has comparable or better performance than classical end-to-end supervised models. Furthermore, we find that the embeddings generated by a model trained with our procedures lead to higher performance on downstream tasks that were not seen during training, and that the episodic training procedure leads to better embeddings even in the single-task setting. We believe this work can be of interest to the whole deep representation learning community, as our method is model agnostic and task agnostic.

Acknowledgments

This work was supported, in part, by MIUR of Italy, under PRIN Project n. 20174LF3T8 AHeAD and grant L. 232 (Dipartimenti di Eccellenza), and by the University of Padova under project “SID 2020: RATED-X”.

Appendix A. Episode Design Algorithm

Algorithm 2 contains the procedure for the creation of the episodes for our meta-learning procedures. The algorithm takes as input a batch of graphs (with graph labels, node labels, and node features) and the loss function balancing weights, and outputs a multi-task episode. We assume that each graph has a set of attributes that can be accessed with a dot-notation (like in most object-oriented programming languages).

Notice how the episodes are created so that only one task is performed on each graph (which implies that we only need labels for one task for each graph). This is important as in the inner loop of our meta-learning procedure, the learner adapts and tests the adapted parameters on one task at a time. The outer loop then updates the parameters, optimizing for a representation that leads to fast single-task adaptation. This procedure bypasses the problem of learning parameters that directly solve multiple tasks, which can be very challenging.

Another important aspect to notice is that the support and target sets are designed as if they were the training and validation splits for training a single-task model with the classical procedure. This way the meta-objective becomes to train a model that can generalize well.
Algorithm 2 Episode Design Algorithm

Input: Batch of \( n \) randomly sampled graphs \( \mathcal{B} = \{ \mathcal{G}_1, \ldots, \mathcal{G}_n \} \)
Loss weights \( \lambda^{(GC)}, \lambda^{(NC)}, \lambda^{(LP)} \in [0, 1] \)
Output: Episode \( \mathcal{E}_i = (\mathcal{L}^{(m)}_{\mathcal{E}_i}, \mathcal{S}^{(m)}_{\mathcal{E}_i}, \mathcal{T}^{(m)}_{\mathcal{E}_i}) \)
\( \mathcal{B}^{(GC)}, \mathcal{B}^{(NC)}, \mathcal{B}^{(LP)} \leftarrow \) equally divide the graphs in \( \mathcal{B} \) in three sets

\{Graph Classification\}
\( \mathcal{S}^{(GC)}_{\mathcal{E}_i}, \mathcal{T}^{(GC)}_{\mathcal{E}_i} \leftarrow \) randomly divide \( \mathcal{B}^{(GC)} \) with a 60/40 split

\{Node Classification\}
for \( \mathcal{G}_i \) in \( \mathcal{B}^{(NC)} \) do
  \( \text{num\_labelled\_nodes} \leftarrow \mathcal{G}_i\text{.num\_nodes} \times 0.3 \)
  \( \mathcal{N} \leftarrow \) divide nodes per class, then iteratively randomly sample one node per class
  without replacement and add it to \( \mathcal{N} \) until \( |\mathcal{N}| = \text{num\_labelled\_nodes} \)
  \( \mathcal{G}_i' \leftarrow \) copy(\( \mathcal{G}_i \))
  \( \mathcal{G}_i\text{.labelled\_nodes} \leftarrow \mathcal{N}; \quad \mathcal{G}_i'\text{.labelled\_nodes} \leftarrow \mathcal{G}_i\text{.nodes} \setminus \mathcal{N} \)
  \( \mathcal{S}^{(NC)}_{\mathcal{E}_i}\text{.add}(\mathcal{G}_i); \quad \mathcal{T}^{(NC)}_{\mathcal{E}_i}\text{.add}(\mathcal{G}_i') \)
end for

\{Link Prediction\}
for \( \mathcal{G}_i \) in \( \mathcal{B}^{(LP)} \) do
  \( \mathcal{E}^{(N)}_i \leftarrow \) randomly pick negative samples (edges that are not in the graph; possibly in the same number as the number of edges in the graph)
  \( \mathcal{E}^{(1)}_i, \mathcal{E}^{(2)}_i \leftarrow \) divide \( \mathcal{E}^{(N)}_i \) with an 80/20 split
  \( \mathcal{E}^{(P)}_i \leftarrow \) randomly remove 20% of the edges in \( \mathcal{G}_i \)
  \( \mathcal{G}_i' \leftarrow \) copy(\( \mathcal{E}^{(P)}_i \))
  \( \mathcal{G}_i'^{(1)} \leftarrow \mathcal{G}_i'^{(1)}\text{.edges}; \quad \mathcal{G}_i'^{(2)}\text{.negative\_edges} \leftarrow \mathcal{E}^{(P)}_i \)
  \( \mathcal{G}_i'^{(1)}\text{.positive\_edges} \leftarrow \mathcal{E}^{(1)}_i\text{.edges}; \quad \mathcal{G}_i'^{(2)}\text{.negative\_edges} \leftarrow \mathcal{E}^{(2)}_i\text{.edges} \)
  \( \mathcal{S}^{(LP)}_{\mathcal{E}_i}\text{.add}(\mathcal{G}_i'^{(1)}); \quad \mathcal{T}^{(LP)}_{\mathcal{E}_i}\text{.add}(\mathcal{G}_i'^{(2)} \)
end for

\( \mathcal{S}^{(m)}_{\mathcal{E}_i} \leftarrow \{ \mathcal{S}^{(GC)}_{\mathcal{E}_i}, \mathcal{S}^{(NC)}_{\mathcal{E}_i}, \mathcal{S}^{(LP)}_{\mathcal{E}_i} \} \)
\( \mathcal{T}^{(m)}_{\mathcal{E}_i} \leftarrow \{ \mathcal{T}^{(GC)}_{\mathcal{E}_i}, \mathcal{T}^{(NC)}_{\mathcal{E}_i}, \mathcal{T}^{(LP)}_{\mathcal{E}_i} \} \)
\( \mathcal{L}^{(GC)}_{\mathcal{T}_i} \leftarrow \text{Cross-Entropy}(\cdot); \quad \mathcal{L}^{(NC)}_{\mathcal{T}_i} \leftarrow \text{Cross-Entropy}(\cdot) \)
\( \mathcal{L}^{(LP)}_{\mathcal{T}_i} \leftarrow \text{Binary Cross-Entropy}(\cdot) \)
\( \mathcal{L}^{(m)}_{\mathcal{E}_i} = \lambda^{(GC)} \mathcal{L}^{(GC)}_{\mathcal{T}_i} + \lambda^{(NC)} \mathcal{L}^{(NC)}_{\mathcal{T}_i} + \lambda^{(LP)} \mathcal{L}^{(LP)}_{\mathcal{T}_i} \)
Return \( \mathcal{E} = (\mathcal{L}^{(m)}_{\mathcal{E}_i}, \mathcal{S}^{(m)}_{\mathcal{E}_i}, \mathcal{T}^{(m)}_{\mathcal{E}_i}) \)
Appendix B. Additional Experimental Details

In this section we provide additional information on the implementation of the models used in our experimental section. We implement our models using PyTorch (Paszke et al., 2019), PyTorch Geometric (Fey and Lenssen, 2019) and Torchmeta (Deleu et al., 2019). For all models the number and structure of the layers is as described in Section 4.2 of the paper, where we use 256-dimensional node embeddings at every layer.

At every cross-validation fold the datasets are split into 70% for training, 10% for validation, and 20% for testing. For each model we perform 100 iterations of hyperparameter optimization over the same search space (for shared parameters) using Ax (Bakshy et al., 2018).

We tried some sophisticated methods to balance the contribution of loss functions during multi-task training like GradNorm (Chen et al., 2018) and Uncertainty Weights (Kendall et al., 2018), but we saw that usually they do not positively impact performance. As an example, a GNN model trained for GC and LP with the classical procedure and using GradNorm, achieves results on GC, NC, and LP, that are on average 0.5% higher than the same model trained without GradNorm. However, a GNN model trained for NC and LP with the classical procedure and using GradNorm achieves results that are 0.8% lower than the same model trained without GradNorm. A similar behaviour happens by applying Uncertainty Weights, and, when the improvements were positive, they would never be higher than 1.7%. Vandenhende et al. (2020) also observe that when the multiple losses are of the same form, e.g. all cross-entropies, then these techniques tend to not bring any performance improvements. Furthermore, in the few cases where they increase performance, they work for both classically trained models, and for models trained with our proposed procedures. We then set the balancing weights to $\lambda^{(GC)} = \lambda^{(NC)} = \lambda^{(LP)} = 1$ to provide better comparisons between the training strategies.

The experiments were run on a Nvidia 1080Ti GPU, and on a CPU cluster equipped with 8 cpus 12-Core Intel Xeon Gold 5118 @2.30GHz, with 1.5Tb of RAM.

**Linear Model.** The linear model trained on the embeddings produced by our proposed method is a standard linear SVM. In particular we use the implementation available in Scikit-learn (Pedregosa et al., 2011) with default hyperparameters. For graph classification, we take the mean of the node embeddings as input. For link prediction we take the concatenation of the embeddings of two nodes. For node classification we keep the embeddings unaltered.

**Deep Learning Baselines.** We train the single task models for 1000 epochs, and the multi-task models for 5000 epochs, with early stopping on the validation set (for multi-task models we use the sum of the task validation losses or accuracies as metrics for early-stopping). Optimization is done using Adam (Kingma and Ba, 2015). For node classification and link prediction we found that normalizing the node embeddings to unit norm in between GCN layers helps performance.

**Our Meta-Learning Procedure.** We train the single task models for 5000 epochs, and the multi-task models for 15000 epochs, with early stopping on the validation set (for multi-task models we use the sum of the task validation losses or accuracies as metrics for early-stopping). Early stopping is very important in this case as it is the only way to
Table 3: Results of a neural network trained on the embeddings generated by a multi-task model, to perform a task that was not seen during training by the multi-task model. “$x$,$y$ ->$z$” indicates that the multi-task model was trained on tasks $x$ and $y$, and the neural network is performing task $z$.

| Task       | Model     | Dataset  | ENZYMES | PROTEINS | DHFR    | COX2    |
|------------|-----------|----------|---------|----------|---------|---------|
| GC,NC ->LP | iSAME     |          | 77.3 ± 4.5 | 88.5 ± 1.8 | 99.8 ± 1.8 | 97.1 ± 2.0 |
|            | eSAME     |          | 78.9 ± 2.8 | 89.1 ± 1.5 | 99.7 ± 2.2 | 95.8 ± 3.3 |
| GC,LP ->NC | iSAME     |          | 73.3 ± 2.1 | 59.2 ± 2.5 | 77.6 ± 1.6 | 78.1 ± 4.6 |
|            | eSAME     |          | 79.1 ± 1.7 | 64.7 ± 3.0 | 76.1 ± 2.7 | 76.9 ± 3.3 |
| NC,LP ->GC | iSAME     |          | 48.5 ± 5.5 | 76.1 ± 2.3 | 76.1 ± 3.7 | 79.7 ± 5.1 |
|            | eSAME     |          | 56.6 ± 3.1 | 74.6 ± 2.7 | 77.1 ± 3.6 | 79.3 ± 6.2 |

check if the meta-learned model is overfitting the training data. The inner loop adaptation consists of 1 step of gradient descent. Optimization in the outer loop is done using Adam (Kingma and Ba, 2015). We found that normalizing the node embeddings to unit norm in between GCN layers helps performance.

Algorithm 3 Classical Multi-Task Training Procedure.

Input: Model $f_{\theta}$; Batches $B = \{B_1, .., B_n\}$
init($\theta$)

for $B_i$ in $B$ do

loss $\leftarrow$ concurrently perform all tasks on all graphs in $B_i$, calculate the loss for each task, and sum the losses together

$\theta \leftarrow$ UPDATE($\theta$, loss)

end for

Appendix C. Comparison with Traditional Training Approaches

Classical Multi-Task Training Our proposed meta-learning approach is significantly different from the classical multi-task training strategy (Algorithm 3). The classical training approach for multi-task models takes as input a batch of graphs, which is simply a set of graphs, where on each graph the model has to execute all the tasks. Based on the cumulative loss on all tasks

$$\mathcal{L} = \lambda^{(GC)}\mathcal{L}^{(GC)} + \lambda^{(NC)}\mathcal{L}^{(NC)} + \lambda^{(LP)}\mathcal{L}^{(LP)}$$

for all the graphs in the batch, the parameters are updated with some form of gradient descent, and the procedure is repeated for each batch. This requires the model to learn to solve all tasks concurrently, while our proposed approaches removes this requirement.
Table 4: Results for a single-task model trained in a classical supervised manner (Cl), and a linear classifier trained on the embeddings generated by a model trained with an ablated “single-task” version our meta-learning strategies ((a)iSAME, (a)eSAME).

| Task | Model  | Dataset  | ENZYMES | PROTEINS | DHFR | COX2 |
|------|--------|----------|---------|----------|------|------|
|      | Cl     |          | 87.5 ± 1.9 | 72.3 ± 4.4 | 97.3 ± 0.2 | 96.4 ± 0.3 |
| NC   | (a)iSAME |          | 87.3 ± 0.8   | 81.8 ± 1.6   | 96.6 ± 0.3 | 96.1 ± 0.4 |
|      | (a)eSAME |          | 87.8 ± 0.7   | 82.4 ± 1.6   | 96.8 ± 0.2 | 96.5 ± 0.6 |
| GC   | Cl     |          | 51.6 ± 4.2   | 73.3 ± 3.6   | 71.5 ± 2.3 | 76.7 ± 4.7 |
|      | (a)iSAME |          | 50.8 ± 2.9   | 73.5 ± 1.2   | 73.2 ± 3.2 | 76.3 ± 4.6 |
|      | (a)eSAME |          | 52.1 ± 5.0   | 72.6 ± 1.6   | 71.6 ± 2.4 | 75.6 ± 4.1 |
| LP   | Cl     |          | 75.5 ± 3.0   | 85.6 ± 0.8   | 98.8 ± 0.7 | 98.3 ± 0.8 |
|      | (a)iSAME |          | 81.7 ± 1.7   | 84.0 ± 1.1   | 99.2 ± 0.4 | 99.1 ± 0.5 |
|      | (a)eSAME |          | 80.1 ± 3.4   | 84.1 ± 0.9   | 99.2 ± 0.3 | 99.2 ± 0.7 |

Appendix D. Full Results for the Generalization of Node Embeddings

Table 3 contains results for a neural network, trained on the embeddings generated by a multi-task model, to perform a task that was not seen during the training of the multi-task model. Accuracy (%) is used for node classification (NC) and graph classification (GC); ROC AUC (%) is used for link prediction (LP). The embeddings produced by a model trained with SAME lead to higher performance (up to 35%), showing that our procedures lead to models that can generate more informative node embeddings with respect to the classical end-to-end training procedure.

Appendix E. Ablation Study - Full Results

Table 4 shows the results for the ablated “single-task” versions of SAME (i.e., the full results related to Figure 4). For every task, we train a linear classifier on top of the embeddings produced by a model trained using our proposed methods, and compare against a network with the same architecture trained in a classical manner. For all three tasks, a linear classifier on the embeddings produced by a model trained with our methods achieves comparable, if not superior, performance to an end-to-end model. In fact, the linear classifier is never outperformed by more than 2%, and it can outperform the classical end-to-end model by up to 12%. These results highlight the impact of designing support and target sets to encourage generalization.

Table 5 presents the results of a neural network trained on the embeddings generated by a model trained with an ablated version of iSAME and eSAME to perform a task that was unseen during training. The ablated version of iSAME and eSAME is obtained by using the support and target set design that encourage generalization, but by not applying the multiple separate single-task adaptations in the inner loop. In particular all tasks are performed concurrently on all graphs both in the inner loop and the outer loop (leading to a multi-task version of the traditional MAML and ANIL procedure, but with our design of support and target sets). Finally, Table 6 shows the results in terms of the multi-task
Table 5: Results of a neural network trained on the embeddings generated by a multi-task model, to perform a task that was not seen during training by the multi-task model. The multi-task model has been trained with an ablated version of iSAME and eSAME (which we refer to as (a)iSAME and (a)eSAME), where no single-task adaptation is performed, but a multi-task version of the traditional meta-learning procedure is applied. “x,y -> z” indicates that the multi-task model was trained on tasks x and y, and the neural network is performing task z.

| Task         | Model  | Dataset  | ENZYMES  | PROTEINS  | DHFR  | COX2  |
|--------------|--------|----------|----------|-----------|-------|-------|
| GC,NC -> LP  | (a)iSAME  | 75.6 ± 3.3 | 88.3 ± 1.2 | 98.4 ± 0.9 | 95.1 ± 1.7 |
|              | (a)eSAME  | 79.4 ± 2.8 | 89.2 ± 1.6 | 97.4 ± 0.7 | 95.3 ± 1.4 |
| GC,LP -> NC  | (a)iSAME  | 71.8 ± 2.5 | 59.7 ± 3.2 | 76.4 ± 2.3 | 79.1 ± 2.3 |
|              | (a)eSAME  | 79.5 ± 1.6 | 63.8 ± 2.1 | 77.0 ± 2.1 | 78.9 ± 2.1 |
| NC,LP -> GC  | (a)iSAME  | 42.3 ± 5.5 | 75.8 ± 2.6 | 76.9 ± 4.4 | 78.3 ± 7.5 |
|              | (a)eSAME  | 53.6 ± 3.5 | 75.6 ± 2.1 | 77.3 ± 2.8 | 77.7 ± 5.2 |

Table 6: $\Delta_m$ (%) results for a linear classifier trained on the node embeddings generated by a model trained with an ablated version of iSAME and eSAME (which we refer to as (a)iSAME and (a)eSAME), where no single-task adaptation is performed, but a multi-task version of the traditional meta-learning procedure is applied.

| Task | Model  | Dataset  | ENZYMES  | PROTEINS  | DHFR  | COX2  |
|------|--------|----------|----------|-----------|-------|-------|
| GC   | ✓      | ✓        | (a)iSAME | -3.2 ± 0.4 | 2.8 ± 1.3 | -0.4 ± 0.3 | -0.5 ± 0.2 |
|      |        |          | (a)eSAME | 0.5 ± 1.1  | 1.7 ± 0.5  | -0.5 ± 1.2 | -1.5 ± 0.5 |
| NC   | ✓      | ✓        | (a)iSAME | 1.5 ± 2.9  | -0.9 ± 1.1 | 0.1 ± 4.1  | -0.2 ± 3.1 |
|      |        |          | (a)eSAME | 3.0 ± 1.7  | -2.5 ± 1.6 | -0.4 ± 3.5 | -0.4 ± 4.2 |
| LP   | ✓      | ✓        | (a)iSAME | 4.3 ± 2.8  | 4.5 ± 1.1  | -0.2 ± 6.2 | -0.6 ± 4.2 |
|      |        |          | (a)eSAME | 3.1 ± 0.4  | 5.0 ± 1.1  | -0.1 ± 5.9 | -0.5 ± 4.1 |
|      | ✓      | ✓        | (a)iSAME | 1.0 ± 1.2  | 2.7 ± 0.3  | -1.2 ± 2.4 | -1.1 ± 2.9 |
|      |        |          | (a)eSAME | 0.4 ± 1.2  | 1.1 ± 0.3  | -1.3 ± 1.1 | -0.9 ± 1.1 |

performance ($\Delta_m$) metric (Maninis et al., 2019) of the latter ablated version of SAME. For both experiments, we notice that the results are not significantly different from those of the non-ablated iSAME and eSAME (Table 3 in Appendix, and Table 2 of the paper), indicating that iSAME and eSAME increase the sample efficiency of the training procedure as they can lead to a model generating embeddings that can reach the same results but by only applying one task per graph (and hence only requiring the labels for one task per graph).

References

Ferran Alet, Erica Weng, Tomas Lozano-Perez, and L. Kaelbling. Neural relational inference with fast modular meta-learning. In NeurIPS, 2019.
Pedro Avelar, Henrique Lemos, Marcelo Prates, and Luis Lamb. Multitask learning on graph neural networks: Learning multiple graph centrality measures with a unified network. In *ICANN Workshop and Special Sessions*. 2019.

Eytan Bakshy, Lili Dworkin, Brian Karrer, Konstantin Kashin, Benjamin Letham, Ashwin Murthy, and Shaun Singh. Ae: A domain-agnostic platform for adaptive experimentation. In *NeurIPS Systems for ML Workshop*, 2018.

Avishek Joey Bose, Ankit Jain, Piero Molino, and William L Hamilton. Meta-graph: Few shot link prediction via meta learning. *arXiv*, 2019.

Michael M. Bronstein, Joan Bruna, Yann LeCun, Arthur Szlam, and Pierre Vandergheynst. Geometric deep learning: Going beyond euclidean data. *IEEE Signal Processing Magazine*, 2017.

Ines Chami, Sami Abu-El-Haija, Bryan Perozzi, Christopher Ré, and K. Murphy. Machine learning on graphs: A model and comprehensive taxonomy. *arXiv*, 2020.

Zhao Chen, Vijay Badrinarayanan, Chen-Yu Lee, and Andrew Rabinovich. Gradnorm: Gradient normalization for adaptive loss balancing in deep multitask networks. In *ICML*, 2018.

Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering. In *NeurIPS*, 2016.

Tristan Deleu, Tobias Würfl, Mandana Samiei, Joseph Paul Cohen, and Yoshua Bengio. Torchmeta: A Meta-Learning library for PyTorch. *arXiv*, 2019.

Paul D. Dobson and Andrew J. Doig. Distinguishing enzyme structures from non-enzymes without alignments. *Journal of Molecular Biology*, 2003.

Matthias Fey and Jan E. Lenssen. Fast graph representation learning with PyTorch Geometric. In *ICLR Workshop on Representation Learning on Graphs and Manifolds*, 2019.

Chelsea Finn, Pieter Abbeel, and Sergey Levine. Model-agnostic meta-learning for fast adaptation of deep networks. In *ICML*, 2017.

Victor Garcia and Joan Bruna. Few-shot learning with graph neural networks. In *ICLR*, 2018.

Justin Gilmer, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl. Neural message passing for quantum chemistry. In *ICML*, 2017.

William L Hamilton, Rex Ying, and Jure Leskovec. Representation learning on graphs: Methods and applications. *IEEE Data Engineering Bulletin*, 2017.

Lu Haonan, Seth H. Huang, Tian Ye, and Guo Xiuyan. Graph star net for generalized multi-task learning. *arXiv*, 2019.

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *CVPR*, 2016.
Buffelli and Vandin

Chester Holtz, Onur Atan, Ryan Carey, and Tushit Jain. Multi-task learning on graphs with node and graph level labels. In NeurIPS Workshop on Graph Representation Learning, 2019.

Timothy Hospedales, Antreas Antoniou, Paul Micaelli, and Amos Storkey. Meta-learning in neural networks: A survey. arXiv, 2020.

Alex Kendall, Yarin Gal, and Roberto Cipolla. Multi-task learning using uncertainty to weigh losses for scene geometry and semantics. In CVPR, 2018.

Jongmin Kim, Taesup Kim, S. Kim, and C. Yoo. Edge-labeling graph neural network for few-shot learning. In CVPR, 2019.

Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In ICLR, 2015.

Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. In ICLR, 2017.

Diya Li and Heng Ji. Syntax-aware multi-task graph convolutional networks for biomedical relation extraction. In LOUIH, 2019.

Lu Liu, Tianyi Zhou, Guodong Long, Jing Jiang, and Chengqi Zhang. Learning to propagate for graph meta-learning. In NeurIPS, 2019a.

Pengfei Liu, J. Fu, Y. Dong, Xipeng Qiu, and J. Cheung. Learning multi-task communication with message passing for sequence learning. In AAAI, 2019b.

Kaushalya Madhawa and Tsuyoshi Murata. Active learning on graphs via meta learning. In ICML Workshop on Graph Representation Learning and Beyond, ICML, 2020.

Kevis-Kokitsi Maninis, Ilija Radosavovic, and Iasonas Kokkinos. Attentive single-tasking of multiple tasks. In CVPR, 2019.

Floriane Montanari, Lara Kuhnke, Antonius Ter Laak, and Djork-Arné Clevert. Modeling physico-chemical ADMET endpoints with multitask graph convolutional networks. Molecules, 2019.

Christopher Morris, Nils M. Kriege, Franka Bause, Kristian Kersting, Petra Mutzel, and Marion Neumann. Tudataset: A collection of benchmark datasets for learning with graphs. In ICML Workshop on Graph Representation Learning and Beyond, 2020.

Cuong Q. Nguyen, Constantine Kreatsoulas, and Branson Kim M. Meta-learning gnn initializations for low-resource molecular property prediction. In ICML Workshop on Graph Representation Learning and Beyond, ICML, 2020.

Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library. In NeurIPS. 2019.
Fabian Pedregosa, Gaël Varoquaux, Alexandre Gramfort, Vincent Michel, Bertrand Thirion, Olivier Grisel, Mathieu Blondel, Peter Prettenhofer, Ron Weiss, Vincent Dubourg, Jake Vanderplas, Alexandre Passos, David Cournapeau, Matthieu Brucher, Matthieu Perrot, and Édouard Duchesnay. Scikit-learn: Machine learning in Python. Journal of Machine Learning Research, 2011.

Aniruddh Raghu, Maithra Raghu, Samy Bengio, and Oriol Vinyals. Rapid learning or feature reuse? towards understanding the effectiveness of maml. In ICLR, 2020.

Franco Scarselli, Marco Gori, Ah Chung Tsoi, Markus Hagenbuchner, and Gabriele Monfardini. The graph neural network model. IEEE Transactions on Neural Networks, 2009.

Ida Schomburg, Antje Chang, Christian Ebeling, Marion Gremse, Christian Heldt, Gregor Huhn, and Dietmar Schomburg. Brenda, the enzyme database: updates and major new developments. Nucleic acids research, 2004.

Trevor Standley, Amir R. Zamir, Dawn Chen, Leonidas Guibas, Jitendra Malik, and Silvio Savarese. Which tasks should be learned together in multi-task learning? In ICML, 2020.

Qiuling Suo, Jingyuan Chou, Weida Zhong, and Aidong Zhang. Tadanet: Task-adaptive network for graph-enriched meta-learning. In ACM SIGKDD, 2020.

Jeffrey J. Sutherland, Lee A. O’Brien, and Donald F. Weaver. Spline-fitting with a genetic algorithm: A method for developing classification structure-activity relationships. Journal of Chemical Information and Computer Sciences, 2003.

Simon Vandenhende, Stamatios Georgoulis, Marc Proesmans, Dengxin Dai, and Luc Van Gool. Revisiting multi-task learning in the deep learning era. arXiv, 2020.

Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. Graph Attention Networks. In ICLR, 2018.

Shanfeng Wang, Qixiang Wang, and Maoguo Gong. Multi-task learning based network embedding. Frontiers in Neuroscience, 2020.

Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and Philip S. Yu. A comprehensive survey on graph neural networks. IEEE Transactions on Neural Networks and Learning Systems, 2020.

Yu Xie, Maoguo Gong, Yuan Gao, A. K. Qin, and Xiaolong Fan. A multi-task representation learning architecture for enhanced graph classification. Frontiers in Neuroscience, 2020.

Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In ICLR, 2019.

Huaxiu Yao, Chuxu Zhang, Ying Wei, Meng Jiang, Suhang Wang, Junzhou Huang, Nitesh V. Chawla, and Zhenhui Li. Graph few-shot learning via knowledge transfer. In AAAI, 2020.

Yu Zhang, Ying Wei, and Qiang Yang. Learning to multitask. In NeurIPS, 2018.
Fan Zhou, Chengtao Cao, Kunpeng Zhang, Goce Trajcevski, Ting Zhong, and Ji Geng. Meta-gnn: On few-shot node classification in graph meta-learning. In *CIKM*, 2019.

Daniel Zügner and Stephan Günnemann. Adversarial attacks on graph neural networks via meta learning. In *ICLR*, 2019.