## FOUNDATION MODELS FOR BOOLEAN LOGIC

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## Abstract

Boolean logic is fundamental to solving various computational problems, such as Boolean satisfiability (SAT) and model counting, but existing machine learning (ML) approaches for automating algorithm design are computationally expensive and data-intensive. We propose the first foundation model for Boolean logic, leveraging a multi-task dataset of one million instances spanning sixteen tasks and using graph neural networks (GNNs). We evaluated the generalization of the foundation models on held-out tasks; we found that models fine-tuned from the foundation model were substantially more sample efficient and converged much faster than models trained from scratch. We identified a number of crucial design components for training these models, in particular the choice of normalization layer. We showed that a hybrid of different normalization techniques across layers is much more effective than any single normalization layer.

1 INTRODUCTION

Boolean logic—binary operations  $\land$  (AND),  $\lor$  (OR), and  $\neg$  (NOT) over Boolean variables—is a fundamental mathematical language for describing many real-world settings. There are a variety of computational problems over logical formulae commonly solved in practice:

- Boolean Satisfiability (SAT): Determining if there exists a satisfying assignment. Example: Finding valid channel assignments for TV stations in spectrum auctions (Fréchette et al., 2016).
- Model Counting (#SAT): Calculating the number of satisfying assignments. Example: Determining the probability that a sequence of actions achieves a goal in probabilistic planning (Domshlak & Hoffmann, 2006).
- Unsatisfiable Core Extraction (unsat core): Identifying the smallest set of variables that prove no satisfying assignment exists. Example: Finding the minimal conflict in circuit configurations to aid system debugging (Sülflow et al., 2008).

Despite their computational hardness, efficient heuristic algorithms have been developed over 038 decades of empirically driven research to solve these problems at scale. The performance of different algorithms often depends on the specific structure of problem instances, leading to designs tailored for "typical-case" scenarios. This creates a data-dependent algorithm design challenge: 040 how can we design efficient algorithms for particular distributions of problems? Manual approaches 041 are limited and time intensive, naturally steering us toward machine learning to leverage the rich 042 structure of formulae. Just as machine learning has surpassed human capabilities in tasks like im-043 age recognition by identifying complex patterns, it can similarly be employed to discover effective 044 algorithms for Boolean logic. 045

Traditionally, leveraging machine learning for algorithm design has relied on computing handcrafted instance features based on expert domain knowledge. For example, practitioners build *algorithm selector* models that use such features to make a per-instance choie among a portfolio of off-the-shelf algorithms, leveraging their complementary strengths. Features used in Boolean logic range from simple metrics like problem size to complex ones like the diameter of the variable-clause graph or statistics from short probing runs of local-search and CDCL solvers (Xu et al., 2008). While powerful, such features can be expensive to compute and difficult to transfer to new domains.

Recent work has demonstrated the promise of leveraging modern "end-to-end" ML techniques to learn features directly from data. To give some examples of approaches that achieved state-of-the-

054 art performance in given settings, Selsam & Bjørner (2019) predicted unsatisfiable cores to guide 055 branching decisions, Wang et al. (2021) predicted the polarity of backbone variables to choose vari-056 able assignments in tree search, and Cameron et al. (2024) learned branching policies via reinforce-057 ment learning to minimize downstream decisions. A key idea unifying all of these approaches is a reliance on message-passing architectures, such as graph neural networks (GNNs) (Scarselli et al., 058 2008) and exchangeable nets (Hartford et al., 2018). Such architectures impose a helpful inductive bias, corresponding to the invariances of Boolean logic in conjunctive normal form (CNF): (1) logi-060 cal equivalence under reordering of clauses and literals, and (2) variability in the number of literals 061 and clauses. 062

063 The downside of these approaches is that they are extremely data hungry. For example, all of the 064 approaches described above required many CPU years of computation to generate training data. To achieve strong performance, practitioners must gather huge datasets for specific prediction tasks, 065 where the offline computation costs can be prohibitive. In other fields, large pretrained models 066 trained on massive, multi-task datasets-known as foundation models-can be fine-tuned to specific 067 applications to massively decrease training costs. (Betker et al., 2023; Achiam et al., 2023). These 068 models leverage shared information across multiple tasks to learn richer and more generalizable 069 representations. 070

For the first time, we developed foundation models for Boolean logic, demonstrating strong fine-071 tuning performance on held-out tasks. We compiled a massive dataset of one million small in-072 stances encompassing ten different categories (sixteen tasks in total) of Boolean logic-based tasks: 073 four well-known computational problems (satisfiability, backbone, unsat core, and model counting), 074 a linear programming relaxation, a branch prediction task based on reinforcement learning, three 075 that are statistics of probing runs from SAT solvers (DPLL, local search, and survey propagation), 076 and one predicting graph structure. Notably, some tasks are only applicable to either satisfiable or 077 unsatisfiable instances—backbones are defined solely for satisfiable instances, while unsatisfiable cores apply exclusively to unsatisfiable ones. We trained ten different Graph Neural Network (GNN) 079 foundation models, each with a distinct held-out task. Foundation models were consistently more 080 data efficient and converged faster when fine-tuned on the same held-out tasks relative to models 081 trained from scratch.

082 The major challenge of building a foundation model is to find one architecture that works well 083 across many diverse kinds of tasks. We found that architectures that performed well on one task 084 can perform poorly on another. A major contribution of this work was finding an architecture that 085 performed well across all tasks. First, we found that all commonly used normalization layers (i.e, 086 layer norm, batch norm, graph norm) had some failure cases. Layer norm was unable to learn 087 graph-level tasks at all and for batch and graph norm we observed erratic training behaviour, which 880 we attributed to the high-variance batch statistics. We found that using a hybrid norm-batch norm for GNN layers and layer norm for the feed-forward model— substantially improved performance 089 and training efficiency. We provided some empirical evidence that the success of hybrid norm is 090 in its ability to avoid both the numerical instability that can occur with batch norm as well as the 091 over-smoothing of node embeddings we observed with layer norm. The success of this hybrid norm 092 approach could be of significant interest to the GNN community more broadly. We also found 093 that both dropout and mean pooling often substantially degraded performance and we observed 094 consistent performance improvement by adding self-attention over node embeddings between GNN 095 layers. We found using sum pooling and turning off dropout was the best configuration for all tasks. 096

We used a hydrid GNN transformer models based on GPS++ (Masters et al., 2022), which is among the state-of-the-art models for standard graph benchmarks. Our final foundation model had eight layers and 122 million parameters, with each layer comprising a GPS message-passing component followed by self-attention over node embeddings. We add a feed-forward head for each of the sixteen total tasks: seven graph-level (one classification, six regression) and nine node-level (three classification, eight regression).

This work serves as a major step towards building foundation models for Boolean logic. We found an architecture that works well across a wide-variety of tasks which will make future work much more accessible. We envision a future with large, GPT-like pretrained Boolean logic models with billions of parameters that can be fine-tuned for a wide range of tasks.

## 108 2 PRELIMINARIES AND RELATED WORK

# 110 2.1 HAND-CRAFTED ML

112 Prior to Selsam et al. (2019)'s first attempt to learn a model to represent Boolean logic, hand-crafted 113 features were exclusively used for making per-instance predictions (typically predicting solver run-114 ning times) and still dominate the research today. For example, algorithm selection is still an active 115 area of research and it was only until very recently (Zhang et al., 2024; Leeson & Dwyer, 2024) that 116 GNNs have been applied to that problem. Nudelman et al. (2004) introduced a set of hand-crafted features that were expanded by Xu et al. (2008), later again by Hutter et al. (2014), and have been 117 recently upgraded to be more informative (e.g., smartly choosing timeouts on probing runs) (Shavit 118 & Hoos, 2024). They have been proven to be effective for building empirical hardness models of 119 algorithms (Hutter et al., 2014) and for algorithm selection (Xu et al., 2008; Lindauer et al., 2015). 120 These features were derived from various sources: known heuristics (e.g., the ratio of positive to 121 negative clause occurrences and per-variable statistics), tractable subclasses (such as the proximity 122 to Horn formulae), graph-based features (like properties extracted from the clause-variable inci-123 dence graph), and other proxies for problem complexity (including statistics about the progress of 124 SAT solvers and linear programming relaxations of the SAT problem). The computational complex-125 ity of these features spans a wide range, from trivial calculations (like determining the size of the 126 problem) to more computationally intensive tasks (such as computing LP relaxations or extracting 127 specific graph-based features, which can be roughly cubic in complexity). Many other combinatorial problems like MIP and TSP (Hutter et al., 2014) have relied on similar hand-crafted features. 128

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2.2 GNNs

132 The ML for Boolean logic community has converged on representing logical formulae as graphs and 133 using GNNs. Selsam et al. (2019) pioneered this by encoding CNF SAT formulae as graphs with 134 variables, clauses, and true/false literals as nodes, connecting variables and clauses if a variable participates in a clause, and linking literals to their variables. Their approach used two message-passing 135 operations-between clauses and variables, and between variables and literals-achieving high ac-136 curacy in predicting satisfiability and deriving solutions for small random SAT problems. Cameron 137 et al. (2020) instead represent CNF as an exchangeable matrix, using an architecture equivalent to a 138 bipartite variable-clause graph (Hartford et al., 2018). For broader insights on representing combi-139 natorial problems as graphs, see Boisvert et al. (2024). 140

GNNs have been used to predict unsatisfiable cores (Selsam & Bjørner, 2019), predict satisfiability (Cameron et al., 2020), predict branching variables (Kurin et al., 2019; Cameron et al., 2024), and for algorithm selection (Zhang et al., 2024; Leeson & Dwyer, 2024). Perhaps the closest work to our own is on predicting backbones, where Wang et al. (2021) first pretrained on a large dataset of backbones from small instances and fine-tuned on larger instances. Also relevant is the recent work of Li et al. (2023) who compiled a large benchmark of instances and tasks to benchmark GNN performance in Boolean logic.

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## 149 2.3 MULTI-TASK LEARNING AND FOUNDATION MODELS

150 The advent of foundation models—large-scale pretrained models capable of being fine-tuned for a 151 multitude of downstream tasks—has revolutionized fields like natural language processing (Brown, 152 2020) and computer vision (Betker et al., 2023). Typically, the multi-task aspect of foundation mod-153 els in vision and language is implicit. For example, Large Language Models (LLMs) like GPT are 154 primarily framed to predict the next word in a sequence; this objective inherently requires solving a 155 variety of implicit tasks depending on the context provided within the input text. Multi-task learning 156 (MTL) explicitly defines and optimizes multiple tasks simultaneously for a given input (Yu et al., 157 2024). In contrast to foundation models where tasks are inferred from context, MTL frameworks 158 require distinct task definitions integrated into the model architecture. Typically, this involves de-159 signing models with shared layers that learn a common representation, alongside task-specific heads that handle individual objectives. As one notable example, Beaini et al. (2023) built a multitask 160 foundation model over a variety of molecule prediction tasks and datasets. Our implementation is 161 based off their graphium package.

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Figure 1: Our foundation model architecture. One-hot encoded SAT instance goes into feed-forward pre-NN encoders followed by a sequence of hybrid MPNN+transformer layers. GNN output then goes through a global pooling and concat operation across nodes, and feed into feed-forward task heads for different tasks.

#### 3 METHODS: END-TO-END BOOLEAN LOGIC MODELLING

Given a set of k tasks  $T = \{T_1, ..., T_k\}$  and instance distribution  $\mathbb{P}$ , our goal is to learn a function  $\phi^*$  that minimizes the mean over |T| loss functions

$$\mathcal{L}(\phi; \mathbb{P}) = \frac{1}{|T|} \sum_{i=1}^{|T|} \mathcal{L}_i(T_i, \phi).$$

190 We define losses for each task based on its category: mean squared loss for regression tasks and 191 cross-entropy loss for classification tasks, averaged over nodes if it is predicting per node metrics. 192 For detailed description of the losses, see Appendix B.

193 Instances in our case are Boolean logical formulae in conjunctive normal form (CNF). We represent 194 CNFs with the well-known and lossless clause-variable bipartite graph, allowing us to model  $\phi$  as 195 a GNN which takes a graphical representation directly as input. We one-hot encode the intut CNF 196 and pass the encoded node and edge embedding matrices  $\mathbf{X}^0$  and  $\mathbf{E}^0$  as inputs to the model. For a 197 detailed description of how we encoded the CNF, see Appendix C.

GNNs involve a sequence of message-passing operations over nodes/edges, where a given node/edge 199 representation is updated by aggregating (i.e., any commutative function) over its neighbouring 200 nodes/edge representations and sending the aggregation through a multi-layer perceptron (MLP). 201 Our GNN instantiation is adapted from GPS++ (Masters et al., 2022). Our network takes as input a 202 graph  $(\mathbf{X}^0, \mathbf{E}^0, g^0)$ , where g is a graph embedding that is represented as a "virtual" node connected 203 to every other node. Our network consists of (1) a pre-GNN node and edge encoder that learns an embedding for each node/edge type followed by (2) a sequence of message-passing layers that 204 iteratively update node and edge embeddings, (3) a shared-embedding layer that pools and concats 205 graph and node level embeddings and (4)  $\left|T\right|$  task heads that map the node embedding representation 206 down to the target shape of the task. See figure 1 for a visualization of our end-to-end model 207 architecture and Appendix D for a detailed description of each layer. 208

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#### 4 **EXPERIMENT SETUP**

#### 212 4.1 DATASET

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We built a dataset of one million uniform-random 3SAT instances at the solubility phase transition 214 (Cheeseman et al., 1991), each with 100 variables. This allowed us to generate an arbitrary number 215 of challenging training examples. The computing cost of gathering target labels can scale exponentially with instance size, and model training resources scale linearly in both memory and time with
 the size of the formulae. By training our foundation model on smaller formulae, we were able to
 train much larger models and we were able to collect much more training data.

219 We compiled sixteen prediction tasks spanning ten different categories, all of which have been previ-220 ously studied in the context of machine learning for Boolean logic. Four of these tasks—unsat core, 221 backbone, RL branching, and model counting-have been used to directly improve SAT solver per-222 formance by informing branching decisions during tree search. One task, satisfiability, has been 223 extensively studied as a testbed for end-to-end learning on Boolean formulae. The remaining five 224 tasks have been employed as computationally inexpensive features for meta-algorithmic approaches 225 to solving SAT, such as algorithm selection. Below, we describe for each task (1) its prior use in 226 machine learning for Boolean logic and (2) how we computed its ground truth labels. For formal definitions of each task, please refer to Appendix A. 227

Predicting satisfiability Selsam et al. (2019) were the first to demonstrate how GNNs could be used for end-to-end learning for Boolean logic by predicting satisfiability. Cameron et al. (2020) later showed how GNNs could beat expert hand-engineered features for SAT prediction and there have been several later follow up works (Chang et al., 2022; Li et al., 2023). We used the model counting computation below to identify satisfiability. If the model count was zero, the instance is usatisfiable, otherwise it is satisfiable.

- Model counting Vaezipoor et al. (2021) train a neural network to make branching decisions to solve
   model counting. We used the Sharpsat (Thurley, 2006) solver to compute model counts.
- Backbone Wang et al. (2022) predicted backbones which they used to assign polarity to branching variables in CDCL solvers. We used the Cadiback (Biere et al., 2023) solver to compute backbones. Only defined for satisfiable instances.
- Unsatisfiable Core Selsam & Bjørner (2019) learned a GNN model to predict unsatisfiable cores
  which they then used to make branching decisions in CDCL solvers (i.e., branch of the variable predicted to be most likely to belong to smallest core); they acheived state-of-the-art performance. We
  used the z 3 program (De Moura & Bjørner, 2008) to compute approximately minimal unsatisfiable
  cores. Only defined for unsatisfiable instances.
- RL-based branching Cameron et al. (2024) used an RL procedure to learn a model to estimate the relative effectiveness of branching on each variable (which they then used as a branching policy to improve SAT solvers). We ran MCFS at the root of the tree for 100,000 lookaheads with identical settings to Cameron et al. (2024) and measured variable counts and tree-size estimates. Only defined for unsatisfiable instances.
- Instance-level properties Leyton-Brown et al. (2003); Xu et al. (2008); Hutter et al. (2014) developed a number of features for representing Boolean logic that have been used to build prediction
  models to predict solver running times (Hutter et al., 2014), select amongst a set of algorithms Xu
  et al. (2012), and to configure SAT solvers (Hutter et al., 2011). We partitioned these features into
  five tasks: graphical structure, linear programming relaxation, and statistics from probing runs of
  three types of SAT solvers (local search, dpll probing, survey propagation). We use the feature
  generation script from (Hutter et al., 2014).
- Variable/Clause properties The features from (Hutter et al., 2014) are on the intance level and
   many are aggregations across variables or clause statistics. We developed finer-grained variations of
   these features at the level of variables and clauses as well as other features that don't make sense at
   an instance level (e.g., number of times variable is flipped in local search).
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We computed the ground truth for each task on every instance, except for tasks that are defined only for satisfiable/unsatisfiable instances. We used 2.40 GHz 2 x AMD Rome 7532 CPUs with 8GB of RAM. The dataset required 20 CPU years in total to label. We divided our dataset into an 80:10:10 train, validation, and test split.

We will make this dataset publicly available on hugging face to help facilitate further research. We
 believe that this dataset can serve as an excellent test bed for evaluating various GNN approaches in the context of Boolean logic.

## 4.2 WITHIN DISTRIBUTION TASK GENERALIZATION

We evaluated our foundation model first on how effectively we could fine-tune to new tasks. We evaluated how (1) data-efficient and (2) training-time efficient fine-tuning was relative to training from scratch. We then evaluated whether efficiency gains from fine-tuning were a consequence of the diversity of pretraining tasks. We compared fine-tuning from foundation model vs fine-tuning from pretrainged models from single tasks.

**Data Efficiency** We trained ten foundation models with each task category held out on the all one million instances. We then randomly subsampled the training set at 100, 1000, 10000, and 100000 instances. For each dataset size and task category, we trained two models with identical architecture: (1) fine-tuning from corresponding foundation model for held-out task and (2) training from scratch.

Faster Convergence For each task category, we evaluated fine-tuning against training from scratch on the full dataset. We ran two variants of finetuning in each case. One where we fine-tuned all of the parameters, and another where we froze the shared architecture and only trained the task head. This latter setting is much less demanding on GPU resources, especially for much larger Boolean logical formulae we might encounter in practice. We measured validation performance at regular intervals and compared training-time efficiency.

Finetuning from single-task pretraining For five different tasks (SAT, #SAT, bakebone, unsat core and RL branching), we built pretrained single-task models. We fine-tuned each task from each pretrained model and compared performance relative to fine-tuning from the foundation model. We froze the shared architecture in each fine-tuning experiment.

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## 4.3 OUT-OF-DISTRIBUTION GENERALIZATION

We fine-tuned on evaluation to seven new distributions, three of which are non random. The nonrandom distributions are small-world graph colouring Hutter et al. (2014), quasi group completion Hutter et al. (2014), and spectrum repacking Fréchette et al. (2016). The other are uniform random 4SAT, uniform random 5SAT, and controlled and minimal backbone which are random instance with controlled backbone. We also fine-tune on eight larger size-datasets from the same distribution on variable 150-600 at intervals of 50 variables.

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  - 4.4 MODEL TRAINING

302 We pretrained the model using a two-layer MLP for edge and node encoding, followed by eight 303 message-passing layers and a two-layer MLP for each dataset-specific head. Each dataset was as-304 signed a unique MLP head appended to the shared message-passing layers. The network used leaky 305 ReLU activations and maintained 64-dimensional embeddings for nodes and edges. Optimization 306 employed the Adam optimizer (Kingma & Ba, 2014) with a learning rate of 0.0001, batch normal-307 ization (used with batching during validation to reduce high variance) in GNN layers, and layer 308 normalization in MLP layers. Training used a batch size of 20 (80,000 nodes + edges), with batches 309 sampled uniformly at random. Losses were masked for undefined or missing tasks (e.g., backbone 310 loss on unsat instances). Pretraining, fine-tuning, and frozen fine-tuning runs were allocated 24, 6, 311 and 2 hours, respectively. Performance was evaluated on a validation set per epoch, with the best model tested on a held-out test set. Experiments ran on A100 GPUs. 312

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## 5 Results

# 316<br/>3175.1WITHIN DISTRIBUTION TASK GENERALIZATION

Table 1 shows the improvement in fine-tuning on each hold-out task on the pretraining instance
distribution on a small subset of the training set (1000 examples). Except when performance did not
exceed the trivial baseline for both approaches (DPLL Probing, Var LP, Local Search), fine-tuning
performed at least as well as training from scratch. This is most prominent for the four tasks that
correspond to NP-hard computational problems. Fine-tuning had 10%, 8%, and 1% better accuracy
in predicting satisfiability, backbone variables, and unsat core, respectively. It also performed three
times better in terms of r<sup>2</sup> value for predicting model counting. Performance tended to be poor

324 on tasks from probing runs of SAT solvers (DPLL, Local Search). We suspect that these tasks are 325 fundamentally difficult to predict. For a homogeneous distribution like uniform random, differences 326 in these probing statistics across instances are likely to be dominated by noise. We also note the 327 improvement in the RL-for-branching task (4% better accuracy in predicting a variable in the top 328 10). The loss differential appears minimal but in fact is a substantial difference. The target is the distribution of Q values across the actions (variables) in an RL procedure, which tends to be very 329 close to uniform because it takes a lot of samples to pull apart the actions. Small differences in 330 Q-value predictions are meaningful but not captured well by the magnitude of the cross entropy 331 loss. 332

Held-out Task	Туре	Metric	Fine-tuning		From Scratch	
			Loss	Metric	Loss	Metric
SAT	Graph Classification	Accuracy	0.538	0.738	0.632	0.644
Backbone Unsat Core	Node Classification	Accuracy	0.832 0.134	0.619 0.902	0.953 0.14	0.535 0.895
RL Branching	Node Selection	Top-10 Accuracy	4.6084	0.396	4.6086	0.359
Var Structural Clause Structural Var Local Search Clause Local Search Var LP Clause LP	Node Regression	R2 Score	0.990 0.431 1.771 0.494 0.146 0.088	0.099 0.972 0.057 0.705 -0.001 0.796	<b>0.989</b> 0.434 1.800 0.612 0.146 0.171	0.099 0.971 0.041 0.634 <b>0.004</b> 0.602
#SAT Local Search LP DPLL Probing Survey Propagation Graph Structural	Graph Regression	R2 Score	1.168 2.878 1.086 0.993 0.369 0.529	0.327 -16.749 0.044 -0.134 0.274 0.147	1.551 11.155 1.128 <b>0.886</b> 0.424 0.622	0.107 -67.792 0.007 <b>-0.011</b> 0.166 -0.003

Table 1: Performance comparison between fine-tuning and training from scratch on each task held out for a subsampled training set of 1000 examples.

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It is very common in practice to have just a few hundred or thousand instances to train from (e.g. 356 Bischl et al. (2016)) so performance at these dataset sizes is much more indicative of real-world 357 performance. Figure 2a shows the complete results of the data efficiency experiments at the four 358 orders of magnitude of dataset size. The base of the y-axis represents performance of the trivial 359 baseline (random guessing for classification and predicting the mean for regression). In many cases, 360 fine-tuning was an order of magnitude more data efficient, achieving better performance at 1000 361 examples than training from scratch achieved with 10,0000 examples. Satisfiability prediction was 362 the most striking; fine-tuning from 100 examples outperformed training from scratch on 100,000 363 examples. In almost all cases, training from scratch eventually reached fine-tuning performance with a sufficiently large training set; datasets of this size are unlikely to be readily available for 364 particular downstream applications. 365

We now show that fine-tuning performance also tended to converge much faster. Figure 2b shows validation performance over training runs comparing fine-tuning and training from scratch on the full dataset. For all four of the NP-hard computational tasks, fine-tuning is more than an order of magnitude faster; performance of fine-tuning after 1000 steps exceeded performance of training from scratch after 10,000 steps. The plot also shows performance of fine-tuning with the shared parameters frozen and just the task-head parameters are learnable. In many cases, this frozen model exceeds the performance of training all parameters from scratch before 10,000 steps.

Next, we evaluated whether fine-tuning from single-task pretrained models could achieve similar
results to pretraining on all tasks. We found that in general that is not the case suggesting that the
combination of pretraining tasks is leading to a more generalizable representation. See Table 2 for
results. The left-most column lists the pretrained models and each column represents the tasks we
are fine-tuning to. In every case, the foundation model trained on all but the fine-tuning task achieved best performance.



(a) Performance as a function of training set size. (b) Validation performance over training run.

Figure 2: Performance of fine-tuning and training from scratch on each held-out task.

We also observed a clear distinction between tasks trained only on unsatisfiable instances (unsat core, RL branching) and the others. SAT, model counting, and backbone were mutually complementary but models trained on these tasks tended to fine-tune poorly to tasks on unsatisfiable tasks and vice versa. This is evidence that predictive features are very different between satisfiable and unsatisfiable instances. 

			Held-out Tasks		
Model	SAT Acc	<b># SAT</b> R <sup>2</sup>	Backbone Acc	Unsat Core Acc	RL Branching Top-10 Acc
Foundation	0.743	0.432	0.614	0.894	0.408
Sat		0.362	0.586	0.889	0.388
Model Counting	0.727		0.592	0.872	0.385
Backbone	0.721	0.346		0.886	0.363
Unsat Core	0.685	0.208	0.552		0.406
RL Branching	0.630	0.091	0.522	0.890	

Table 2: Performance for finetuning task heads with frozen graph layers on six models (one foun-dation model trained on all but one task and five models trained on single tasks) and five held-out tasks. Colors are normalized by the max (green) and min (red) metric of each task. Foundation model outperformed all single task models. 

#### 5.2 **OUT-OF-DISTRIBUTION GENERALIZATION**

Table 3 shows out-of-distribution fine-tuning performance for 15 different settings. Finetuning con-sistently showed better performance. In the three nonrandom distributions, fine-tuning achieved 0.3 (vs. 0.11)  $r^2$  for model counting (QGC), 0.992 (vs 0.986) auroc for unsat core (SATFC), and 0.09 (vs -0.07)  $r^2$  for model counting (SWGC). We also showed a consistent fine-tuning improvement for upward-size scaling for SAT prediction. For example, for 550 variables, fine-tuning achieved 85% accuracy compared 71% from training from scratch.

5.3 NORMALIZATION 

We found that the performance of the foundation model was sensitive to the choice of specific combi-nations of normalization layers. We evaluated the performance of the foundation model for different normalization techniques: batch normalization (Ioffe & Szegedy, 2015), layer normalization (Ba et al., 2016) and what we call hybrid normalization, which uses batch normalization in GNN and layer normalization in feed-forward head networks. We show in Table 4 that hybrid normalization outperformed all other normalization techniques for most Boolean logic tasks when training from scratch.

Distribution	Mean #Var	Task	Metric Type	Four	dation	From	Scratch
				Loss	Metric	Loss	Metric
	150			0.492	0.759	0.600	0.660
	200	SAT	Accuracy	0.436	0.793	0.594	0.662
	250			0.451	0.788	0.591	0.682
Uniform Random 3SAT	300			0.439	0.802	0.577	0.694
emonin Random 55/A	350	5/11		0.416	0.823	0.566	0.698
	400			0.448	0.784	0.582	0.666
	550			0.411	0.854	0.572	0.711
	600			0.394	0.829	0.555	0.712
Uniform Double of AT	00	Backbone	Accuracy	0.676	0.727	0.731	0.713
Uniform Random 45A1	90	#SAT	R2 score	0.508	0.407	0.635	0.258
Uniform Random 5SAT	65	#SAT	R2 score	0.201	0.368	0.191	0.399
Dealthan Minimal Sectionstance	100	Backbone	Accuracy	1.001	0.504	1.006	0.509
Backbone Minimal Subinstance	100	#SAT	R2 score	2.698	0.209	3.452	-0.011
	100	Backbone	Accuracy	0.798	0.633	0.856	0.596
Controlled Backbone Size	100	#SAT	R2 score	0.967	0.329	1.304	0.095
Quasi Group Completion (QGC)	1299	#SAT	R2 score	1.188	0.315	1.539	0.112
Spectrum Repacking Problem (SATFC)	782	Unsat Core	AUROC	0.116	0.992	0.128	0.986
Small-world Graph Colouring (SWGC)	1332	#SAT	R2 score	1.884	0.093	2.231	-0.074

Table 3: Out-of-distribution finetuning on seven new distributions and eight upward-size generalization datasets of the same pretraining distribution.

Normalization	SAT	# SAT	Backbone	<b>Unsat Core</b>	<b>RL Branching</b>
	Acc	$\mathbb{R}^2$	Acc	Acc	Loss*
Batch	0.646	0.130	0.535	0.867	0.0460878
Layer	0.651	0.137	0.537	0.877	0.0460876
Hybrid	0.756	0.448	0.634	0.904	0.0460860

Table 4: Foundation model performance (val loss) for each normalization layer type: batch normalization, layer normalization, and hybrid normalization (batch norm for GNN layers + layer norm for feed-forward heads). \* Had issue with RL branching metric; We will have it for camera ready.

467 Batch normalization and layer normalization are two widely adopted normalization techniques in 468 deep learning models and we observed significant limitations in both. For batch normalization, 469 we observed high variance for graph embeddings of the same random chosen graph throughout 470 training, which caused stability issues during optimization. For layer norm, it struggled to learn 471 in most graph-level tasks which we hypothesize is related to the oversmoothing effect described in 472 Zhao & Akoglu (2020) and Cai & Wang (2020). We proposed hybrid normalization to address both 473 issues. We found that (1) unlike layer normalization, hybrid normalization maintains high separation between node embeddings throughout training, while (2) variance of node embedding for a given 474 graph across batches is much more controlled compared to batch normalization. 475

476 We monitored two key metrics during foundation model training for each of the 3 choices of nor-477 malization techniques.

478 (1) Cosine similarity between neighboring training steps of the node embeddings for the same graph. 479 Let  $H_t \in \mathbb{R}^{n \times d}$  be the embedding matrix for a chosen graph at training step  $t, H_{t,i} \in \mathbb{R}^d$  be the 480 node embedding for node i, the metric is defined as 481

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 $\text{cosine\_similarity}(H_t, H_{t-1}) = \frac{\sum_i H_{t,i} H_{t-1,i}}{\sqrt{\sum_i H_{t,i}^2} \sqrt{\sum_i H_{t-1,i}^2}}$ (1)

This measures how much the graph embedding of a given graph changes during training.

486 (2) Pairwise distances between node embeddings from the output of GNN layers. ("row-diff" mea-487 sure from (Zhao & Akoglu, 2020) Let  $H \in \mathbb{R}^{n \times d}$  be the embedding matrix output by GNN layers, 488  $h_i \in \mathbb{R}^d$  be the *i*-th row of H, then row-diff is defined as the average of all pairwise distances 489 between node embeddings:

> pairwise\_dist(H) =  $\frac{1}{n^2} \sum_{i,j \in [n]} ||h_i - h_j||^2$ . (2)

This is an indicator of how well the GNN can separate node embeddings from each other.

As shown in Figures 3a and 3b, batch norm showed high separability of nodes, however, the cosine similarity of graph embeddings changes drastically during training, which is indicative of unstable learning.In contrast, layer normalization maintained a consistent rate of change for the cosine similarity measure after training stabilized but exhibited lower and narrower node separability, which could be linked to the over-smoothing phenomenon. Hybrid normalization maintained relatively high node separability across training while the variance of cosine similarity appears to be much more controlled than batch normalization.



over batches throughout training.



(b) Cosine similarity between graph embeddings from neighboring training steps.



#### DISCUSSION, LIMITATIONS AND FUTURE DIRECTIONS 6

520 Our work demonstrates the promise of foundation models for Boolean logic but is currently lim-521 ited to small-scale problems, far smaller than typical industrial cases. Working with large instances 522 becomes difficult in multiple ways, it is computationally hard to acquire large enough datasets and 523 the large size of the instances constrains the amount of memory available for an expressive enough 524 network. However, our fine-tuning results suggest that there might be a way to circumvent both of 525 these obstacles. Our results on generalization to unseen tasks with more efficient training suggest that generalizing to unseen problem sizes might also not require massive new datasets. Furthermore, 526 our results using frozen shared representations suggest that fine-tuning only a smaller head network 527 might be sufficient for achieving good performance alleviating the need for massive memory inten-528 sive networks at training time. 529

530 By solving the hurdles of generalizing to larger problem sizes, we would also expand the diversity 531 of instances we would be able to study. Incorporating a richer class of problem instances could also provide a yet richer shared representation, which could benefit performance even in the regime we 532 currently study. We restricted ourselves to small instance distributions so we could evaluate very 533 large GNN architectures; distributions of small instances, which are difficult across the variety of 534 tasks we study are limited. 535

536 Further investigation into the hybrid normalization architecture is potentially exciting. We have empirically demonstrated that hybrid normalization outperforms other normalization techniques when used in isolation, and we have provided a hypothesis to explain these results. It would be interesting 538 to evaluate this method on other graph datasets and to explore the theoretical foundations behind its success.

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## A TASK DETAILS

- We hereby give the detailed definitions of each task use in model training and evaluation. First, we define a SAT formula S as a set of clauses  $C = \{c_1, \ldots, c_m\}$  over a set of variables  $V = \{v_1, \ldots, v_n\}$ . Each clause consists of a set of Boolean *literals*, defined as either a variable  $v_i$  or its negation  $\neg v_i$ . The set of literals in a clause are joined by OR operators and the set of clauses are joined by AND operators.
- 698 A.1 MODEL COUNTING

For a given SAT formula S, its **model count** is defined as the number of distinct truth assignments to variables for which the formula evaluates to true. Formally:

 $ModelCount(S) = |\{\mathbf{t} \in \{True, False\}^n \mid S(\mathbf{t}) = True\}|$ 

Graph-Level Regression Tasks		
Task	Description	Output Shape
Model Counting	Predicting the number of satisfying assignments for the SAT instance.	$\phi_{\mathrm{MC}}(S) \in \mathbb{R}$
Instance-wise Structural Features	C	
– Graph Features	Basic graph statistics (e.g., average degree, clustering coefficient).	$\phi_{\rm GF}(S) \in \mathbb{R}^{48}$
– Linear Programming Relaxation	Features from LP relaxation of the SAT problem.	$\phi_{\mathrm{LP}}(S) \in \mathbb{R}^6$
– Local Search Probing	Summary stats of probes of saps and gsat solvers.	$\phi_{\mathrm{LS}}(S) \in \mathbb{R}^{22}$
– DPLL Probing	Propagation/depth of dpll probes.	$\phi_{\mathrm{DP}}(S) \in \mathbb{R}^5$
– Survey Propagation Probing	Summary stats from probes of a survey propagation algorithm.	$\phi_{\mathrm{SP}}(S) \in \mathbb{R}^{18}$
Graph-Level Classification Tasks		
Predicting Satisfiability	Determining whether the SAT in- stance is satisfiable or unsatisfiable.	$\phi_{SAT}(S) \in \mathbb{R}$
Node-Level Regression Tasks		
Variable Features		
– Graph Features	Node-specific statistics (e.g., node degree, betweenness centrality).	$\phi_{\mathrm{GFV}}(S) \in \mathbb{R}^{n \times n}$
– Linear Programming Relaxation	Variable assignments for optimal solution.	$\phi_{\mathrm{NSF}}(S) \in \mathbb{R}^n$
– Local Search Probing	Stats of variable flip counts/weights in local search probes.	$\phi_{\rm LSV}(S) \in \mathbb{R}^{n \times n}$
Clause Features	I I I I I I I I I I I I I I I I I I I	
– Graph Features	Clause node-specific statistics (e.g., node degree, betweenness central-	$\phi_{\rm GFC}(S) \in \mathbb{R}^{n \times n}$
- Linear Programming Relaxation	Ry). Constraint slacks	$\phi_{\mathrm{MGE}}(S) \in \mathbb{R}^n$
– Local Search Probing	clause penalties and frequency sat- isfied	$\phi_{\rm LSC}(S) \in \mathbb{R}^{n \times n}$
Node-Level Classification Tasks		
Backbone Prediction	Predicting the backbone status (non-backbone, true, false) of each variable.	$\phi_{\rm BB}(S) \in \mathbb{R}^{n \times 3}$
Unsatisfiable Core Detection	Predicting probability of variable belonging to unsat core	$\phi_{\mathrm{UC}}(S) \in \mathbb{R}^n$
RL Branching	Predicting MCTS-related proper- ties for each node (visit counts, value estimates)	$\phi_{\mathrm{MCTS}}(S) \in \mathbb{R}^n$

Table 5: Categorization of task into graph and node-level regression and classification along with brief descriptions and output shape of each corresponding task head.

## A.2 INSTANCE-WISE GRAPH FEATURES

From Hutter et al. (2014). A SAT problem can be represented as different graph representations.
First, a variable-clause graph is a bipartite graph where the two disjoint sets of nodes correspond to variables and clauses. An edge connects a variable node to a clause node if the variable appears (positively or negatively) in the clause. Second, a variable graph have each node corresponds to a variable, and an edge exists between two nodes if the corresponding variables appear in the same

756	Graph representation Metrics
757	variable-clause graph variable node degree, clause node degree
758	variable graph node degree, diameter
759	clause graph node degree, clustering coefficient
760	
761	Table 6: Graph metrics
762	
763	alouse. Third, a cloure graph have each node corresponds to a cloure, and an edge is drawn between
764	two nodes if the corresponding clauses share at least one variable.
765	We have $1^{1}$ C $1^{1}$ T $1^{1}$ C $1^{1}$ C $1^{1}$ T $1^{1}$ C $1^{1}$ C $1^{1}$ T $1^{1}$ C $1^{1}$
767	We collect different graph metrics in Table 6 from each graph representation, and for each metric
768	compute its mean, variation coefficient, min, max and entropy.
769	
770	A.3 INSTANCE-WISE LINEAR PROGRAMMING RELAXATION
771	SAT instance can also be represented as linear programming problem.
772	
773	Variables
774	
775	$x_j \in [0,1],  orall j \in \{1,\ldots,n\}$
776	$s_i \ge 0,  \forall i \in \{1, \dots, m\}$
777	
778	where $x_j$ is the boolean variable, $s_i$ is the slack variable for clause $C_i$ , measuring the degree of
779	under-satisfaction of the clause.
780	
781	<b>Objective:</b> As a constraint satisfaction problem, there's no objective.
782	Construction for each along $C$ the following in quality must hold
78/	<b>Constraints:</b> For each clause $C_i$ , the following inequality must hold.
785	$\sum x_i + \sum (1 - x_i) + s_i \ge 1$ $s_i \ge 0$ $\forall i \in \{1, \dots, m\}$
786	$\sum_{j \in \text{Pos}(i)} x_j + \sum_{j \in \text{Neg}(i)} (1 - x_j) + b_i \ge 1,  b_i \ge 0,  \forall e \in \{1, \dots, ne\}$
787 788	where $Pos(i)$ is the set of variables that appear positively in clause $C_i$ , $Neg(i)$ is the set of variables that appear negatively in clause $C_i$ .
789	We compute the mean variation coefficient min and may for the Integer cleak vector of the I.D.
790 791	problem, along with ratio of integer vars in LP solution and objective value of LP solution.
792	
793	A.4 INSTANCE-WISE LOCAL SEARCH PROBING
794	
795	SAPS Hutter et al. (2002) is a dynamic local search algorithm for SAT solving. We run 2 seconds
796	of the solver on the sat instance and record:
797	
798	• Number of steps to the best local minimum in a run
799	<ul> <li>Average improvement per step to best local minimum in a run</li> </ul>
800 801	• Fraction of overall improvement due to first local minimum
802	Best solution
803	
804	A 5 INSTANCE-WISE DPLI PROBING
805	1.5 INSTANCE-WISE DI LE I ROBINO
806	From Hutter et al. (2014). DPLL is a fundamental algorithm for SAT solving. A sequence of variable
807	assignments are made until a contradiction is encountered. After each assignment, unit propagation
808	is called, which means literals in a clause by themselves are assigned to true. We make random

probes of depth 1, 4, 16, 64 and 256 and measure the number of unit propagations. We also take a number of random probes until a contradiction is encountered and measure average depth.

# 810 A.6 SURVEY PROPAGATION PROBING

From Hutter et al. (2014). Run a survey propagation algorithm Braunstein et al. (2005). Then for
each variable, compute the higher of P(true)/P(false) or P(false)/P(true). Then compute statistics
across variables: mean, variation coefficient, min, max, 10%, 25%, 50%, 75%, and 90% quantiles.

## 816 A.7 PREDICTING SATISFIABILITY

A Boolean formula S is **satisfiable** if there exists an assignment  $\mathbf{V} \in {\text{True}, \text{False}}^n$  to the variables  $V = {v_1, \ldots, v_n}$ , such that the formula S evaluates to True. Formally:

 $\operatorname{Satisfiable}(S) \iff \exists \mathbf{t} \in {\operatorname{True}, \operatorname{False}}^n \text{ s.t. } S(\mathbf{t}) = \operatorname{True}.$ 

### A.8 BACKBONE PREDICTION

The **backbone** of a satisfiable formula S is the set of variables that are true in all satisfying assignments of S. Formally:

Backbone(S) = { $v \mid \text{variable } v = \text{True } \forall \mathbf{t} \in {\text{True, False}}^n \text{ s.t. } S(\mathbf{t}) = \text{True}$ }.

### A.9 MINIMAL UNSATISFIABLE CORE

Given an unsatisfiable SAT formula represented in CNF form, a minimal UNSAT core of S is the smallest subset of its clauses  $C_{core} \subseteq C$  such that  $S_{core}$  is unsatisfiable. Formally:

$$\underset{C_{core}}{\arg\min} |C_{core}| \ s.t. \ C_{core} \subseteq C, \quad S_{core} = \bigwedge_{c \in C_{core}} c \ \text{s.t. Satisfiable}(S_{core}) = False$$

### A.10 RL BRANCHING

MCFS Cameron et al. (2024) is a Monte Carlo Tree Search based algorithm aims to find the optimal branching policy (i.e choosing which variable to search next) for SAT solving. After an offline search and rollouts for SAT instance S, we get two measurements from the search tree: variable counts and tree-size estimates. **variable counts**  $\in \mathbb{R}^n$  measures how many times each variable was chosen during the search. **tree-size**  $\in \mathbb{R}^n$  measures the estimated size of the search tree for each variable.

## B Loss

For each task  $T_i$ , the loss  $\mathcal{L}_i$  is defined based on the task type  $\tau(T_i) \in \{\text{node, graph}\}\)$  and category  $\ell(T_i) \in \{\text{regression, classification}\}\)$ .  $\tau(T_i)$  defines whether the model makes predictions for every node or a global prediction of entire graph and category  $\ell(T_i) \in \{\text{regression, classification}\}\)$  defines whether we use mean-squared error or cross entropy loss

 $\mathcal{L}_{i}(T_{i},\phi) = \begin{cases} \mathbb{E}_{S \sim \mathbb{P}} \left[ (T_{i}(S) - \phi_{i}(S))^{2} \right] & \text{if } \tau(T_{i}) = \text{graph}, \ell(T_{i}) = \text{regression}, \\ \mathbb{E}_{S \sim \mathbb{P}} \left[ -\sum_{c=1}^{C} T_{i}(S)_{c} \log \phi_{i}(S)_{c} \right] & \text{if } \tau(T_{i}) = \text{graph}, \ell(T_{i}) = \text{classif}, \\ \mathbb{E}_{S \sim \mathbb{P}} \left[ \frac{1}{N} \sum_{i=1}^{N} (T_{i}(v_{j}) - \phi_{i}(v_{j}))^{2} \right] & \text{if } \tau(T_{i}) = \text{node}, \ell(T_{i}) = \text{regression}, \end{cases}$ 

$$\left(\mathbb{E}_{S\sim\mathbb{P}}\left[\frac{1}{N}\sum_{j=1}^{N}\left(-\sum_{c=1}^{C}T_{i}(v_{j})_{c}\log\phi_{i}(v_{j})_{c}\right)\right] \quad \text{if } \tau(T_{i}) = \text{node}, \ell(T_{i}) = \text{classif.}$$

<sup>864</sup>  $T_i(S)$  is the ground truth result for task  $T_i$  on instance  $S, T_i(x)_c$  is an indicator if class c is the true <sup>865</sup> class,  $\phi_i$  is the task head for task  $i, \phi_i(x')_c$  is the predicted probability of class c where x' could be <sup>866</sup> a logical formula S or a variable  $v_j \in S$ . We would like to learn some  $\phi$  that takes S or a lossless <sup>867</sup> representation of S directly as input.

## C SAT ENCODING

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871 A CNF SAT instance S is defined by a set of clauses  $C = \{c_1, \ldots, c_m\}$  over a set of variables 872  $V = \{v_1, \ldots, v_n\}$ . Each clause consists of a set of Boolean *literals*, defined as either a variable 873  $v_i$  or its negation  $\neg v_i$ . The set of literals in a clause are joined by OR operators and the set of 874 clauses are joined by AND operators. We represented a CNF SAT instance with n clauses and m875 variables as an  $n \times m$  bipartite graph, where each node and edge is represented as a d-dimensional 876 trainable embedding. Variable and clause nodes are represented with embedding vectors  $v^0$  and  $c^0$ respectively and each edge (i, j) is represented with embedding  $e_t$  if the true literal for variable i 877 appears in clause j and  $e_f$  if the false literal for variable i appears in clause j. 878

### D MODEL ARCHITECTURE

**Pre-GNN encoder** We first map each node and edge embedding with a MLP:  $\forall x : x^1 = \text{MLP}_{\text{pre-node}}(x^0), \forall u, v : e_{u,v}^1 = \text{MLP}_{\text{pre-edge}}(e_{u,v}^0), g^1 = \text{MLP}_{\text{pre-global}}(g^0).$ 

**Message-passing layers** We take in  $(\mathbf{X}^{\ell}, \mathbf{E}^{\ell}, g^{\ell})$  and output  $(\mathbf{X}^{\ell+1}, \mathbf{E}^{\ell+1}, g^{\ell+1})$  as follows:

$$\forall u, v : \bar{e}_{u,v}^{\ell} = \mathrm{MLP}_{\mathrm{edge}}([x_{u}^{\ell}|x_{v}^{\ell}|e_{u,v}^{\ell}|g^{\ell}])$$

$$\forall i : \bar{x}_{i}^{\ell} = \mathrm{MLP}_{\mathrm{node}} \left( \left[ x_{i}^{\ell} \middle| \sum_{u,i} [\bar{e}_{u,i}^{\ell}|x_{u}^{\ell}] \middle| \sum_{i,v} [\bar{e}_{i,v}^{\ell}|x_{v}^{\ell}] \middle|_{g_{i,v}^{\ell}} \right]$$

$$g^{\ell+1} = \mathrm{MLP}_{\mathrm{global}}\left(g^{\ell} \left|\sum_{j} \bar{x}_{j}^{\ell}\right| \sum_{u,v} \bar{e}_{u,v}^{\ell}\right)$$

$$\bar{\mathbf{X}}^{\ell} = \text{SelfAttention}(\bar{\mathbf{X}}^{\ell})$$
$$\forall u, v : e_{u,v}^{\ell+1} = e_{u,v}^{\ell} + \bar{e}_{u,v}^{\ell}$$

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$$\forall u, v : e_{u,v} = e_{u,v} + e_i$$
$$\forall i : x_i^{\ell+1} = x_i^{\ell} + \bar{x}_i^{\ell},$$

where | denotes the concatenation of vectors.

**Shared-embedding layer** We take the node embedding output of k Message-passing layers  $X^k$ , pass through a row-wise sum pooling layer to get the graph level embedding

$$emb_{graph} = \sum_{i=1}^{m} X_{i,}^{k}$$

scatter across rows

$$S = \mathbf{1}_m s$$

and concat back to the node embedding  $X^k$ 

$$emb_{\text{shared}} = X^k \mid S$$

where  $1_m \in \mathbb{R}^m$  denotes a column vector of 1s and | denotes the concatenation of vectors.

**Head networks** We have a head network for each task in the foundation model and a single head for finetuning and single task training. We first describe the head networks according to task type

- Graph-level tasks: The final prediction is a global sum pooling of all node representations followed by an MLP that maps to output shape according to the specific task:  $\bar{y} = \text{Dropout}_p(\text{MLP}_{\text{head}}(\sum_i x_i)).$
- Node-level tasks: The final prediction is an MLP that maps each node embedding to output shape according to the specific task:  $\bar{y}_i = \text{Dropout}_p(\text{MLP}_{\text{head}}(x_i))$ , where  $\text{Dropout}_p$  masks each parameter with probability p.

Table 5 in the appendix describes the output space for each of the sixteen task heads.

