Reptile for Multitask Graph Execution

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Introduction

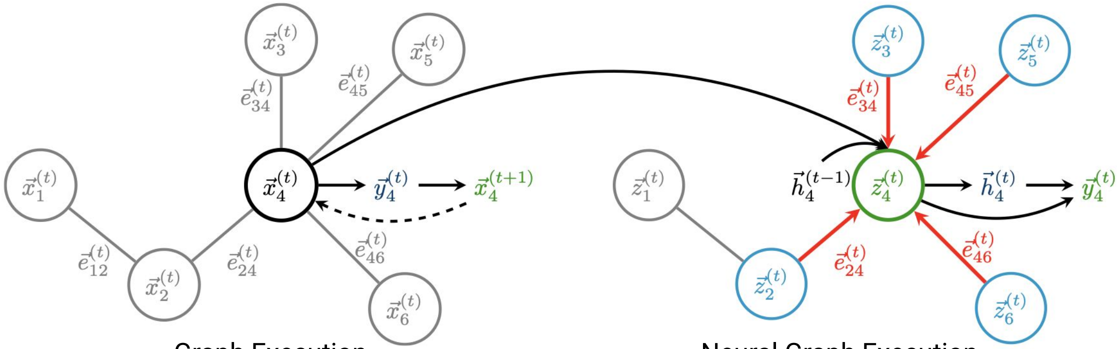
- Neural Algorithmic Reasoning incorporates the theoretical guarantees of classical computer science algorithms with the flexibility of deep learning
- Neural Reasoning typically relies only on the final state as the training signal
- Recent approaches have begun to incorporate intermediate steps to improve the accuracy of the solution

Neural Execution of Graph Algorithms

- Many classical graph algorithms (e.g. Bellman-ford, Breadth-first search, Dijkstra) share common subroutines
    - Ex. Enumerating sets of edges adjacent to a given node
- Intuition: learning multiple graph algorithms simultaneously is the best way to leverage subroutines
- The supervision signals in the learning process are the intermediate outputs of the classical algorithms we're trying to learn

Neural Execution

- The neural executor utilizes an encoder-processor-decoder architecture



Graph Execution

Neural Graph Execution

Encoder $\vec{z}_i^{(t)} = f_A(\vec{x}_i^{(t)}, \vec{h}_i^{(t-1)})$

Processor $\mathbf{H}^{(t)} = P(\mathbf{Z}^{(t)}, \mathbf{E}^{(t)})$

Decoder $\vec{y}_i^{(t)} = g_A(\vec{z}_i^{(t)}, \vec{h}_i^{(t)})$

Termination $\tau^{(t)} = \sigma(T_A(\mathbf{H}^{(t)}, \overline{\mathbf{H}^{(t)}}))$

- The loss for each task is aggregated during each training iteration
  - The parameters for the shared processor network as well as the task-specific encoder/decoder networks are all updated at once using the aggregate loss
  - Dissimilarity between task gradients makes learning more difficult

Sequential Reptile

- A learning framework that seeks to maximize the knowledge transfer when learning multiple tasks simultaneously
- Main observation: it is crucial to align gradients between tasks in order to maximize knowledge transfer while minimizing negative transfer (forgetting)
- Method: assume the model is trained on ***T*** tasks
- For each outer iteration: perform ***K*** updates (inner iterations) on a copy of the current model parameters to compute meta gradient (MG)
- For each inner iteration: sample a task $\boldsymbol{t_k}$ from a categorical distribution, then sample a batch $\boldsymbol{B_{tk}^{(k)}}$ from task $\boldsymbol{t_k}$

$$\theta^{(0)} = \phi, \qquad \theta^{(k)} = \theta^{(k-1)} - \alpha \frac{\partial \mathcal{L}(\theta^{(k-1)}; \mathcal{B}_{t_k}^{(k)})}{\partial \theta^{(k-1)}}$$

- After K inner iterations (1 outer iteration):

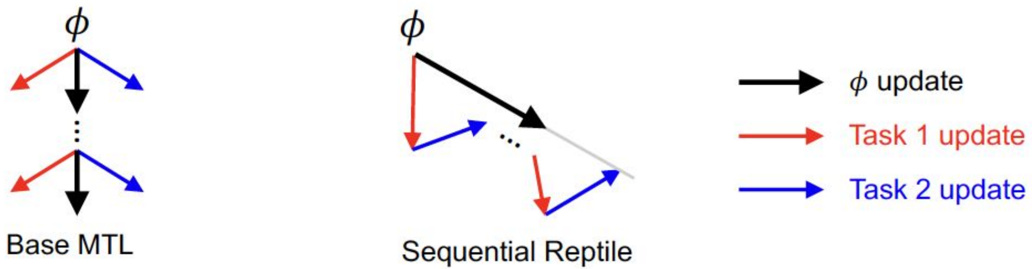
$$\phi \leftarrow \phi - \eta \cdot \mathrm{MG}(\phi), \quad \text{where} \quad \mathrm{MG}(\phi) = \phi - \theta^{(K)}$$

- Advantage:

$$\mathbb{E}\left[\mathrm{MG}(\phi)\right] \approx \frac{\partial}{\partial \phi}\mathbb{E}\left[\sum_{k=1}^{K} \mathcal{L}(\phi; \mathcal{B}_{t_k}^{(k)}) - \frac{\alpha}{2}\sum_{k=1}^{K}\sum_{j=1}^{k-1}\left\langle \frac{\partial \mathcal{L}(\phi; \mathcal{B}_{t_k}^{(k)})}{\partial \phi}, \frac{\partial \mathcal{L}(\phi; \mathcal{B}_{t_j}^{(j)})}{\partial \phi} \right\rangle\right]$$

Problem Statement

- We want to align the gradients from each algorithm learning task to leverage inter-algorithm features in a multi-task learning setting to improve performance
    - Ex. common subroutines: shortest path computation via Bellman-Ford and breadth-first search both enumerate sets of edges adjacent to a particular node



Training Procedure

- Incorporate sequential reptile with neural execution baseline for multi-task learning
- For each iteration: perform K updates on a copy of the current model parameters
  - For each update: sample a task t_k (BFS or Bellman-Ford) from a categorical distribution / specified order, then sample a batch $B_{tk}^{(k)}$ from task t_k and taking gradient steps with them (learning rate = 5e-4)
  - After K updates
    - we meta-update Φ with learning rate = 1
- Also, the percentage of graph numbers w.r.t. different algorithms varies (imbalanced data settings)

Experiment Settings

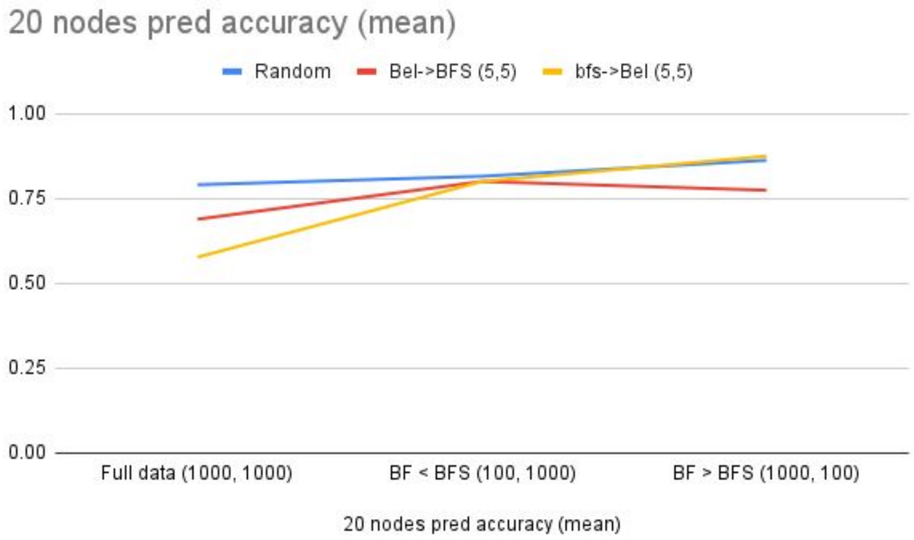
- Algorithms: We are currently focusing on two parallel algorithms, **BELLMAN-FORD** and **BREADTH-FIRST SEARCH**
- Our datasets:
  - Graph Types: Most experiments are done on **Erdós Rényi** graphs
  - Train Set: number of graph for each algorithm = 1000 (or 100 imbalance case); number of nodes = 20
  - Validation Set: number of graph for each algorithm = 100; number of nodes = 20
  - Test Set: number of graph for each algorithm = 200; number of nodes = 20, 50
- Performance metrics:
  - BFS: reachability mean step accuracy; reachability last step accuracy; termination accuracy
  - Bellman-Ford: mean squared error, last step mean squared error; predecessors mean step accuracy: predecessors last step accuracy; termination accuracy

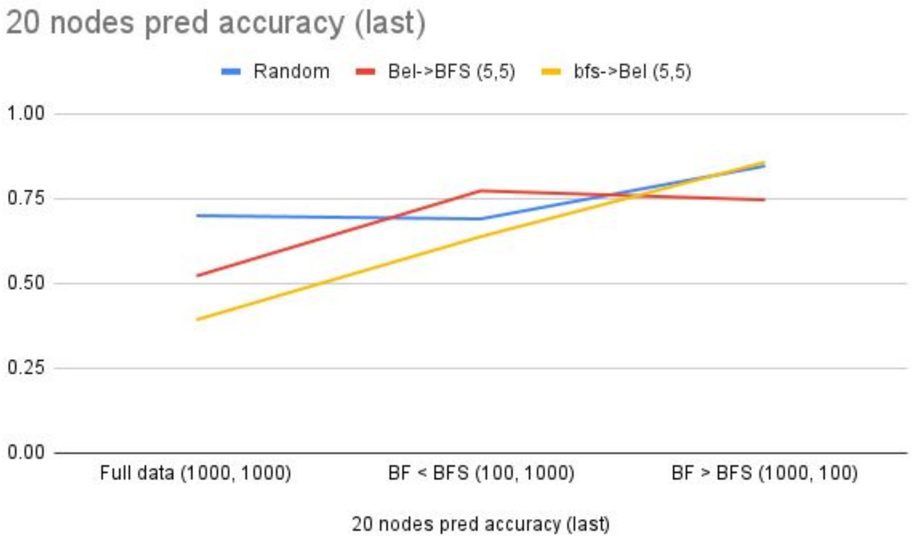
Seq Reptile vs Vanilla Multitasking

20 Nodes	Reachability Acc (mean/last)	Predecessor Acc (mean/last)	MSE (mean/last)	Termination Acc (BF/BFS)
Sequential Reptile	0.9882/0.9882	0.8628/0.8460	0.08/0.08	0.8240/0.772
Vanilla Multitasking	0.9921/0.9799	0.7365/0.6999	0.147/0.151	0.7544/0.7544

50 Nodes	Reachability Acc (mean/last)	Predecessor Acc (mean/last)	MSE (mean/last)	Termination Acc (BF/BFS)
Sequential Reptile	0.9970/ 0.9970	0.8356/0.8076	0.2593/0.3359	0.8828/0.78
Vanilla Multitasking	0.9979/0.9595	0.6954/0.6889	0.5378/1.2226	0.6751/0.6751

Data Imbalanced Setting





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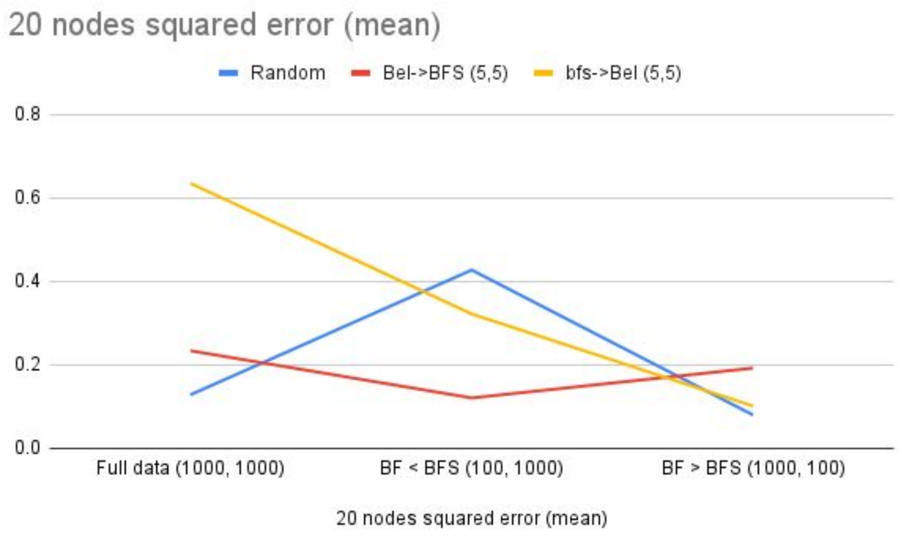
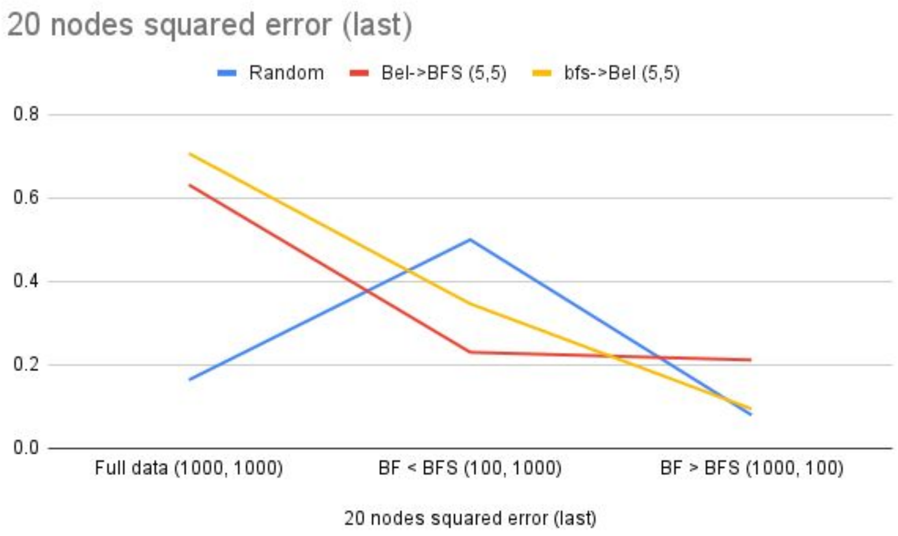
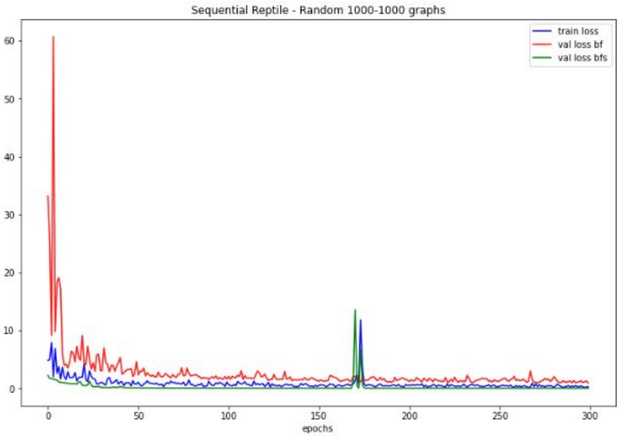
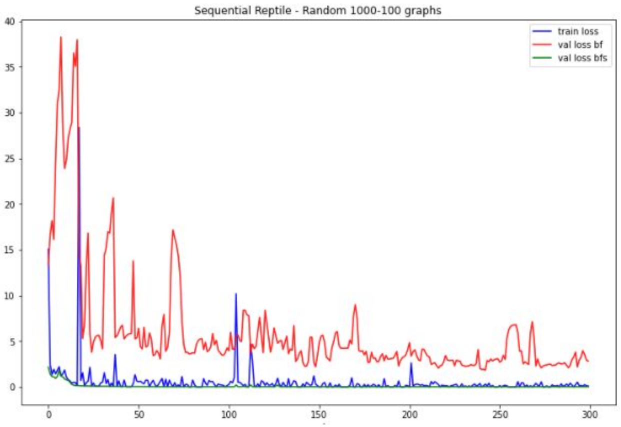
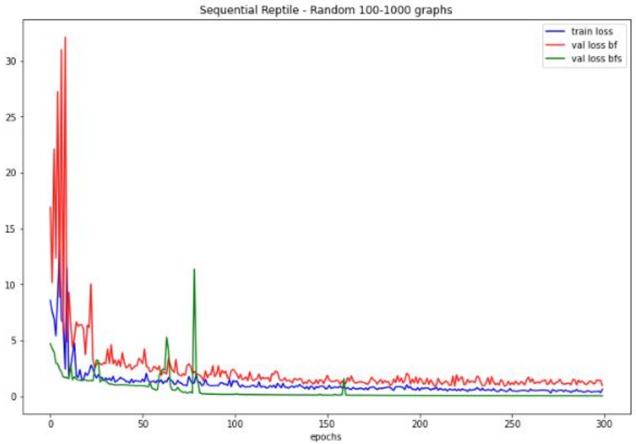




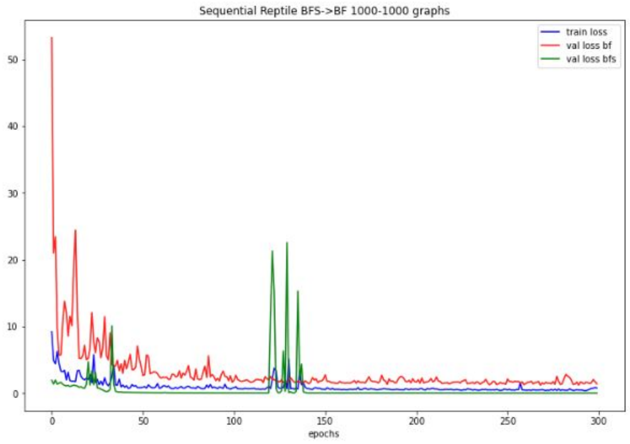
Training vs Validation Loss Curve: Random

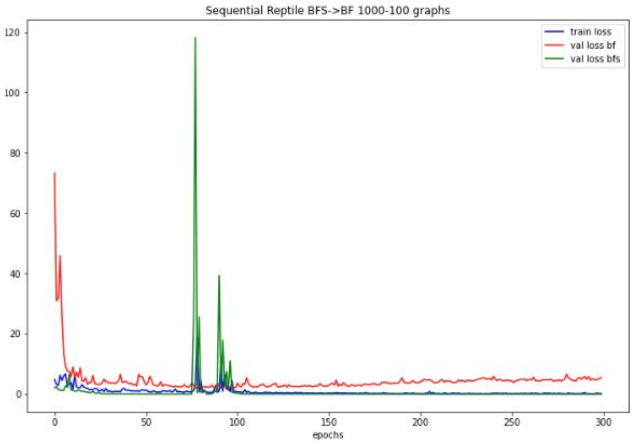


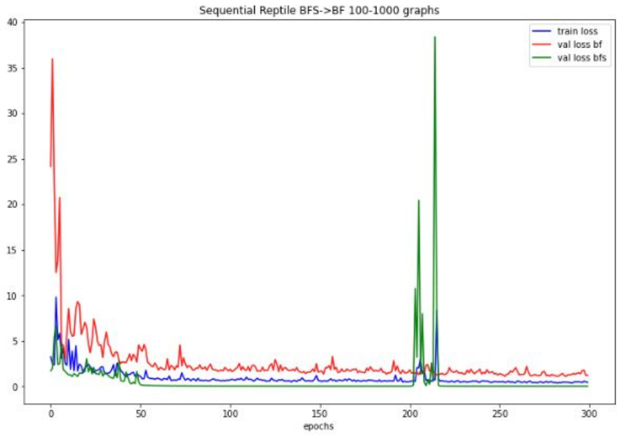




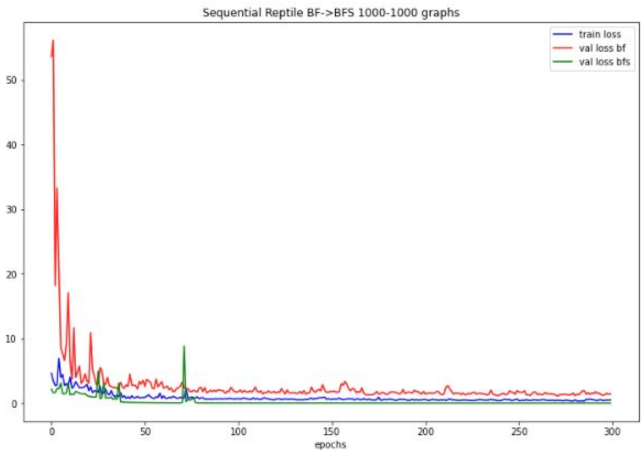
Training vs Validation Loss Curve: BFS->BF

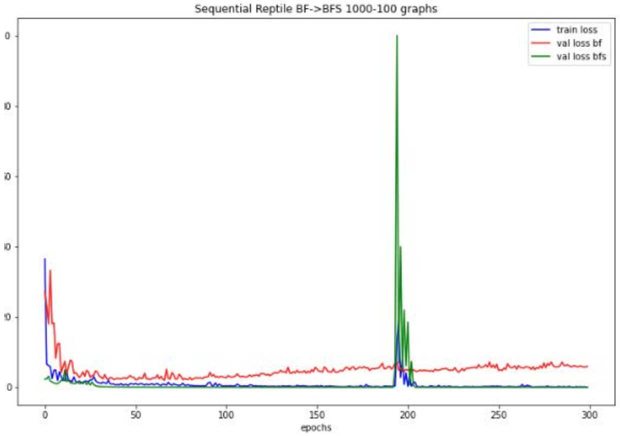


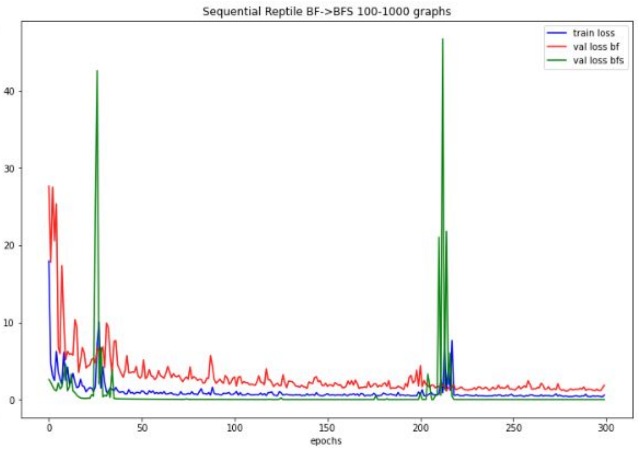




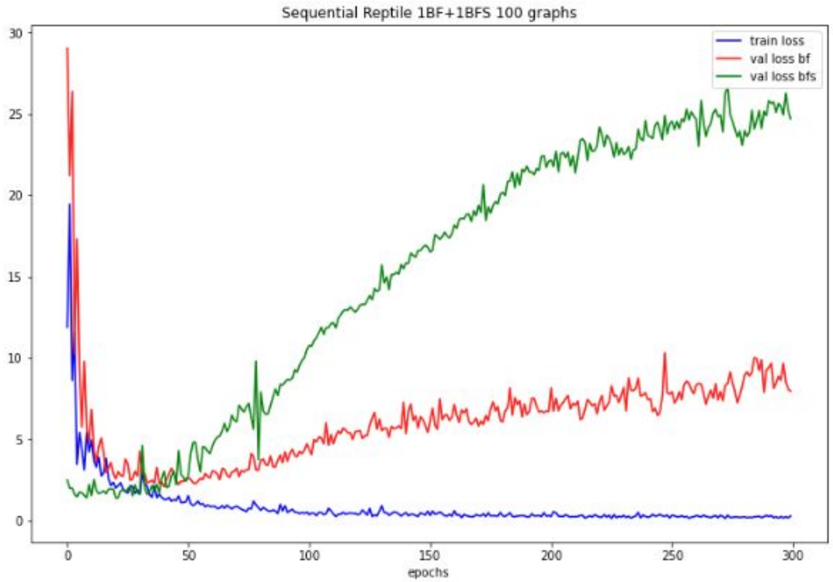
Training vs Validation Loss Curve: BF->BFS

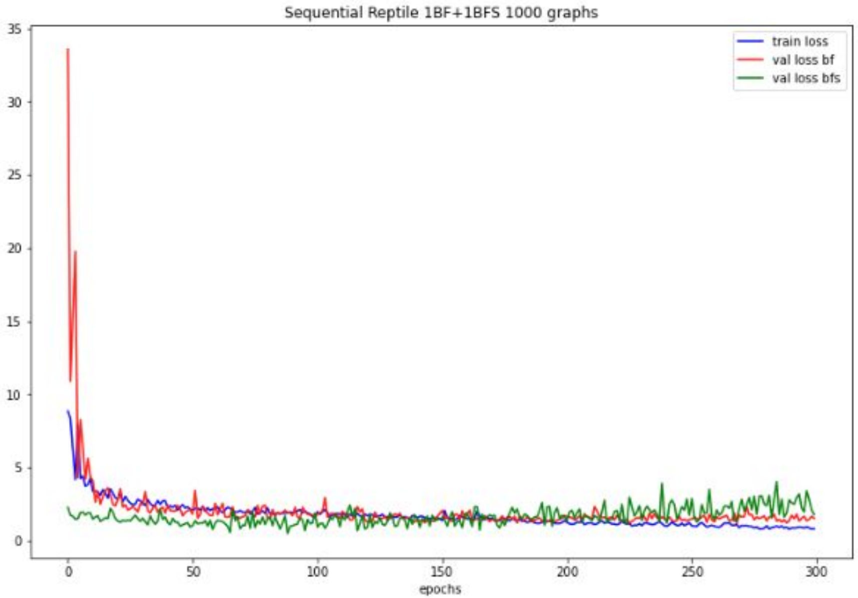




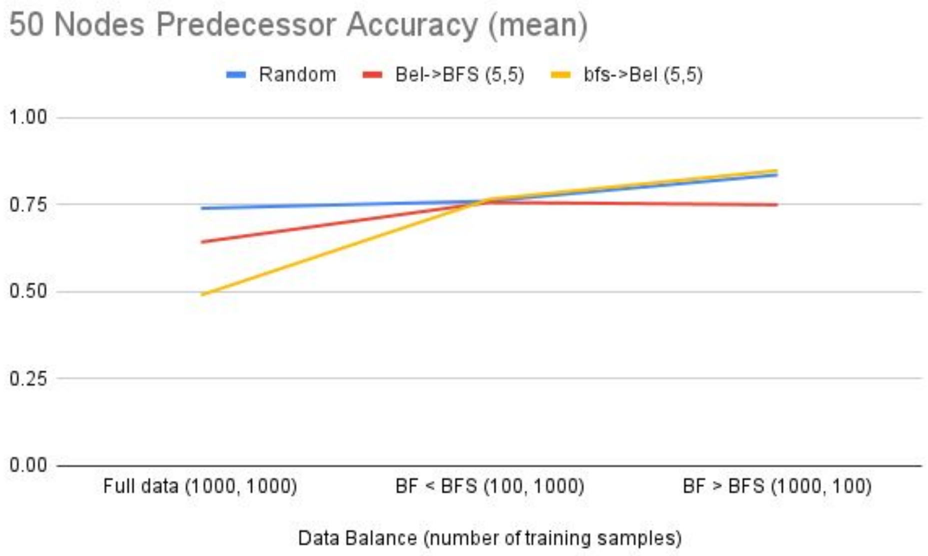


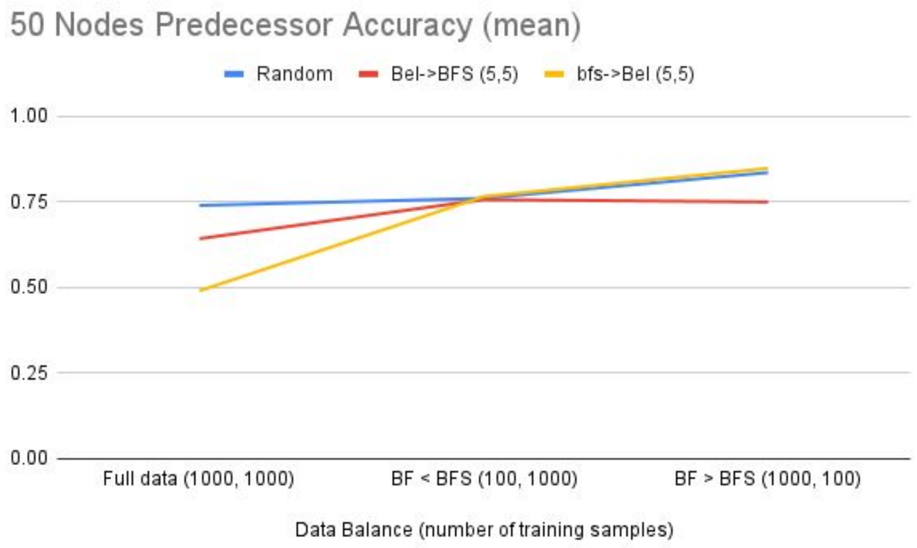
Training vs Validation Loss Curve:1BF+1BFS





Data Imbalanced Setting





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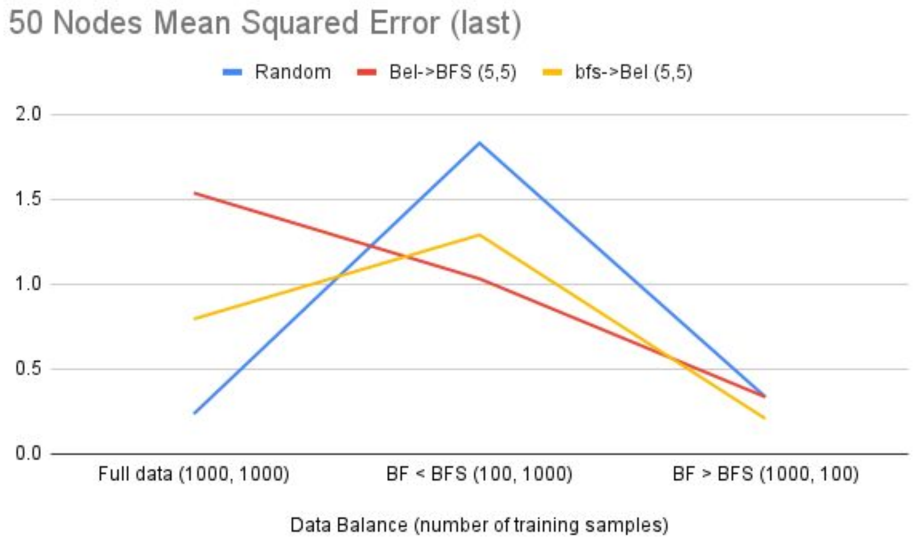

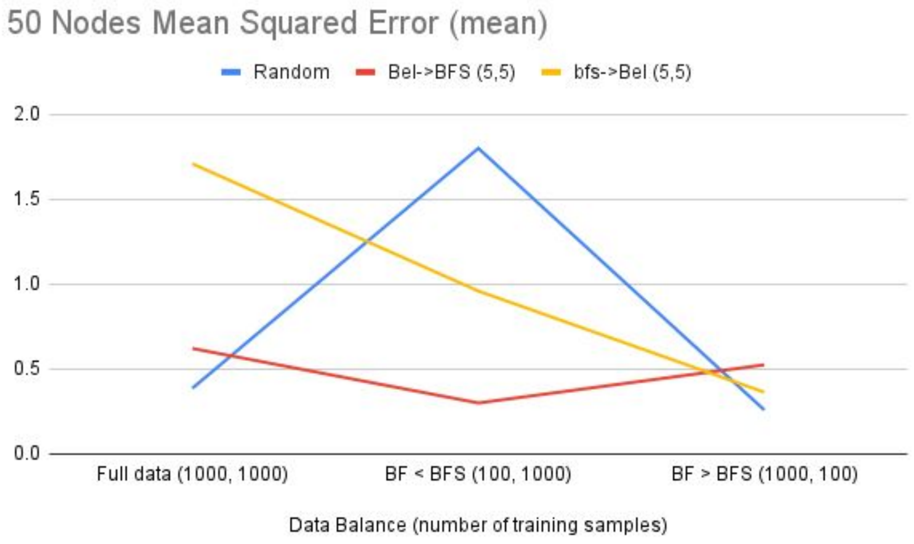

Future Works

- Compare the convergence rate of Sequential Reptile with vanilla multitask learning in the context of neural graph execution
    - The number of graphs needed to achieve comparable performance
- Make Sequential Reptile more suitable for the context of neural graph execution
    - Currently for each step in the inner loop, the distribution the next task is sampled from a distribution based on the sizes of training datasets for each task
    - Can utilize domain specific knowledge to serve as a prior for the task distribution. E.g. use GNN to extract features of the graphs in the training set and utilize these features
- Experiment with training on more algorithms
    - Parallel: Widest
    - Sequential: Prims, Dijkstra
- Experiment with other multitask learning frameworks
    - Adaptive scheduling using validation performance to leverage the benefits of ordering tasks

Thank You

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Related Work

- Multi-task learning has shown success in applications such as:
    - Natural language processing (learning multiple languages simultaneously) Xue et al.
    - Visual classification X. Yuan and S. Yan
    - Identifying influenza variants Han et al.
- Sequential reptile can improve the optimization process of multi-task learning in these instances
- More specific to our case, effectively applying sequential reptile to multi-task learning with graph neural networks can open doors to other multi-task graph problems (e.g. molecule generation, physical simulations, social networks)