

Graph Neural Thompson Sampling

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Abstract

We consider an online decision-making problem with a reward function defined over graph-structured data. We formally formulate the problem as an instance of graph action bandit. We then propose **GNN-TS**, a Graph Neural Network (GNN) powered Thompson Sampling (TS) algorithm which employs a GNN approximator for estimating the mean reward function and the graph neural tangent features for uncertainty estimation. We prove that, under certain boundness assumptions on the reward function, **GNN-TS** achieves a state-of-the-art regret bound which is (1) sub-linear of order $\tilde{O}((\tilde{d}T)^{1/2})$ in the number of interaction rounds, T , and a notion of effective dimension \tilde{d} , and (2) independent of the number of graph nodes. Empirical results validate that our proposed **GNN-TS** exhibits competitive performance and scales well on graph action bandit problems.

1 Introduction

Thompson Sampling (Thompson, 1933) is a widely adopted and effective technique in sequential decision-making problems, known for its ease of implementation and practical success (Chapelle and Li, 2011; Kawale et al., 2015; Russo et al., 2018; Riquelme et al., 2018). The fundamental concept behind Thompson Sampling (TS) is to compute the posterior probability of each action being optimal for the present context, followed by the selection of an action from this distribution. Previous research has extended TS or developed variants of it to incorporate increasingly complex models of the reward function, such as Linear TS (Agrawal and Goyal, 2013; Abeille and Lazaric, 2017), Kernelized TS (Chowdhury and Gopalan, 2017), and Neural TS (Zhang et al., 2020). However, these efforts have mainly focused on conventional data types. In contrast, the application of sequential learning to graph-structured data, such as molecular or biological graph representations, introduces unique challenges that merit further investigation.

Recently, there has been a growing interest in studying bandit optimization over graphs. Several researchers have initiated this line of work by addressing the challenge of encoding graph structures in bandit problems (Gómez-Bombarelli et al., 2018; Jin et al., 2018; Griffiths and Hernández-Lobato, 2020; Korovina et al., 2020). More recently, Graph Neural Network (GNN) bandits have been proposed, which leverage expressive GNNs to approximate reward functions on graphs (Kassraie et al., 2022). Despite these advancements, the GNN bandits remain relatively unexplored compared to the extensive research on Neural bandits. Firstly, a formal formulation of this sequential graph selection problem is yet to be proposed. More importantly, there is a significant lack of comprehensive theoretical and empirical investigations regarding the use of TS in sequential graph selection.

Contribution. In this work, we address the online decision-making problem over graph-structured data by contributing a novel algorithm called **GNN-TS**. We begin by formulating the sequential graph selection as graph action bandit. We then propose Graph Neural Thompson Sampling, **GNN-TS**, to incorporate TS exploration with graph neural networks. We establish a regret bound for the proposed algorithm with sub-linear growth of order $\tilde{O}((\tilde{d}T)^{1/2})$ with respect to the effective dimension \tilde{d} and the number of interaction round T , and independent of the number of graph nodes. Finally, we corroborate the analysis with an empirical evaluation of the algorithm in simulations. Experiments

show that GNN-TS yields competitive performance and scalability, compared to the state-of-the-art baselines, underscoring its practical value in addition to its strong theoretical guarantees.

Notations. Let $[n] = \{1, 2, \dots, n\}$. For a set or event E , we denote its complement as E^c . $I_n \in \mathbb{R}^{n \times n}$ is the identity matrix. For a matrix A , A_i and A_j denote its i -th row and j -th column, respectively. $\lambda_{\max}(A)$ and $\lambda_{\min}(A)$ represents the maximum and minimum eigenvalues of the matrix A . For any vector x and square matrix A , $\|x\|_A = \sqrt{x^T A x}$. We denote the history of randomness up to (but not including) round t as F_t and write $P_t(\cdot) := P(\cdot | F_t)$ and $E_t(\cdot) := E[\cdot | F_t]$ for the conditional probability and expectation given F_t . We use \lesssim and big-O, to denote less than, up to a constant factor. We further use $\tilde{O}(\cdot)$ for big-O up to logarithmic factor.

2 Related Works

Graph Bandit. Multiple works have studied graph bandit problems, which can be classified into two categories: graph as structure across arms and graph as data. Most research focuses on the former category, starting from spectral bandit (Kocák et al., 2014; 2020) to graphical bandit (Liu et al., 2018; Yu et al., 2020; Gou et al., 2023; Toni and Frossard, 2023). Within this field, bandit problems with graph feedback have garnered significant attention (Tossou et al., 2017; Dann et al., 2020; Chen et al., 2021; Kong et al., 2022), where learners observe rewards from selected nodes and their neighborhoods. The primary focus of these works have been improving sample efficiency (Bellemare et al., 2019; Waradpande et al., 2020; Idé et al., 2022), with some assuming that payoffs are shared according to the graph Laplacian (Esposito et al., 2022; Lee et al., 2020; Lykouris et al., 2020; Thaker et al., 2022; Yang et al., 2020). While the existing literature primarily aims to optimize over geometrical signal domains, our work focuses on optimization within graph domains. Specifically, we investigate the online graph selection problem, aligning with the second category of research that considers the entire graph as input data. A related recent work (Kassraie et al., 2022) proposed a GNN bandit approach with regret bound based on information gain and an elimination-based algorithm. In contrast, our work explores regret bound based on the effective dimension and builds upon the foundation of Thompson Sampling. This second category of research also encompasses empirical works (Upadhyay et al., 2020; Qi et al., 2022; 2023), particularly those centered around molecule optimization (Wang-Henderson et al., 2023a;b).

Neural Bandit. Our work contributes to the research on neural bandits, where deep neural networks are utilized to estimate the reward function. The work of Zahavy and Mannor (2019); Xu et al. (2020) investigated the Neural Linear bandit, while Zhou et al. (2020) developed Neural Upper Confidence Bound (UCB), an extension of Linear UCB. Zhang et al. (2020) adapted TS with deep neural networks, proposing Neural TS. Dai et al. (2022) makes improvements to neural bandit algorithms to overcome practical limitations. Nguyen-Tang et al. (2021) explores neural bandit in an online contextual bandit setting and (Gu et al., 2024) examines batched learning for neural bandit. Our work can be seen as an extension of Neural TS (Zhang et al., 2020), incorporating significant improvements such as the utilization of graph neural tangent kernel and a distinct definition of effective dimension.

3 Problem Formulation and Methodology

3.1 Graph Action Bandit Problem

We consider an online decision-making problem in which the learner aims to optimize an unknown reward function by sequentially interacting with a stochastic environment. We identify the actions with graphs from an action space \mathcal{G} and assume that the size of this action space, denoted $|\mathcal{G}|$, is finite. At time $t \in [T]$, the learner selects a graph G_t from the action space \mathcal{G} . The learner then observes a noisy reward $r_t = f(G_t) + \epsilon_t$ where $f: \mathcal{G} \rightarrow \mathbb{R}$ is the true (unknown) reward function and $\{\epsilon_t\}_{t \in [T]}$ are i.i.d zero-mean sub-gaussian noise with variance proxy σ^2 . The goal of the learner is to maximize the expected cumulative reward in T rounds, which equivalently entails minimizing the expected (pseudo-)regret denoted as $R_T = \sum_{t=1}^T E[f(G_t^*) - f(G_t)]$ where $G_t^* = \operatorname{argmax}_{G \in \mathcal{G}} f(G)$ represents the optimal graph at time t .

The graph space \mathcal{G} is a finite set of undirected graphs with at most N nodes. Note that the graphs with less than N nodes can be treated by adding auxiliary isolated nodes with no features. We denote an undirected attributed graph with N nodes as $G = (X; A)$, where $X \in \mathbb{R}^{N \times d}$ represents the feature matrix with d features, and $A \in \mathbb{R}^{N \times N}$ is the unweighted adjacency matrix. The rows of X correspond to node features. The size of the node set of a graph G is denoted as $|V(G)| = N$.

Graph action bandit has several applications such as chemical molecules optimization. Consider the graph structures representing the molecules (Weininger, 1988) and rewards are molecular properties. The goal is to sequentially recommend the optimal molecules for experimental testing.

3.2 Graph Neural Network Model

We propose to learn the unknown reward function $r(\cdot)$ by fitting a Graph Neural Network (GNN). We consider a relatively simple GNN architecture where the output of a single graph convolution layer is normalized (to unit ℓ_2 norm) and passed through a multilayer perceptron (MLP). A single-layer graph convolution can be compactly stated as AX using the adjacency matrix A of the network. Additionally, we normalize each row of the resulting matrix to have a unit ℓ_2 norm. Letting $u(x) = \frac{x}{\|x\|_2}$ denote the normalization operator, the aggregated feature of node i in a graph G is $h_i^G = u((AX)_i) = u(\sum_{j \in N_i} X_j)$ where N_j is the neighborhood of node j . Our GNN also consists of an L -layer m -width MLP neural network f_{MLP} which is defined recursively as follows

$$\begin{aligned} f^{(1)}(h_i^G) &= W^{(1)} h_i^G; \quad i \in [N]; \\ f^{(l)}(h_i^G) &= \frac{1}{m} W^{(l)} \text{ReLU}(f^{(l-1)}(h_i^G)); \quad 2 \leq l \leq L; \\ f_{\text{MLP}}(h_i^G; \theta) &= f^{(L)}(h_i^G); \end{aligned} \quad (1)$$

Here, $\text{ReLU}(\cdot) = \max(\cdot, 0)$, $W^{(1)} \in \mathbb{R}^{m \times d}$, $W^{(l)} \in \mathbb{R}^{1 \times m}$, $W^{(l)} \in \mathbb{R}^{m \times m}$ for any $1 < l < L$ are weight matrices of the MLP and $\theta := (W^{(1)}; \dots; W^{(L)}) \in \mathbb{R}^p$ is the collection of parameters of the neural network where $p = dm + (L - 2)m^2 + m$. Our GNN model to estimate the reward function is

$$f_{\text{GNN}}(G; \theta) := \frac{1}{N} \sum_{i=1}^N f_{\text{MLP}}(h_i^G; \theta); \quad (2)$$

The gradient of $\nabla_{\theta} f_{\text{GNN}}(G; \theta)$ denoted as $g(G; \theta) := \nabla_{\theta} f_{\text{GNN}}(G; \theta)$ will play a key role in uncertainty quantification, which will be discussed in Section 3.3. The GNN model (2) is trained by minimizing the mean-squared loss with ℓ_2 penalty, described concretely in (6). A hyperparameter is used to tune the strength of ℓ_2 regularization. For the simplicity of exposition, in the theoretical analysis, we solve the optimization via gradient descent with learning rate η , total number of iterations J and initialize parameters θ_0 such that $f_{\text{GNN}}(G; \theta_0) = 0$ for all $G \in \mathcal{G}$, which can be fulfilled based on the work of Zhou et al. (2020); Kassraie and Krause (2022).

3.3 Graph Neural Thompson Sampling

We adapt Thompson Sampling (TS) for graph exploration, due to its robust performance in balancing exploration against exploitation. Algorithm 1 outlines our proposed GNN Thompson sampling, following the idea of NeuralTS in Zhang et al. (2020). The key step is the sampling of an estimated reward mean $\hat{b}_t(G)$ for each graph G in the action space at time t , from a normal distribution as in equation (4). The mean of the normal distribution in (4) is our current estimate, $f_{\text{GNN}}(G; \theta_{t-1})$, of the true mean reward for graph G (i.e., $r(G)$). This estimate is obtained by fitting the GNN to all the past data as in (6). The variance of the normal distribution $\hat{\Sigma}_t^2(G)$ is our current measure of uncertainty about the true reward of graph G . Note that

$$\hat{\Sigma}_t^2(G) = \frac{1}{m} \text{kg}(G; \theta_{t-1})_{U_{t-1}}^2, \quad \text{where } U_{t-1} = I_p + \frac{1}{m} \sum_{i=1}^{X-1} g(G_i; \theta_{i-1})g(G_i; \theta_{i-1})^\top; \quad (3)$$

Algorithm 1 Graph Neural Thompson Sampling (GNN-TS)

- 1: Input: T, μ, σ, ρ
 - 2: Initialization: $\mu_0, U_0 = I_p$.
 - 3: for $t = 1; \dots; T$ do
 - 4: Compute $\hat{\Sigma}_t(G) := \frac{1}{m} \text{kg}(G; \mu_{t-1}) k_{U_{t-1}}^2$ and sample

$$b_t(G) \sim N(f_{\text{GNN}}(G; \mu_{t-1}); \hat{\Sigma}_t(G)); \text{ for all } G \in \mathcal{G}. \quad (4)$$
 - 5: Select graph $G_t = \text{argmax}_{G \in \mathcal{G}} b_t(G)$, and collect reward $y_t := r(G_t) + \mu_t$.
 - 6: Update uncertainty estimate as

$$U_t = U_{t-1} + g(G_t; \mu_{t-1}) g(G_t; \mu_{t-1})^\top = m. \quad (5)$$
 - 7: Update the parameter estimate as

$$\mu_t = \text{argmin}_{\mu} \frac{1}{2t} \sum_{i=1}^t f_{\text{GNN}}(G_i; \mu) - y_i)^2 + \frac{m}{2} \text{tr}(k_{\mu}^2). \quad (6)$$
 - 8: end for
-

The rationale behind $\hat{\Sigma}_t(G)$ comes from a linear approximation of $f_{\text{GNN}}(G; \mu)$. In particular, the idea is that (6) approximately looks like a linear ridge regression problem, with features $\phi(G; \mu) = \frac{1}{m} \text{kg}(G; \mu)$. The expression (3) is then the familiar estimated covariance matrix from linear bandits after we make this identification. This approximation can be made rigorous via the neural tangent kernel idea, as discussed in Section 4.

The sampled reward mean $b_t(G)$ is the index for decision-making. The learner selects the graph with the highest index, i.e., $G_t = \text{argmax}_{G \in \mathcal{G}} b_t(G)$. The randomness in $b_t(G)$, due to the positive variance of the sampling distribution, is what allows TS to efficiently explore the action space. We want the uncertainty, as captured by $\hat{\Sigma}_t(G)$ not to be too small early on, to allow for effective exploration, but not too large either to miss out on the optimal choice too often. Lemma 5.2 in Section 5 captures the two sides of this trade-off in our theory.

It is worth noting that our proposed Algorithm 1 is not exact TS. In our approach, (4) serves as an approximation to a posterior for mean reward function, rather than a true posterior. The difference between our proposed method and an exact Bayesian method will be smaller if the GNN model is better approximated by a linear model.

Lastly, we note that $b_t(G)$ is also referred to as the perturbed mean reward, as it can be expressed as: $b_t(G) = f_{\text{GNN}}(G; \mu_{t-1}) + \mu_t(G)z$ where $z \sim N(0, 1)$. This perturbed reward includes both the estimated part ($f_{\text{GNN}}(G; \mu_{t-1})$) and the random perturbation part ($\mu_t(G)z$). The use of perturbations for exploration has been shown to be a strong strategy in previous works (Kim and Tewari, 2019; Kveton et al., 2019a). Algorithm 1 can be summarized as greedily selecting the graph with the highest perturbed mean reward.

4 Regret Bound for GNN-TS

Graph Neural Tangent Kernel. Let us briefly review the idea of graph neural tangent kernel (GNTK) (Kassraie et al., 2022) which is based on the neural tangent kernel (NTK) of (Jacot et al., 2018). The tangent kernel on graph space \mathcal{G} , induced by initialization μ_0 , is defined as the inner product of the gradient at initialization, i.e. $k(G; G^0) := g(G; \mu_0)^\top g(G^0; \mu_0)$ for any $G; G^0 \in \mathcal{G}$. The GNTK is the limiting kernel of $k(G; G^0) = m$. We define the finite-width (empirical) and infinite-width GNTK as

$$\hat{k}(G; G^0) := \frac{1}{m} \text{hg}(G; \mu_0); g(G^0; \mu_0)i; \quad k(G; G^0) := \lim_{m \rightarrow \infty} \frac{1}{m} \text{hg}(G; \mu_0); g(G^0; \mu_0)i; \quad (7)$$

We assume the reward function falls within the RKHS corresponding to the GNTK k defined in (7). Define $K \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$ as the GNTK matrix with entries $k(G; G^0)$ for all $G; G^0 \in \mathcal{G}$ and

$\mathbf{r} = (r_{\mathbf{G}})_{\mathbf{G} \in \mathcal{G}}$ as the reward function vector. The kernel matrix \mathbf{K} is positive definite with maximum eigenvalue $\lambda_{\max} := \lambda_{\max}(\mathbf{K})$ and minimum eigenvalue $\lambda_{\min} := \lambda_{\min}(\mathbf{K})$. We also define the finite-width GNTK matrix $\hat{\mathbf{K}} \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$ with entries $\hat{K}(\mathbf{G}; \mathbf{G}^0)$ for all $\mathbf{G}, \mathbf{G}^0 \in \mathcal{G}$ and maximum eigenvalues $\hat{\lambda}_{\max} = \lambda_{\max}(\hat{\mathbf{K}})$. Note that $\hat{\mathbf{K}} \preceq \mathbf{K}$ as $m \leq 1$.

Effective Dimension. We define the effective dimension \mathfrak{d} of the GNTK matrix \mathbf{K} with regularization as

$$\mathfrak{d} := \frac{\log \det(\mathbf{I}_{|\mathcal{G}|} + \mathbf{T} \mathbf{K})}{\log(1 + \mathbf{T} \lambda_{\max})}. \tag{8}$$

This quantity, which appears in our regret bound, measures the actual underlying dimension of the reward function space as seen by the bandit problem (Valko et al., 2013; Bietti and Mairal, 2019). Our definition is adapted from (Yang and Wang, 2020). The key difference is that our \mathfrak{d} does not directly depend on $|\mathcal{G}|$, which is replaced by λ_{\max} , compared to the definition in (Zhang et al., 2020). Our definition is the ratio of the sum over the maximum of the sequence of log-eigenvalues of matrix $\mathbf{I}_{|\mathcal{G}|} + \mathbf{T} \mathbf{K}$. As such, it is a robust measure of matrix rank. In particular, we always have $\mathfrak{d} \leq |\mathcal{G}|$. Moreover, previous work on GNN bandit (Kassraie et al., 2022) utilized the notion of information gain which we replace with the related, but different, notion of effective dimension \mathfrak{d} .

We will make the following assumptions:

Assumption 1 (Bounded RKHS norm for Reward). The reward function \mathbf{r} has R -bounded RKHS norm with respect to a positive definite kernel k : $\|k\|_{\text{RKHS}} = \sqrt{R} > \sqrt{K^{-1}}$.

Assumption 2 (Bounded Reward Differences). Reward differences between any graph in action space are bounded. Formally $\beta_{\mathbf{G}; \mathbf{G}^0} \leq \beta$ for all $\mathbf{G}, \mathbf{G}^0 \in \mathcal{G}$, for some $\beta \leq 1$.

Assumption 3 (Subgaussian Noise) Noise process $\{\epsilon_t\}_{t \in [T]}$ satisfies $E_t[\epsilon_t] = 0$ and $E_t[\epsilon_t^2] \leq \sigma^2$, $\sigma > 0$.

Assumption 1 aligns with the regularity assumption commonly found in the kernelized and neural bandit literature (Srinivas et al., 2009; Chowdhury and Gopalan, 2017; Kassraie and Krause, 2022). Assumption 2 implies that instantaneous regret is bounded: $|r_{\mathbf{G}_t} - r_{\mathbf{G}_t^0}| \leq \beta$ for all $t \in [T]$ and Assumption 3 is the conditional subgaussian assumption for stochastic processes $\{\epsilon_t\}_{t \in [T]}$.

We are now ready to state our main result. Recall that N is the maximum number of (graph) nodes and L the depth of MLP and m its width.

Theorem 4.1. Suppose Assumption 1, 2 and 3 hold. For a fixed horizon $T \geq N$, let

$$m \leq \frac{\log(T)}{\log(2 + \mathbf{T} \lambda_{\max})} \cdot \frac{1}{\beta} \cdot \frac{1}{R} \cdot \frac{1}{\lambda_{\min}} \cdot \log(TLN |\mathcal{G}|)$$

and learning rate $\eta = (\mathbb{C}mL + m)^{-1}$, for some constant \mathbb{C} . Then, the regret of Algorithm 1 is bounded as

$$R_T \leq \mathbb{C} \beta \frac{1}{\mathfrak{d}} \sqrt{\log(T|\mathcal{G}|)} \log(2 + \mathbf{T} \lambda_{\max})$$

for some universal constant $\mathbb{C} > 0$.

The order of regret upper bound in Theorem 4.1, $\mathcal{O}(\mathfrak{d}T^{1/2})$ matches the state-of-the-art regret bounds in the literature of Thompson Sampling (Agrawal and Goyal, 2013; Chowdhury and Gopalan, 2017; Kveton et al., 2020; Zhang et al., 2020). As in (Kassraie et al., 2022), our regret bound is independent of N , indicating that GNN-TSs valid for large graphs. Moreover, for low complexity reward functions of effective dimension $\mathfrak{d} = \mathcal{O}(1)$, the regret scales as $\sqrt{\log|\mathcal{G}|}$ in the size of the action space, showing the robust scalability of GNN-TS.

5 Proof of the Regret Bound

Similar to the previous literature, the key is to obtain probabilistic control on the 'discrepancy' of the policy in GNN-TS. Consider the following events

$$\begin{aligned}
 E_t &:= \left\{ \left| f_{\text{GNN}}(G; t-1) - \min_{G \in \mathcal{G}_t} f_{\text{GNN}}(G; t-1) \right| \leq c_t(G); \text{ for all } G \in \mathcal{G}_t \right\} \\
 E_t &:= \left\{ \left| b_t(G) - \min_{G \in \mathcal{G}_t} b_t(G) \right| \leq c_t(G); \text{ for all } G \in \mathcal{G}_t \right\} \\
 E_t^a &:= \left\{ b_t(G_t) - \min_{G \in \mathcal{G}_t} b_t(G) > \frac{1}{t} \right\}
 \end{aligned}$$

where $c_t(G) := \frac{1}{t} \left(\min_{G \in \mathcal{G}_t} f_{\text{GNN}}(G; t-1) + \frac{1}{t} \right)$ and $c_t(G) := \frac{1}{t} \left(\min_{G \in \mathcal{G}_t} b_t(G) + \frac{1}{t} \right)$ as well as $\frac{1}{t} = \frac{1}{C_0 L^{9/2} m^{1-6p} \log m} t$ and C_0 is some universal constant. Events E_t and E_t control the discrepancies with constants $c_t(G)$ and $c_t(G)$ respectively: $c_t(G)$ is bounding the estimation discrepancy while $c_t(G)$ is bounding the exploration discrepancy. Note that event E_t^a is only for G_t , the optimal graph at round t .

5.1 Estimation Bound (E_t)

The following lemma ensures that event E_t happens with high probability.

Lemma 5.1. Fix $\epsilon \in (0, 1)$. For $m = \text{poly}(R; \frac{1}{\epsilon}; L; jGj; \frac{1}{\epsilon}; \frac{1}{\min}; \log(TLN jGj))$ and $(\epsilon; \frac{1}{\epsilon})$ satisfying conditions of Theorem 4.1, we have $\mathbb{P}(E_t) \geq 1 - \epsilon$.

In other words, given a large enough width of the GNN (m) and a small enough learning rate (ϵ), there is a high probability upper bound for the estimation error $\left| f_{\text{GNN}}(G; t-1) - \min_{G \in \mathcal{G}_t} f_{\text{GNN}}(G; t-1) \right|$. This Lemma 5.1 also gives an approximate upper confidence bound similar to GNN-UCB (Kassraie et al., 2022): $\min_{G \in \mathcal{G}_t} f_{\text{GNN}}(G; t-1) + \frac{1}{t}$. Since $\frac{1}{t}$ is negligible for large m , the approximate upper confidence bound, $\min_{G \in \mathcal{G}_t} f_{\text{GNN}}(G; t-1)$ is used as the index for GNN-UCB. Note that this lemma controls the estimation error produced by GNNs, hence applicable to all GNN bandit algorithms using model (2). Our $c_t(G) = \frac{1}{t} \left(\min_{G \in \mathcal{G}_t} f_{\text{GNN}}(G; t-1) + \frac{1}{t} \right)$ is similar in form to that of Zhang et al. (2020) which is different from the earlier analysis of TS in Agrawal and Goyal (2013).

5.2 Exploration Bound ($E_t; E_t^a$)

We also need event E_t to quantify the level of exploration achieved by the algorithm. Intuitively, E_t ensures our exploration is moderate. On the other hand, indicated by the regret analysis in (Kveton et al., 2019b), instead of controlling the exploration independently, the relation between two sources of explorations needs to be considered because this relation is critical for finding the optimal action. To meet such observation, we define an extra "good" event for anti-concentration on the optimal actions, which is E_t^a . Under event E_t^a , the policy index $b_t(G_t)$ of the optimal graph has the higher future positive exploration, which guides the learner to have higher chance to pick the optimal graph. A formal lemma for exploration discrepancy using TS is given as below:

Lemma 5.2. For GNN-TS for all $t \geq [T]$, we have $\mathbb{P}_t(E_t) \geq 1 - \epsilon$ and $\mathbb{P}(E_t^a) \geq (4e^{-\epsilon})^{-1}$.

Lemma 5.2 shows that GNN-TS has a positive probability of moderate exploration of the optimal arm, which is beneficial to regret reduction.

5.3 Proof of Theorem 4.1

Let $r_t := \left(\min_{G \in \mathcal{G}_t} f_{\text{GNN}}(G; t-1) + \frac{1}{t} \right)$ be the instantaneous regret. We will need two additional lemmas:

Lemma 5.3 (One Step Regret Bound) Assume the same as Theorem 4.1. Suppose $\mathbb{P}_t(E_t^a) \geq \frac{1}{2}$ and $\mathbb{P}_t(E_t) \geq 1 - \epsilon$. Then for any $t \geq [T]$, almost surely,

$$r_t \leq \frac{1}{\mathbb{P}_t(E_t^a)} \left(\frac{1}{\mathbb{P}_t(E_t)} \left(\min_{G \in \mathcal{G}_t} f_{\text{GNN}}(G; t-1) + \frac{1}{t} \right) + 1 \right) + \frac{1}{\mathbb{P}_t(E_t^a)} \left(\min_{G \in \mathcal{G}_t} b_t(G) + \frac{1}{t} \right) + B \mathbb{P}_t(E_t)$$

where $r_t(G) = c_t(G) + c_t(G)$.

Lemma 5.4 (Cumulative Uncertainty Bound) . Assume the same as Theorem 4.1. Then with probability at least $1 - \frac{1}{T}$,

$$\frac{1}{2} \sum_{t=1}^T \min\{1, \frac{1}{t} \sum_{j=1}^m g_t(j)\} \leq 4 \log(1 + \frac{1}{T} \sum_{j=1}^m \max_{t \in [T]} g_t(j)) + 3C \sum_{j=1}^m \bar{g}_j^{1-\frac{2}{m}}$$

where $\bar{g}_j = o(1)$ as $m \rightarrow \infty$ and C is some constant. We always have $\sum_{j=1}^m \bar{g}_j \leq 1$.

Main Proof. The expected cumulative regret is

$$R_T = \sum_{t=1}^T E[\ell_t] = \sum_{t=1}^T E[\ell_t | \mathcal{E}_t] + \sum_{t=1}^T E[\ell_t | \bar{\mathcal{E}}_t]$$

By Lemma 5.1, letting $P(\mathcal{E}_t) = \frac{1}{T}$ and $\ell_t \leq B$, we have the upper bound for the second term

$$\sum_{t=1}^T E[\ell_t | \bar{\mathcal{E}}_t] \leq BT = B$$

Now our focus is controlling the first summation term. By Lemma 5.3, almost surely, we have

$$E_t[\ell_t | \mathcal{E}_t] \leq \frac{1}{P_t(\mathcal{E}_t^a)} \sum_{j=1}^m \frac{1}{P_t(\mathcal{E}_t)} + 1 \sum_{j=1}^m E_t[\ell_t(G_t)] \leq \frac{1}{P_t(\mathcal{E}_t^a)} \sum_{j=1}^m \frac{1}{P_t(\mathcal{E}_t)} + B P_t(\mathcal{E}_t)$$

where $\ell_t(G) = c_t(G) + \frac{1}{t} \sum_{j=1}^m g_t(j)$. Assuming that $t \geq 5$, we have $\frac{1}{t^2} \leq 5e^{-\frac{1}{t}}$. By Lemma 5.2, $P_t(\mathcal{E}_t^a) \geq \frac{1}{4e^{\frac{1}{t}}} = \frac{1}{4e}$. Then, for $t \geq 5$, dropping $\frac{1}{t^2} \sum_{j=1}^m g_t(j)$ from the bound,

$$E_t[\ell_t | \mathcal{E}_t] \leq 194 E_t[\frac{1}{t} \sum_{j=1}^m g_t(j)] + B t^{-2} \leq 194 E_t[\min\{1, \frac{1}{t} \sum_{j=1}^m g_t(j)\}] + t^{-2} B$$

using $40e^{-\frac{1}{t}} + 1 \leq 194$, $\ell_t \leq B$ and $B \leq 1$. Therefore, we have

$$\sum_{t=1}^T E[E_t[\ell_t | \mathcal{E}_t]] \leq 194B \sum_{t=5}^T E[E_t[\min\{1, \frac{1}{t} \sum_{j=1}^m g_t(j)\}]] + 4B + B \tag{9}$$

using $\sum_{t=1}^T t^{-2} \leq 6$. Note that $\frac{1}{t} \sum_{j=1}^m g_t(j) \leq \frac{1}{t} \sum_{j=1}^m \sqrt{8 \log(T^2 j G_j)} + \frac{1}{t} \sum_{j=1}^m \frac{1}{t} \sum_{j=1}^m g_t(j)$ for all $t \in [T]$. Then by Cauchy-Schwarz inequality,

$$\sum_{t=5}^T \min\{1, \frac{1}{t} \sum_{j=1}^m g_t(j)\} \leq \sqrt{\frac{1}{8T \log(T^2 j G_j)}} \sum_{t=5}^T \min\{1, \frac{1}{t} \sum_{j=1}^m g_t(j)\} + T \frac{1}{T} \sum_{j=1}^m \frac{1}{t} \sum_{j=1}^m g_t(j)$$

By Lemma 5.4 and take m sufficiently large such that $3C \sum_{j=1}^m \bar{g}_j^{1-\frac{2}{m}} \leq \frac{1}{T} \sum_{j=1}^m \max_{t \in [T]} g_t(j)$, we have

$$\sum_{t=1}^T E[\min\{1, \frac{1}{t} \sum_{j=1}^m g_t(j)\}] \leq 4 \log(1 + \frac{1}{T} \sum_{j=1}^m \max_{t \in [T]} g_t(j)) + T \frac{1}{T} \sum_{j=1}^m \max_{t \in [T]} g_t(j)$$

Recall that the $\frac{1}{T} \sum_{j=1}^m \max_{t \in [T]} g_t(j) = C_1 T m^{-\frac{1}{6}} \log m$. Take m large enough we have $\frac{1}{T} \sum_{j=1}^m \max_{t \in [T]} g_t(j) \leq \frac{1}{T}$. Then put the above results back into (9), we have:

$$\sum_{t=1}^T E[E_t[\ell_t | \mathcal{E}_t]] \leq 194B \sqrt{\frac{1}{16T \log(TjGj)}} \sum_{t=5}^T \frac{1}{t} \sum_{j=1}^m g_t(j) + \frac{1}{T} \sum_{j=1}^m \max_{t \in [T]} g_t(j) + 4B + B \tag{10}$$

by using $\log(T^2 j G_j) \geq 2 \log(TjGj)$. Therefore, we have our regret bound:

$$R_T \leq CB \sqrt{\frac{1}{dT \log(TjGj)}} \sum_{t=5}^T \frac{1}{t} \sum_{j=1}^m g_t(j) + \frac{1}{T} \sum_{j=1}^m \max_{t \in [T]} g_t(j)$$

for some universal constant C . We have used $\frac{1}{1+x} \leq 1$ and $B \leq 1$, to simplify the bound. Finally, note that $1 + \log(1+x) \leq 2 \log(2+x)$ for all $x \geq 0$. □

Figure 1: Regret over horizon $T = 1000$ for Erdős Rényi random graphs with $p = 0.4$ and $N = 50$ in the first row and random dot product graphs with $N = 50$. Three columns are three types of reward function generation: linear model, Gaussian process with GNTK, Gaussian process with representation kernel. GNN-TSs competitive and robust to different environment settings.

6 Experiments

We create synthetic graph data and generate the rewards through three different mechanisms. For the graph structures, we use random graph models including Erdős Rényi and random dot product graph models. The features are generated i.i.d. from the $\mathcal{N}(0; 1)$. The noisy reward is assumed to have $\sigma = 0.01$. Our experiments investigate GNN-UCB, GNN-PE, NN-UCB, NN-PE and NN-TS as baselines from [Kassraie et al. \(2022\)](#). All performance curves in our empirical studies show an average of over 10 repetitions with a standard deviation of the corresponding bandit algorithm with horizon $T = 1000$. We assume the graph domain is fully observable $G_t = G$ for all $t \in [T]$. Below is a brief overview of the simulation elements. For more details, see [Appendix D](#).

Random Graph. We use two types of random graphs including Erdős Rényi (ER) random graphs and random dot product graphs (RDPG). ER graphs are generated with edge probability p and number of nodes N . RDPGs are generated by modeling the expected edge probabilities as the function of the inner product of features. In the first row of [Figure 1](#), the graphs in G are from the ER model with $p = 0.4$ and in the second row from an RDPG, both of size $N = 50$.

Reward Function. To generate the rewards, we use models of three different types: linear model, Gaussian Process (GP) with GNTK, Gaussian process with the representation kernel. For the linear model, we have $r(G) = \mathbf{h}^G; \mathbf{h}^G$ with true parameter $\mathbf{h} \sim \mathcal{N}(0; I_d)$ and $\mathbf{h}^G = \prod_{i=1}^N h_i^G = N$. For the GP with GNTK, we fit a GP regression model with empirical GNTK matrix $\mathbf{K} \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$ as the covariance matrix of the prior, trained on $f(G; y_G)_{G \in \mathcal{G}}$ where $f y_G$ are i.i.d. from $\mathcal{N}(0; 1)$. For the GP with the representation kernel, we trained a GNN for a graph property prediction task and used the mean pooling over all the nodes of the last layer representations as the graph representation, denoted as $\mathbf{h}_{\text{rep}}^G$. We then define the representation kernel as $k_{\text{rep}}(G; G^0) := \mathbf{h}_{\text{rep}}^G; \mathbf{h}_{\text{rep}}^{G^0}$ and draw (\cdot) from a zero-mean GP with this covariance function (over G).

Algorithms. We investigate two baselines GNN-UCB and GNN-PE along with our proposed GNN-TS. GNN-PE is the proposed state-of-the-art algorithm that selects the graph with the highest uncertainty and eliminates the graph candidates by the upper confidence bounds. All the algorithms in our work use the loss function (6) which is different from previous work. All gradients used for our experiments are $g(G; \mathbf{t})$, not $g(G; \mathbf{0})$, unless otherwise specified. In addition, in order to show the benefit of considering the graph structure, we include NN-UCB, NN-TS and NN-PE as our baselines. For these NN-based algorithms, we ignore the adjacency matrix of a graph (setting $\mathbf{A} = I_N$), and pass through

the model in (1) and (2) with $h_i^G = X_i$. The MLPs in our experiments have $L = 2$ layers and width $m = 512$. We use SGD as the optimizer, with mini-batch size 5, and train for 30 epochs. For the tuning of the hyperparameters (;) and other algorithmic setup, see Appendix D. The matrix inversion in the algorithms is approximated by diagonal inversion across all policy algorithms.

Regret Experiments. In Figure 1, we show the performance of all the algorithms for the six possible environments: ER or RDPG model coupled with either of the three reward models. We set the size of the graph domain to $|G| = 100$ in Figure 1 and we experiment across different $|G|$ in Appendix D. Figure 1 demonstrates that GNN-TS consistently outperforms the baseline algorithms and is robust to all types of random graph models and reward function generations in our experiment. In addition, GNN-based algorithms are clearly better than NN-based algorithms in graph action bandit settings.

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A Proof for Lemmas in Regret Analysis

A.1 Notations

In the following parts, we further define the some notations to represent the linear and kernelized models:

$$\begin{aligned} G_t &= [g(G_1; \theta_0); \dots; g(G_t; \theta_{t-1})] \in \mathbb{R}^{p \times t} \\ \tilde{G}_t &= [g(G_1; \theta_0); \dots; g(G_t; \theta_0)] \in \mathbb{R}^{p \times t} \\ \mathbf{X}_t &= [(G_1); \dots; (G_t)]^\top \in \mathbb{R}^{t \times 1} \\ \mathbf{y}_t &= [y_1; \dots; y_t]^\top \in \mathbb{R}^{t \times 1} \\ \mathbf{u}_t &= [u_1; \dots; u_t]^\top \in \mathbb{R}^{t \times 1} \end{aligned}$$

Then we define the uncertainty estimate with initial gradient θ_0 :

$$\hat{\Sigma}_t(G) = \frac{1}{m} \text{kg}(G; \theta_0) \mathbf{K}_{U_t}^{-1} \quad \text{and} \quad U_t = I_p + \sum_{i=1}^t g(G_i; \theta_0) g(G_i; \theta_0)^\top = m:$$

A.2 Proof of Lemma 5.1

Let us write

$$\mathbf{e}_{t-1} := U_{t-1}^{-1} G_{t-1} \mathbf{y}_{t-1} = m$$

for the ridge regression solution. We will need the following auxiliary lemmas:

Lemma A.1 (Taylor Approximation of a GNN). Suppose learning rate $\eta \in (0, 1)$ for some constant C , then for any fixed $t \in [T]$ and $G \in \mathbb{R}^{p \times p}$, with probability at least $1 - \delta$

$$\|f_{\text{GNN}}(G; \theta_t^{(j)}) - f_{\text{GNN}}(G; \theta_0) - \eta g(G; \theta_0; \theta_t^{(j)})\| \leq C L^3 \frac{R^2 + \eta^2}{m} \sqrt{\frac{2=3p}{m \log(m)}}$$

where C is some constant independent of m and t .

Lemma A.2. Suppose $\eta \in (0, 1)$ and $\log(LN \eta G) \leq \frac{1}{\min\{\eta, 1\}}$ given a fixed $\eta \in (0, 1)$ and learning rate $\eta \in (0, 1)$ for some constant C . For $G \in \mathbb{R}^{p \times p}$ and $t > 1$, with probability at least $1 - \delta$,

$$\| \eta g(G; \theta_0; \theta_{t-1}) - \eta g(G; \theta_0; \theta_{t-1}) \| \leq C \eta (G)$$

where $C = (C_1(2 - m)^J + C_2) \frac{\eta^2 + R^2}{2} (1 + \frac{3 \max}{2})$ with $C_1 = O(1)$ and $C_2 = O(\eta^{-3})$.

Lemma A.3. Fix $\eta \in (0, 1)$ and let $m = \lceil \frac{L^{10} T^4 \eta^6}{\min\{\eta, 1\}} \log(LN \eta G) \rceil$: Then, there exists $\tilde{m} \in \mathbb{R}^p$ with $\frac{\tilde{m}}{k_2} \leq \frac{2R}{2R}$ such that with probability at least $1 - \delta$,

$$\begin{aligned} (G) &= \eta g(G; \theta_0; \theta_i); \quad \text{for all } G \in \mathbb{R}^{p \times p} \\ \log \det(U_t) &= \log \det(I_{jG} + U_t K) + 1: \end{aligned}$$

Lemma A.4. With probability at least $1 - \delta$, we have

$$\| \hat{\Sigma}_t(G) - \hat{\Sigma}_t(G) \| \leq C t^{-1} L^{9=2} (R^2 + \eta^2)^{1=6} m^{-1=6} \sqrt{\frac{p}{\log(m)}}:$$

We choose an arbitrary small $\eta \in (0, 1)$ and set $\eta_i = \eta(5T)$ for $i = 1, \dots, 5$. For all $G \in \mathbb{R}^{p \times p}$, we have

$$\|f_{\text{GNN}}(G; \theta_{t-1}) - (G)\| \leq \underbrace{\|f_{\text{GNN}}(G; \theta_{t-1}) - \eta g(G; \theta_0; \theta_{t-1})\|}_{:= I_1} + \underbrace{\| \eta g(G; \theta_0; \theta_{t-1}) - (G) \|}_{:= I_2}:$$

We then turn to bounding I_1 and I_2 . Throughout the proof, let

$$m := m^{-1=6} \sqrt{\frac{p}{\log(m)}}$$

Bounding I_1 : By Lemma A.1 and Lemma A.2, with probability at least $1 - \epsilon_2$,

$$I_1 = \mathbb{E} \left[\sum_{i,j} \left(f_{\text{GNN}}(G; \mathbf{t}_1) - h(g(G; \mathbf{0}); \mathbf{e}_{\mathbf{t}_1}) \right)_{ij} \right]$$

$$\leq \sum_{i,j} \left(f_{\text{GNN}}(G; \mathbf{t}_1) - h(g(G; \mathbf{0}); \mathbf{t}_1) \right)_{ij} + \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); \mathbf{t}_1) - h(g(G; \mathbf{0}); \mathbf{e}_{\mathbf{t}_1}) \right)_{ij} \right]$$

$$\leq C_0 L^3 m + \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); \mathbf{t}_1) - h(g(G; \mathbf{0}); \mathbf{e}_{\mathbf{t}_1}) \right)_{ij} \right]$$

where $C_0 := C_1 \frac{R^2 + \epsilon^2}{2} \epsilon^{2-3}$ and $C_2 := (C_1(2 - m)^J + C_2 \epsilon^{1-3}) \frac{q}{\epsilon^2 + R^2} (1 + \frac{3}{2} \epsilon_{\max})$ for some constant C_1, C_2 . For $\epsilon < (\frac{\epsilon^2}{2} + R^2)^3 + \epsilon_{\max}$, we have $C_0, C_2 \leq 1$ subject to the constraint in Lemma A.2. Thus, we obtain

$$I_1 \leq L^3 m + \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); \mathbf{t}_1) - h(g(G; \mathbf{0}); \mathbf{e}_{\mathbf{t}_1}) \right)_{ij} \right]$$

Bounding I_2 : By Lemma B.5, with at least probability $1 - \epsilon_3$, for all $G \in \mathcal{G}$, we have

$$I_2 = \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); \mathbf{y}_{\mathbf{t}_1}) - h(g(G; \mathbf{0}); \mathbf{e}_{\mathbf{t}_1}) \right)_{ij} \right]$$

Recall that $\mathbf{y}_{\mathbf{t}_1} = \mathbf{t}_1 + \mathbf{t}_1$ and by Lemma A.3, we have $\mathbf{t}_1 = G_{\mathbf{t}_1}^>$. Then,

$$\mathbf{e}_{\mathbf{t}_1} = U_{\mathbf{t}_1}^{-1} G_{\mathbf{t}_1} G_{\mathbf{t}_1}^> = m + U_{\mathbf{t}_1}^{-1} G_{\mathbf{t}_1} \mathbf{t}_1 = m$$

We have $U_{\mathbf{t}_1} = I_p + G_{\mathbf{t}_1} G_{\mathbf{t}_1}^> = m$. Hence, $U_{\mathbf{t}_1}^{-1} G_{\mathbf{t}_1} G_{\mathbf{t}_1}^> = m = U_{\mathbf{t}_1}^{-1} (U_{\mathbf{t}_1} - I_p) = I_p - U_{\mathbf{t}_1}^{-1}$. This gives

$$\mathbf{e}_{\mathbf{t}_1} = U_{\mathbf{t}_1}^{-1} + \frac{1}{m} U_{\mathbf{t}_1}^{-1} S_{\mathbf{t}_1}$$

where we have defined $S_{\mathbf{t}_1} := \frac{1}{m} G_{\mathbf{t}_1} \mathbf{t}_1$. Thus, we have

$$I_2 = \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1})_{ij} + \frac{1}{m} \sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1} S_{\mathbf{t}_1})_{ij} \right) \right) \right] \tag{10}$$

Recall that $\frac{1}{m} \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1})_{ij} \right) \right] = \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1})_{ij} \right) \right]$. Since $U_{\mathbf{t}_1}^{-1} \leq \frac{1}{4} I_p$, for any vector v , we have $\|v\|_{U_{\mathbf{t}_1}^{-1}} \leq \frac{1}{4} \|v\|$. Then, for the first term in (10), we have

$$\mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1})_{ij} \right) \right] \leq \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1})_{ij} \right) \right]$$

$$\leq \frac{1}{m} \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1})_{ij} \right) \right] \leq \frac{1}{m} \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1})_{ij} \right) \right]$$

where we have used Cauchy-Schwarz inequality for $\| \cdot \|_{U_{\mathbf{t}_1}^{-1}}$ and Lemma A.3. For the second term in (10), we have

$$\frac{1}{m} \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1} S_{\mathbf{t}_1})_{ij} \right) \right] \leq \frac{1}{m} \mathbb{E} \left[\sum_{i,j} \left(h(g(G; \mathbf{0}); U_{\mathbf{t}_1}^{-1} S_{\mathbf{t}_1})_{ij} \right) \right]$$

By Theorem 20.4 of Lattimore and Szepesvári (2020), with probability at least $1 - \epsilon_4$, we have

$$\frac{1}{2} k S_{\mathbf{t}_1} k_{U_{\mathbf{t}_1}^{-1}}^2 \leq 2 \log(1 - \epsilon_4) + \log \deg(\mathbf{t}_1 U_{\mathbf{t}_1}); \text{ for all } \mathbf{t}_2 \in \mathcal{N}$$

By Lemma A.3, with high probability,

$$\log \det(\mathbf{t}_1 U_{\mathbf{t}_1}) \leq \log \det(I_{|G|} + T K) + 1 \leq 2d \log(1 + T \max_{i,j} K_{ij})$$

Using ϵ_{\max} , we have $\log \det(\mathbf{t}_1 U_{\mathbf{t}_1}) \leq d \log(T) + 1 \leq d \log(T)$. We also have $\log(1 - \epsilon_4) = \log(5T) - \log(T) - d \log(T)$.

Putting the pieces together, we have

$$\frac{1}{m} \mathbb{E} [jg(G; \theta) > U_{t-1} S_{t-1} j] \leq \frac{q}{d \log T} \mathbb{E} [t(G)]:$$

Combining with the first term, we obtain

$$I_2 \leq \frac{q}{d \log T} + \frac{p}{R} \mathbb{E} [t(G)]:$$

Combining with the bound on I_1 , we have

$$\begin{aligned} |f_{\text{GNN}}(G; t-1) - (G)| &\leq L^3 m + 1 + \frac{q}{d \log T} + \frac{p}{R} \mathbb{E} [t(G)] \\ &=: L^3 m + t(G) \end{aligned}$$

where we have set $t := 1 + \frac{p}{d \log T} + \frac{p}{R}$ for simplicity.

By Lemma A.4, with probability at least $1 - \delta$,

$$t(G) \leq t(G) \leq Ct L^{9=2} \frac{R^2 + \frac{2}{m}}{1=6} \cdot t L^{9=2} m$$

using the assumption $R^2 + \frac{2}{m}$. We obtain

$$\begin{aligned} |f_{\text{GNN}}(G; t-1) - (G)| &\leq L^3 m + t L^{9=2} m + t(G) \\ &\leq 2t L^{9=2} m + t(G) \end{aligned}$$

since $t \geq 1$ and $t \geq 1$. Taking $t \geq 1$ finishes the proof.

A.3 Proof of Lemma 5.2

Proof of Lemma 5.2. Conditioned on F_t , we have

$$b_t(G) | F_t \sim N(f_{\text{GNN}}(G; t-1); \frac{2}{t} \mathbb{E} [t(G)]):$$

Using standard Gaussian tail bound, followed by a union bound gives

$$P_t(|b_t(G) - f_{\text{GNN}}(G; t-1)| \geq t(G) u) \leq jG_t j e^{-u^2=2}$$

which shows the first assertion by letting $u = \frac{p}{2 \log(t^2 jG_t j)}$.

For the second assertion, it is enough to note that $P(Z \geq 1) \leq (4e^{-p})^{-1}$ for $Z \sim N(0; 1)$. \square

A.4 Proof of Lemma 5.3

Proof of Lemma 5.3. Our proof is inspired from the proof in Wu et al. (2022). Recall that $c_t(G) = \frac{1}{t} \mathbb{E} [t(G) + \epsilon(t; m)]$ and $c_t(G) := \frac{1}{t} \mathbb{E} [t(G) + \frac{2}{2 \log(t^2 jG_t j)}]$ and

$$\begin{aligned} E_t &= \{G \mid |f_{\text{GNN}}(G; t-1) - (G)| \leq c_t(G)g\} \\ E_t &= \{G \mid |b_t(G) - f_{\text{GNN}}(G; t-1)| \leq c_t(G)g\} \end{aligned}$$

Let $t(G) = c_t(G) + c_t(G)$ and $c_t(G) = \frac{1}{t} \mathbb{E} [t(G) + \epsilon(t; m)]$. Then, on $E_t \setminus E_t^a$, by triangle inequality,

$$|b_t(G) - (G)| \leq t(G) \tag{11}$$

We also recall that $E_t^a := \{G \mid |b_t(G) - f_{\text{GNN}}(G; t-1)| > \frac{1}{t} \mathbb{E} [t(G)]g\}$. Then, on $E_t \setminus E_t^a$, we have

$$\begin{aligned} b_t(G) &> f_{\text{GNN}}(G; t-1) + \frac{1}{t} \mathbb{E} [t(G)]g \\ &= (G) - c_t(G) + \frac{1}{t} \mathbb{E} [t(G)]g \\ &= (G) - \epsilon(t; m) \end{aligned} \tag{12}$$

Recall that $U_t := \{G_t\} \cup \{G_t\}$ for convenience. Consider the set of unsaturated actions

$$U_t = \{G \in \mathcal{G} : c_t(G) < c_t(G_t) + \alpha_t(G)\}$$

and let G_t be the least uncertain unsaturated action at time t :

$$G_t := \operatorname{argmin}_{G \in U_t} c_t(G)$$

By $G_t \in U_t$, we have $c_t(G_t) < c_t(G_t) + \alpha_t(G_t) = c_t(G_t)$: Applying (11), twice, on $E_t \setminus E_{t-1}$, we have

$$\begin{aligned} c_t(G_t) &\leq c_t(G_t) + \alpha_t(G_t) + \alpha_t(G_t) + b_t(G_t) - b_t(G_t) \\ &\leq c_t(G) + \alpha_t(G) + \alpha_t(G_t) \end{aligned}$$

for all $G \in U_t$ where the second inequality follows since G_t maximizes $b_t(\cdot)$ over \mathcal{G} , by design.

Recall that $E_t[\cdot] = E[\cdot | F_t]$, where F_t is the history up to (but not including) time t . Given F_t , the event E_t is deterministic while E_{t-1} is only random due to the independent randomness in the sampling step (4). Next, we have

$$\begin{aligned} E_t[c_t(G_t) | E_{t-1}] &= I_{E_t} E_t[c_t(G_t)] \\ &= I_{E_t} (E_t[c_t(G_t) | E_{t-1}] + E_t[\alpha_t(G_t) | E_{t-1}]) \\ &= I_{E_t} (E_t[c_t(G_t) | E_{t-1}] + B P_t(E_{t-1})) \end{aligned} \tag{13}$$

using the boundedness Assumption 2. Here, we are using the fact that α_t is measurable w.r.t. F_t , hence it is deterministic conditioned on F_t . Due to factor I_{E_t} in the above, the bound is trivial when E_t fails, so for the rest of the proof we assume that E_t holds (conditioned on F_t).

We have

$$\begin{aligned} E_t[c_t(G_t) | E_{t-1}] &\leq c_t(G_t) + \alpha_t(G_t) + E_t[\alpha_t(G_t) | E_{t-1}] \\ &\leq 2\alpha_t(G_t) + \alpha_t(G_t) + E_t[\alpha_t(G_t) | E_{t-1}] \end{aligned}$$

where we have used the definition of $\alpha_t(\cdot)$ and dropped the indicator I_{E_t} to get a further upper bound. It remains to bound $\alpha_t(G_t)$ in terms of $\alpha_t(G_t)$.

Since G_t is the least uncertain unsaturated action, we have

$$\alpha_t(G_t) \leq \alpha_t(G_t)$$

Multiplying both sides by I_{E_t} , taking $E_t[\cdot]$, and rearranging

$$\alpha_t(G_t) \leq \frac{E_t[\alpha_t(G_t) | E_{t-1}]}{P_t(\{G \in U_t \setminus E_{t-1}\})} \leq \frac{E_t[\alpha_t(G_t)]}{P_t(\{G \in U_t \setminus E_{t-1}\})}$$

It remains to bound the denominator.

Recall that G_t maximizes $b_t(\cdot)$ over the entire \mathcal{G} . Thus, if

$$b_t(G_t) > \max_{G \in U_t} b_t(G) \tag{14}$$

then G_t cannot belong to U_t , hence $G_t \in U_t$. On $E_t \setminus E_{t-1}$, for any $G \in U_t$, we have

$$\begin{aligned} b_t(G) &\leq c_t(G) + \alpha_t(G) - \alpha_t(G_t) \\ &\leq c_t(G) + \alpha_t(G) - \alpha_t(G_t) \end{aligned}$$

where the second inequality is by the definition of U_t . Then for (14) to hold on $E_t \setminus E_t^a$, it is enough to have $b_t(G_t) > \beta(t; m)$. But this holds on $E_t \setminus E_t^a$ by (12). That is,

$$\begin{aligned} E_t^a \setminus E_t \setminus E_t & \text{ f } b_t(G_t) > \beta(t; m) g \setminus E_t \setminus E_t \\ & \text{ f } b_t(G_t) > \max_{G \in U_t} b(G) g \setminus E_t \setminus E_t \\ & \text{ f } G_t \in U_t g \setminus E_t \setminus E_t : \end{aligned}$$

Assuming as before that E_t holds, we have

$$P_t(E_t^a \setminus E_t) = P_t(\text{f } G_t \in U_t g \setminus E_t):$$

We have $P_t(E_t^a \setminus E_t) = P_t(E_t^a) - P_t(E_t)$. Putting the pieces together

$$q_t(G_t) = \frac{E_t[\beta_t(G_t)]}{P_t(E_t^a) - P_t(E_t)}$$

and we obtain

$$E_t[\beta_t | E_t] \leq \frac{2}{P_t(E_t^a) - P_t(E_t)} + 1 \cdot E_t[\beta_t(G_t)] \quad \beta(t; m)$$

Combining with (13) the result follows. □

A.5 Proof of Lemma 5.4

Proof of Lemma 5.4. For simplicity, we define

$$g_t := \frac{1}{m} g(G_t; t-1); \quad g_t := \frac{1}{m} g(G_t; 0):$$

Then, recall that

$$\beta_t^2(G_t) = k g_t k_{U_{t-1}}^2; \quad U_t = I_p + \sum_{i=1}^{X-1} g_t g_t^>$$

Note that $U_t = U_{t-1} + g_t g_t^>$.

Then we introduce following Lemmas:

Lemma A.5 (Elliptical Potential). Assume that $U_t = U_{t-1} + g_t g_t^>$ for all $t \in [T]$. Then,

$$\sum_{t=1}^{X-1} \min\{1; k g_t k_{U_{t-1}}^2\} \geq 2 \log \frac{\det U_T}{\det U_0} :$$

Lemma A.6. Let $A = [a_1 \ a_2 \ \dots \ a_n]$ and $A = [a_1 \ a_2 \ \dots \ a_n]$ be $p \times n$ matrices, with columns $f a_i g$ and $f a_i g$, respectively. Assume that for $\epsilon \in (0, C]$, we have

$$k a_i - a_i k \leq \epsilon; \quad k a_i k \leq C$$

for all i . Then,

$$\begin{aligned} \log \det(I_p + A A^>) & \leq \log \det(I_p + A A^>) + p \log(1 + 3Cn) \\ \log \det(I_p + A A^>) & \leq \log \det(I_n + A^> A) + 3Cn^{3-2n} \end{aligned}$$

By Lemma A.5, we have

$$\frac{1}{2} \sum_{t=1}^{X-1} \min\{1; \beta_t^2(G_t)\} \geq \log \frac{\det U_T}{\det U_0} = \log \det(I_p^{-1} U_T) = \log \det(V_T)$$

using $\det(U_0) = \det(I_p) = 1$, and defining $V_t := U_t^{-1}$.

Let $G = \{G^j : j \in [G]\}$ be the collection of all the graphs and $n_j(t)$ be the number of graphs which are equal to G^j in our selection of graphs up to and including time t , i.e. $n_j(t) := \sum_{i=1}^t \mathbb{1}_{G_i = G^j}$. Let

$$c_j := \frac{1}{m} g(G^j; t-1); \quad d_j := \frac{1}{m} g(G^j; 0)$$

and let C and D be the corresponding $j \times j$ matrices with the above columns. Then, we have

$$\sum_{i=1}^T g_i g_i^T = \sum_{j=1}^{|G|} n_j(T) c_j c_j^T = D^{-1} > T^{-1} >$$

where $D \in \mathbb{R}^{j \times j}$ is the diagonal matrix with diagonal elements $n_j(T) c_j c_j^T$ and the last inequality due to $n_j(T) \geq T$ for all $j \in [G]$.

Note that $V_T = I_p + \sum_{i=1}^T g_i g_i^T$, hence

$$\log \det(V_T) = \log \det(I_p + \sum_{i=1}^T g_i g_i^T);$$

By Lemma C.7, $x \in (0, 1)$, we have the following bound for $k_j k_2$ and $k_j \leq k_2$, with probability at least $1 - \epsilon$,

$$k_j k_2 \leq \frac{1}{N} \sum_{i \in V(G^j)} k_{MLP}(h_i^{G^j}; t-1) \leq \bar{m} k_2 + C$$

$$k_j \leq k_2 \leq \frac{1}{N} \sum_{i \in V(G^j)} k_{MLP}(h_i^{G^j}; t-1) \leq \bar{m} g_{MLP}(h_i^{G^j}; 0) \leq \bar{m} k_2 + \epsilon_m$$

where $\epsilon_m = o(1)$ as $m \rightarrow \infty$ and C is $C_7 \bar{L}$ in Lemma C.7.

Then, applying Lemma A.6 with $n = |G|$, $A = \sum_{j=1}^{|G|} c_j c_j^T$, $A = \sum_{j=1}^{|G|} d_j d_j^T$ and ϵ replaced with ϵ_m , we obtain

$$\log \det(V_T) = \log \det(I_{|G|} + \sum_{j=1}^{|G|} c_j c_j^T) + 3C |G|^{3/2} \bar{L}^{-1} \epsilon_m$$

Recall $\hat{K} = \sum_{j=1}^{|G|} c_j c_j^T$ and $\hat{\Lambda}_{\max} = \lambda_{\max}(\hat{K})$ and note that \hat{K} is the nite-width GNTK matrix. By Lemma B.6, with high probability, $\hat{\Lambda}_{\max} \leq \lambda_{\max} + \epsilon_m$ and note that $\epsilon_m = O(m^{-1/4})$. Dropping ϵ_m by large enough m , we have

$$\log \det(I_{|G|} + \sum_{j=1}^{|G|} c_j c_j^T) \geq |G| \log(1 + \hat{\Lambda}_{\max}^{-1});$$

Putting the pieces together with the definition of effective dimension d in (8) finishes the proof. \square

A.6 Proof of Lemma A.5

Proof of Lemma A.5. Since $\min\{1, x\} \geq 2 \log(1+x)$ for $x \geq 0$, we have

$$\sum_{t=1}^T \min\{1, k_t k_{U_{t-1}}^2\} \geq 2 \sum_{t=1}^T \log(1 + k_t k_{U_{t-1}}^2)$$

$$= 2 \sum_{t=1}^T \log \frac{\det U_t}{\det U_{t-1}} = 2 \log \frac{\det U_T}{\det U_0}$$

where the first equality follows from $\det(A + vv^T) = \det(A)(1 + v^T A^{-1}v)$, obtained by an application of Sylvester's determinant identity: $\det(I + AB) = \det(I + BA)$. \square

A.7 Proof of Lemma A.6

Proof of Lemma A.6. Note that

$$\begin{aligned} k a_i a_i^\top - a_i a_i^\top k_{\text{op}} &= k a_i (a_i - a_i)^\top + (a_i - a_i) a_i^\top k_{\text{op}} \\ &= (k a_i k + k a_i k) k a_i - a_i k \leq (2C + \epsilon) \epsilon \leq 3C \epsilon \end{aligned}$$

Let $V = I_p + A A^\top$ and $V = I_p + A A^\top$. We have

$$kV - V k_{\text{op}} = \sum_{i=1}^X k a_i a_i^\top - a_i a_i^\top k_{\text{op}} \leq n \cdot 3C \epsilon$$

Write $\lambda_i(V)$ for the i th eigenvalue of matrix V . By Weyl's inequality $|\lambda_j(V) - \lambda_i(V)| \leq 3C \epsilon$. Then,

$$\begin{aligned} \log \det(V) &= \sum_{i=1}^X \log \lambda_i(V) = \sum_{i=1}^X \log \lambda_i(V) + 3C \epsilon n \\ &= \sum_{i=1}^X \log(\lambda_i(V)) + \sum_{i=1}^X \log \left(1 + \frac{3C \epsilon n}{\lambda_i(V)} \right) \\ &= \log \det(V) + p \log(1 + 3C \epsilon n) \end{aligned}$$

using $\lambda_i(V) \geq 1$. This proves one of the bounds.

For the second bound, let $W = I_n + A^\top A$ and $W = I_n + A^\top A$. Then, then by concavity of the $X \mapsto \log \det(X)$ and the fact that its derivative is X^{-1} over symmetric matrices, we have

$$\log \det(X + \epsilon) - \log \det(X) \leq \text{tr}(X^{-1} \epsilon) \leq k X^{-1} k_F k \epsilon k_F$$

Let $\epsilon = W - W$. We have $\epsilon_{ij} = |h_{a_i} - h_{a_j}| \leq 3C \epsilon$, hence $k \epsilon k_F \leq 3C \epsilon n$. Then,

$$\begin{aligned} \log \det(V) - \log \det(W) &\stackrel{(a)}{\leq} \log \det(W) - \log \det(W) \\ &\leq \text{tr}(W^{-1} \epsilon) \\ &\leq p \overline{n} k W^{-1} k_{\text{op}} k \epsilon k_F \stackrel{(b)}{\leq} p \overline{n} \cdot 3C \epsilon n \end{aligned}$$

where (a) is by Sylvester's identity and (b) uses the fact that $W \succeq I_n$, hence $W^{-1} \preceq I_n$ giving $k W^{-1} k_{\text{op}} \leq 1$. \square

B Technical Lemmas

In this Section, we provide the Proof for Lemmas in Appendix A and other Technical Lemmas supporting the proofs. Most technical Lemmas are related to NTK and optimization in deep learning theory, mainly modified from the GNN helper Lemmas in (Kassraie et al., 2022) and technical Lemmas in Zhou et al. (2020); Vakili et al. (2021).

B.1 Notations for MLP

Recall our GNN with one layer of linear graph convolution and a MLP:

$$\begin{aligned} f^{(1)}(h_i^G) &= W^{(1)} h_i^G; \quad i \in [N]; \\ f^{(l)}(h_i^G) &= \frac{1}{m} W^{(l)} \text{ReLU}(f^{(l-1)}(h_i^G)); \quad 2 \leq l \leq L; \\ f_{\text{MLP}}(h_i^G; \cdot) &= f^{(L)}(h_i^G) \\ f_{\text{GNN}}(G; \cdot) &= \frac{1}{N} \sum_{i=1}^N f_{\text{MLP}}(h_i^G; \cdot); \end{aligned}$$

We denote the gradients for GNN and associated MLP as

$$g(G; \cdot) := \nabla_{\theta} f_{\text{GNN}}(G; \cdot)$$

$$g_{\text{MLP}}(\cdot; \cdot) := \nabla_{\theta} f_{\text{MLP}}(\cdot; \cdot)$$

and the connection between gradients for the MLP and the gradient for the whole GNN is

$$g(G; \cdot) = \frac{1}{N} \sum_{i=1}^N g_{\text{MLP}}(h_i^G; \cdot)$$

Similarly, we define a tangent kernel for the a MLP as

$$k_{\text{MLP}}(x; x^0) := g_{\text{MLP}}(G; x)^{\top} g_{\text{MLP}}(G^0; x^0)$$

for any MLP inputs x, x^0 and the associated neural tangent kernel $k_{\text{MLP}}(x; x^0)$ is defined as limiting kernel of $k_{\text{MLP}}(x; x^0) = m$:

$$k_{\text{MLP}}(x; x^0) := \lim_{m \rightarrow \infty} k_{\text{MLP}}(x; x^0) = m$$

By the connection between f_{GNN} and f_{MLP} , we have

$$k(G; G^0) = \frac{1}{N^2} \sum_{i, j} k_{\text{MLP}}(h_i^G; h_j^{G^0}):$$

B.2 Proof for Lemmas in Appendix A

Proof of Lemma A.1. By Lemma C.7, with probability at least $1 - \epsilon$ (0; 1)

$$\begin{aligned} |f_{\text{GNN}}(G; \cdot^{(j)}) - f_{\text{GNN}}(G; \cdot^0) - \langle g(G; \cdot^0); \cdot^{(j)} - \cdot^0 \rangle| & \\ \leq \frac{1}{N} \sum_{j=1}^N |f_{\text{MLP}}(h_j^G; \cdot^{(j)}) - f_{\text{MLP}}(h_j^G; \cdot^0) - \langle g_{\text{MLP}}(h_j^G; \cdot^0); \cdot^{(j)} - \cdot^0 \rangle| & \\ \leq C_1 \frac{L^{4+3} \rho^{3p}}{m \log(m)} & \\ \leq C_1 \frac{\rho^p}{(R^2 + \rho^2)^{2+3p}} \frac{L^{4+3} \rho^{3p}}{m \log(m)} & \end{aligned}$$

where the last inequality is from the choice of $\rho = \frac{\epsilon^p}{(R^2 + \rho^2)^{2+3p}}$ such that $k(\cdot^{(j)}; \cdot^0) \leq \epsilon$. Since $\rho / (1 + \rho) \geq \frac{\epsilon}{2}$, it can be verified that technical condition (23) in Lemma C.7 is satisfied when m is large. Therefore, set $C_2 = C_1 \epsilon^{4+3}$,

$$|f_{\text{GNN}}(G; \cdot^{(j)}) - f_{\text{GNN}}(G; \cdot^0) - \langle g(G; \cdot^0); \cdot^{(j)} - \cdot^0 \rangle| \leq C_2 L^3 \left(\frac{R^2 + \rho^2}{m}\right)^{2+3p} \frac{\rho^{3p}}{m \log(m)}:$$

□

Proof of Lemma A.2. In this proof, set $\epsilon_1 = \epsilon_2 = \epsilon/2$ where $\epsilon/2$ (0; 1) is an arbitrary small real value. We introduce $\tilde{g}_t^{(j)} = \tilde{g}_t^{(j)}$ be the gradient descent update sequence of the following proximal optimization (Kassraie et al., 2022):

$$\min_{\theta} \frac{1}{2t} \sum_{i=1}^t (\langle g(G_i; \cdot^0); \theta - y_i \rangle)^2 + \frac{m}{2} \|\theta\|_2^2$$

and $\tilde{g}_t^{(j)} = \tilde{g}_t^{(j)}$ be the gradient descent update sequence of parameters of our primary optimization (6). In GNN training step in algorithms, we let $\tilde{g}_t := \tilde{g}_t^{(j)}$. Recall that $U_t = I + G_t G_t^{\top} = m$. By

Lemma B.5, with probability at least $1 - \frac{1}{2} (0; 1)$, $U_t \leq 4 \left(1 + \frac{3}{2} \max\right) l$. Therefore,

$$\begin{aligned} \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} G_t y_t = m \mathbb{E} g(G; 0) U_t^{-1} k_t \right) &\geq \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t \right) \\ &\geq \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t \right) \\ &\geq \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t \right) \\ &\geq \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t \right) \end{aligned}$$

By Lemma B.3 and Lemma B.1, with probability at least $1 - \frac{1}{2} (0; 1)$, for some constants C_1 and C_2 , we have

$$\begin{aligned} \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} G_t y_t = m \mathbb{E} g(G; 0) U_t^{-1} k_t \right) &\geq \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t \right) \\ &\geq \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t \right) \\ &\geq \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t \right) \\ &= \mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t \right) \end{aligned}$$

The last equality is obtained from the definition of $\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} G_t y_t$, which is $\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t = \frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t$. Now we let $C = \frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t$. Note that this constant $C = O(1)$ with respect to m since $\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t = O(m^{-1})$. Then we have the desired result:

$$\mathbb{P} \left(\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} G_t y_t = m \mathbb{E} g(G; 0) U_t^{-1} k_t \right) \geq C \frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t$$

where $C = (C_1(2 - m)^J + C_2) \frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t$ with $C_1 = O(1)$ and $C_2 = O(m^{-3})$. □

Proof of Lemma A.3. See Appendix B.4. □

Proof of Lemma A.4. Define function ϕ for vectors $f, v; a_1, \dots, a_{t-1}$ as followed:

$$\phi(v; a_1, \dots, a_{t-1}) := \frac{1}{\sqrt{v^T \left(I + \sum_{i=1}^{t-1} a_i a_i^T \right) v}}$$

and denote the gradients for ϕ as

$$\begin{aligned} r_0 &:= r_v \phi(v; a_1, \dots, a_{t-1}) \\ r_i &:= r_{a_i} \phi(v; a_1, \dots, a_{t-1}); \quad 8i \in [t-1] \end{aligned}$$

By setting $A = \left(I + \sum_{i=1}^{t-1} a_i a_i^T \right)^{-1/2}$ with eigendecomposition $A = V D V^T$. The gradients are bounded as followed

$$\begin{aligned} \|r_0\|_2 &= \frac{\|A v\|_2}{\sqrt{v^T A v}} = \frac{\sqrt{\lambda_{\min}(A)}}{\sqrt{\lambda_{\max}(A)}} \leq 1 \\ \|r_i\|_2 &= \frac{\|A v v^T A a_i\|_2}{\sqrt{v^T A v}} \leq \|a_i\|_2 \frac{\sqrt{\lambda_{\max}(A)}}{\sqrt{\lambda_{\min}(A)}} \leq \|a_i\|_2 \sqrt{\lambda_{\max}(A)} \end{aligned} \tag{15}$$

We can express $\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} G_t y_t$ and $\frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t$ by

$$\begin{aligned} \frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} G_t y_t &= \left(\frac{g(G; 0)}{m}, \frac{g(G; 1)}{m}, \dots, \frac{g(G; t-1)}{m} \right) \\ \frac{1}{m} \sum_{i=1}^m g(G; 0) U_t^{-1} k_t &= \left(\frac{g(G; 0)}{m}, \frac{g(G; 1)}{m}, \dots, \frac{g(G; t-1)}{m} \right) \end{aligned}$$

From Lemma C.7, there exists positive constants such that the gradients and gradient differences are bounded with high probability, which indicates for some constant C_1 with probability greater than $1 - \frac{\epsilon}{2}$,

$$\|g(G; \cdot)\|_2 = k \frac{1}{N} \sum_{j \in \mathcal{V}(G)} g_{MLP}(h_j^G; \cdot) \|k_2\| \leq C_1 \frac{p}{mL} \quad (16)$$

Note that \mathcal{G}_t is Lipschitz continuous, then with high probability, we have

$$\begin{aligned} \| \mathcal{G}_t(G; \cdot) - \mathcal{G}_t(G; \cdot) \| &= \left\| \left(\frac{g(G; \cdot; t-1)}{p \frac{m}{m}}; \frac{g(G_{1; \cdot}); t-1}{p \frac{m}{m}}; \dots; \frac{g(G_{t-1; \cdot}); t-1}{p \frac{m}{m}} \right) - \left(\frac{g(G; \cdot; 0)}{p \frac{m}{m}}; \frac{g(G_{1; \cdot}); 0}{p \frac{m}{m}}; \dots; \frac{g(G_{t-1; \cdot}); 0}{p \frac{m}{m}} \right) \right\| \\ &\leq \sup_{\|k\|_0 \leq k_2} \left\| k \frac{g(G; \cdot; t-1)}{p \frac{m}{m}} - \frac{g(G; \cdot; 0)}{p \frac{m}{m}} \right\|_2 + \sum_{i=1}^{X-1} \sup_{\|k\|_i \leq k_2} \left\| k \frac{g(G_i; \cdot; i)}{p \frac{m}{m}} - \frac{g(G_i; \cdot; 0)}{p \frac{m}{m}} \right\|_2 \\ &\leq \frac{1}{p} \left\| k \frac{g(G; \cdot; t-1)}{p \frac{m}{m}} - \frac{g(G; \cdot; 0)}{p \frac{m}{m}} \right\|_2 + \frac{C_1^2 L}{m} \sum_{i=1}^{X-1} \left\| k \frac{g(G_i; \cdot; i)}{p \frac{m}{m}} - \frac{g(G_i; \cdot; 0)}{p \frac{m}{m}} \right\|_2 \text{ (by (15) and (16))} \\ &\leq C_2 \frac{p}{\log(m)} \frac{1}{m} \leq 3L^3 \|k(G; \cdot; 0)\|_2 = \frac{p}{m} \left(\frac{1}{p} + \frac{C_1^2 L t}{m} \right) \text{ (by Lemma C.7)} \\ &\leq C_1 C_2 \frac{p}{\log(m)} \frac{1}{m} \leq 3L^7 \left(\frac{1}{p} + \frac{C_1^2 L t}{m} \right) \text{ (by (16))} \end{aligned}$$

Therefore, if $C_1^4 L^2 t^2$ and let $\epsilon = C \frac{q}{m^{R^2 + \frac{2}{\epsilon}}}$, $C_3 = 2C C_2 C_1^3$,

$$\| \mathcal{G}_t(G; \cdot) - \mathcal{G}_t(G; \cdot) \| \leq C_3 t^{-7} L^9 \frac{1}{m} \left(R^2 + \frac{2}{\epsilon} \right)^{1+6} m^{-1} \frac{p}{\log(m)}$$

□

B.3 Lemmas for GNN training

Lemma B.1 (Parameter Bound for Primary Optimization). Let $f_t^{(j)} g_{j=1}^J$ be the gradient descent update sequence of parameters of the optimization (6) which is,

$$\min \frac{1}{2t} \sum_{i=1}^X (f_{GNN}(G_i; \cdot) - y_i)^2 + \frac{m}{2} \|k\|_2^2$$

then if $m \geq \text{poly}(R; \epsilon; L; \frac{1}{\epsilon}; \log(\frac{N}{\epsilon}))$ and learning rate $\frac{1}{m} (CmL + m)^{-1}$ for some constant C . Then for a constant $C = O(\frac{1}{\epsilon^3})$ which is independent of m and t , with probability at least $1 - \frac{\epsilon}{2}$

$$\|k_t^{(j)} - \tilde{k}_t^{(j)}\|_2 \leq C \frac{R^2 + \frac{2}{\epsilon}}{m}$$

where $f_t^{(j)} g_{j=1}^J$ be the gradient descent update sequence of parameters of the proximal optimization with loss function $\frac{1}{2t} \sum_{i=1}^X (\mathcal{G}_t(G_i; \cdot); \cdot)_i - y_i)^2 + \frac{m}{2} \|k\|_2^2$. Both optimization have the same initialization at $\tilde{k}_t^{(0)} = k_t^{(0)} = 0$ and same learning rate $\frac{1}{m}$.

Proof. In this proof, set $\epsilon_1 = \epsilon_2 = \frac{\epsilon}{2}$ where $\epsilon \in (0; 1)$ is an arbitrary small real value. Define $G_t^{(j)} := [g(G_1; \cdot; t^{(j)}); \dots; g(G_t; \cdot; t^{(j)})] \in \mathbb{R}^{p \times t}$ as the j -th updates in our primary optimization with loss (6) at round t . Also define $f_{gnn;t}^{(j)} := [f_{GNN}(G_1; \cdot; t^{(j)}); \dots; f_{GNN}(G_t; \cdot; t^{(j)})] \in \mathbb{R}^t$. The gradient descent updates for sequences $f_t^{(j)} g_{j=1}^J$ and $\tilde{f}_t^{(j)} g_{j=1}^J$ are

$$\begin{aligned} f_{t+1}^{(j)} &= f_t^{(j)} - \frac{1}{t} [G_t^{(j)}]^T (f_{gnn;t}^{(j)} - y_t) + m^{-1} f_t^{(j)} \\ \tilde{f}_{t+1}^{(j)} &= \tilde{f}_t^{(j)} - \frac{1}{t} G_t^{(j)} (G_t(\tilde{f}_t^{(j)} - 0) - y_t) + m^{-1} \tilde{f}_t^{(j)} \end{aligned}$$

Therefore,

$$\begin{aligned}
 & k_t^{(j+1)} - \tilde{k}_t^{(j+1)} k_2 \\
 = & k(1 - m) \left(k_t^{(j)} - \tilde{k}_t^{(j)} \right) \frac{1}{t} [G_t^{(j)}]^> (f_{\text{gnn};t}^{(j)} - y_t) + \frac{1}{t} G_t^{>} (G_t(\tilde{k}_t^{(j)} - 0) - y_t) k_2 \\
 = & k(1 - m) \left(k_t^{(j)} - \tilde{k}_t^{(j)} \right) \frac{1}{t} (G_t^{(j)} - G_t)^> (f_{\text{gnn};t}^{(j)} - y_t) - \frac{1}{t} G_t^{>} (f_{\text{gnn};t}^{(j)} - G_t(\tilde{k}_t^{(j)} - 0)) k_2 \\
 = & k(1 - m) \left(k_t^{(j)} - \tilde{k}_t^{(j)} \right) \frac{1}{t} (G_t^{(j)} - G_t)^> (f_{\text{gnn};t}^{(j)} - y_t) - \frac{1}{t} G_t^{>} (f_{\text{gnn};t}^{(j)} - G_t(\tilde{k}_t^{(j)} - 0) + G_t(\tilde{k}_t^{(j)} - k_t^{(j)})) k_2 \\
 = & k \left((1 - m) \mathbb{1} + G_t^{>} G_t = t \right) \left(k_t^{(j)} - \tilde{k}_t^{(j)} \right) \frac{1}{t} (G_t^{(j)} - G_t)^> (f_{\text{gnn};t}^{(j)} - y_t) - \frac{1}{t} G_t^{>} (f_{\text{gnn};t}^{(j)} - G_t(\tilde{k}_t^{(j)} - 0)) k_2 \\
 & \underbrace{k_1 \left((1 - m) \mathbb{1} + G_t^{>} G_t = t \right) k_2 k_t^{(j)} - \tilde{k}_t^{(j)} k_2}_{I_1} + \underbrace{\frac{1}{t} k G_t k_2 k f_{\text{gnn};t}^{(j)} - G_t(\tilde{k}_t^{(j)} - 0) k_2}_{I_2} + \underbrace{\frac{1}{t} k G_t^{(j)} - G_t k_2 k f_{\text{gnn};t}^{(j)} - y_t k_2}_{I_3}
 \end{aligned}$$

For I_1 , due to $G_t^{>} G_t = t < 0$, we have

$$I_1 = k \left((1 - m) \mathbb{1} + G_t^{>} G_t = t \right) k_2 k_t^{(j)} - \tilde{k}_t^{(j)} k_2 = (1 - m) k \left(k_t^{(j)} - \tilde{k}_t^{(j)} \right) k_2$$

For I_2 , by Lemma B.4, set $\epsilon = C^P \frac{1}{(R^2 + \sigma^2)^m}$. Since $\epsilon \mathbb{1} = P \bar{m}$, it can be verified that technical condition (23) in Lemma C.7 is satisfied when m is large. Then with probability at least $1 - \epsilon \mathbb{1} \geq 2(0; 1)$,

$$I_2 = \frac{1}{t} k G_t k_2 k f_{\text{gnn};t}^{(j)} - G_t(\tilde{k}_t^{(j)} - 0) k_2 \leq C_1 \left(C \frac{R^2 + \sigma^2}{m} \right)^{2=3L} L^{7=2} m^P \frac{1}{\log(m)}$$

For I_3 , by Lemma B.2 and Lemma B.4, and Lemma C.7, with probability at least $1 - \epsilon \mathbb{1} \geq 2(0; 1)$,

$$I_3 = \frac{1}{t} k G_t^{(j)} - G_t k_2 k f_{\text{gnn};t}^{(j)} - y_t k_2 \leq C_2 \left(C \frac{R^2 + \sigma^2}{m} \right)^{1=6L} L^{7=2} P \frac{1}{m \log(m)} \frac{1}{R^2 + \sigma^2}$$

Put the upper bound for I_1, I_2, I_3 together and set $C_3 = (\epsilon^{1=3} C_1 + C_2) C = O(\epsilon^{1=3})$, then we get,

$$k_t^{(j+1)} - \tilde{k}_t^{(j+1)} k_2 = (1 - m) k \left(k_t^{(j)} - \tilde{k}_t^{(j)} \right) k_2 + C_3 \left(R^2 + \sigma^2 \right)^{2=3L} L^{7=2} m^{1=3} \frac{1=6P}{\log(m)}$$

Therefore, there exists $m = \text{poly}(R; \sigma; L)$ satisfies that $\left(R^2 + \sigma^2 \right)^{1=6L} L^{7=2} \epsilon^{1=3} \frac{1}{\log(m)} \leq m^{1=6}$, which indicates

$$k_t^{(j)} - \tilde{k}_t^{(j)} k_2 \leq C_3 \left(R^2 + \sigma^2 \right)^{2=3L} L^{7=2} m^{2=3} \frac{1=6P}{\log(m)} \leq C_3^r \frac{R^2 + \sigma^2}{m}$$

□

Lemma B.2 (Prediction Error Bound in Gradient Descent). Let $f_t^{(j)} g_{j=1}^J$ be the gradient descent update sequence of parameters of the optimization (6). Define $f_{\text{gnn};t}^{(j)} := [f_{\text{GNN}}(G_1; \tilde{k}_t^{(j)}); \dots; f_{\text{GNN}}(G_t; \tilde{k}_t^{(j)})]^> \geq 2 R^t \mathbb{1}$. Assume ϵ is set such that $k_t^{(j)} - 0 k_2 \leq \epsilon$ for all t and $8j \leq J$. Suppose $m = \text{poly}(L; \sigma; \epsilon; \log(N))$ where $\epsilon \mathbb{1} \geq 2(0; 1)$ and learning rate $\eta = (CmL + m)^{-1}$ for some constant C , then with probability at least $1 - \epsilon \mathbb{1}$,

$$k f_{\text{gnn};t}^{(j)} - y_t k_2 \leq C^P \frac{1}{t(R^2 + \sigma^2)}$$

where C is some constant which does not depend on m and t .

Proof. Define $f_t(\cdot)$ and $G_t(\cdot)$ as follow

$$\begin{aligned}
 f_t(\cdot) &= [f_{\text{GNN}}(G_1; \cdot); \dots; f_{\text{GNN}}(G_t; \cdot)]^> \geq 2 R^t \mathbb{1} \\
 G_t(\cdot) &= [g(G_1; \cdot); \dots; g(G_t; \cdot)] \geq 2 R^P \mathbb{1}^t
 \end{aligned}$$

Also define $L_t(\cdot) := \frac{1}{2t} \sum_{i=1}^P (f_{\text{GNN}}(G_i; \cdot) - y_i)^2 + \frac{m}{2} k_2^2$ as the loss function in primary optimization. Note that $L_t(\cdot) := \frac{1}{2t} \sum_{i=1}^P (f_t(\cdot) - y_i)^2 + \frac{m}{2} k_2^2$. First notice that loss function $L_t(\cdot)$ is convex due to the strongly convexity of $k_2^2=2$. We are going to use the following two-sided bound from strongly convexity in this proof:

$$\|k_2^2=2\| \cdot \|x - y\| \leq \|x\| + \frac{1}{2} \|y\|$$

By 1-strongly convexity of $k_2^2=2$, we have

$$L_t(\cdot) - L_t(\cdot) = \frac{1}{2t} \sum_{i=1}^P (f_t(\cdot) - y_i)^2 - \frac{1}{2t} \sum_{i=1}^P (f_t(\cdot) - y_i)^2 + \frac{m}{2} k_2^2 - \frac{m}{2} k_2^2$$

$$\frac{1}{t} (f_t(\cdot) - y_t)^\top (f_t(\cdot) - f_t(\cdot)) + \frac{1}{2} \sum_{i=1}^P (f_t(\cdot) - f_t(\cdot))^2 + m \cdot \dots + \frac{1}{2} k_2^2 :$$

Define $e_t := f_t(\cdot) - f_t(\cdot) - G_t^\top(\cdot)(\cdot)$. By Lemma B.4, with probability at least $1 - \epsilon$ (0; 1)

$$L_t(\cdot) - L_t(\cdot)$$

$$\frac{1}{t} (f_t(\cdot) - y_t)^\top (G_t^\top(\cdot)(\cdot) + e_t) + \frac{1}{2t} k G_t^\top(\cdot)(\cdot) + e_t k_2^2 + m \cdot \dots + \frac{1}{2} k_2^2$$

$$= \frac{1}{t} [G_t(\cdot)(f_t(\cdot) - y_t) + m \cdot \dots]^\top (\cdot) + \frac{1}{t} (f_t(\cdot) - y_t)^\top e_t + \frac{1}{2t} k G_t^\top(\cdot)(\cdot) + e_t k_2^2 + \frac{m}{2} k_2^2$$

$$= rL_t(\cdot)^\top (\cdot) + \frac{1}{t} (f_t(\cdot) - y_t)^\top e_t + \frac{1}{2t} k G_t^\top(\cdot)(\cdot) + e_t k_2^2 + \frac{m}{2} k_2^2$$

$$rL_t(\cdot)^\top (\cdot) + \frac{1}{t} \sum_{i=1}^P (f_t(\cdot) - y_i) k_2 e_t k_2 + \frac{1}{t} k G_t(\cdot) k_2^2 k_2^0 k_2^2 + \frac{1}{t} e_t k_2^2 + \frac{m}{2} k_2^2$$

$$rL_t(\cdot)^\top (\cdot) + \frac{1}{t} \sum_{i=1}^P (f_t(\cdot) - y_i) k_2 e_t k_2 + \frac{1}{t} e_t k_2^2 + (C_1^2 m L + m = 2) k_2^0 k_2^2 \quad (\text{by Lemma B.4})$$

(17)

Similarly by 1-strongly convexity of $k_2^2=2$, we also investigate the lower bound:

$$L_t(\cdot) - L_t(\cdot) = \frac{1}{t} (f_t(\cdot) - y_t)^\top (f_t(\cdot) - f_t(\cdot)) + \frac{1}{2} \sum_{i=1}^P (f_t(\cdot) - f_t(\cdot))^2 + m \cdot \dots + \frac{1}{2} k_2^2$$

Using $e_t := f_t(\cdot) - f_t(\cdot) - G_t^\top(\cdot)(\cdot)$, we obtain

$$L_t(\cdot) - L_t(\cdot) = \frac{1}{t} (f_t(\cdot) - y_t)^\top (G_t^\top(\cdot)(\cdot) + e_t) + m \cdot \dots + \frac{m}{2} k_2^2$$

$$= \frac{1}{t} [G_t(\cdot)(f_t(\cdot) - y_t) + m \cdot \dots]^\top (\cdot) + \frac{1}{t} (f_t(\cdot) - y_t)^\top e_t + \frac{m}{2} k_2^2$$

Then using $rL_t(\cdot) = G_t(\cdot)(f_t(\cdot) - y_t) + m \cdot \dots$, we have

$$L_t(\cdot) - L_t(\cdot) = rL_t(\cdot)^\top (\cdot) + \frac{1}{t} (f_t(\cdot) - y_t)^\top e_t + \frac{m}{2} k_2^2$$

$$rL_t(\cdot)^\top (\cdot) + \frac{m}{2} k_2^2 - \frac{1}{t} \sum_{i=1}^P (f_t(\cdot) - y_i) k_2 e_t k_2 \quad (18)$$

$$\frac{krL_t(\cdot) k_2^2}{2m} - \frac{1}{t} \sum_{i=1}^P (f_t(\cdot) - y_i) k_2 e_t k_2 \quad (\text{by Lemma C.1})$$

Now recall the update step $\mathbf{r}_t^{(j+1)} = \mathbf{r}_t^{(j)} + \mathbf{r}_t(\mathbf{r}_t^{(j)})$ and combine the above upper and lower bounds,

$$\begin{aligned}
 & L_t(\mathbf{r}_t^{(j+1)}) - L_t(\mathbf{r}_t^{(j)}) \\
 & \quad \leq \mathbf{r}_t(\mathbf{r}_t^{(j)}) \cdot \mathbf{r}_t^{(j)} + \frac{1}{t} \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2 \mathbf{k}_e \mathbf{k}_2 + \frac{1}{t} \mathbf{k}_e \mathbf{k}_2^2 + \frac{1}{2} (C_1^2 m L + m = 2) \mathbf{r}_t(\mathbf{r}_t^{(j)}) \mathbf{k}_2^2 \quad (\text{by update step and (17)}) \\
 = & \quad \frac{1}{2} (2C_1^2 m L + m) \mathbf{r}_t(\mathbf{r}_t^{(j)}) \mathbf{k}_2^2 + \frac{1}{t} \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2 \mathbf{k}_e \mathbf{k}_2 + \frac{1}{t} \mathbf{k}_e \mathbf{k}_2^2 \\
 & \quad \leq \frac{1}{2} \mathbf{r}_t(\mathbf{r}_t^{(j)}) \mathbf{k}_2^2 + \frac{1}{t} \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2 \mathbf{k}_e \mathbf{k}_2 + \frac{1}{t} \mathbf{k}_e \mathbf{k}_2^2 \quad (\text{by choice of } \epsilon) \\
 & \quad \leq m (L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-1)})) + \frac{1}{t} \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2 \mathbf{k}_e \mathbf{k}_2 + \frac{1}{t} \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2 \mathbf{k}_e \mathbf{k}_2 + \frac{1}{t} \mathbf{k}_e \mathbf{k}_2^2 \quad (\text{by (18)}) \\
 & \quad \leq m (L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-1)})) + \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2^2 = 8t + 2 \mathbf{k}_e \mathbf{k}_2^2 = t + \frac{1}{t} (m \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2^2 = 8 + 2 \mathbf{k}_e \mathbf{k}_2^2 = m) + \frac{1}{t} \mathbf{k}_e \mathbf{k}_2^2 \\
 = & \quad m (L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-1)})) + \frac{m}{4t} \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2^2 + \left(\frac{2m}{t} + \frac{2}{mt} + \frac{1}{t} \right) \mathbf{k}_e \mathbf{k}_2^2 \\
 & \quad \leq m (L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-1)})) + m (L_t(\mathbf{r}_t^{(j-1)}) - L_t(\mathbf{r}_t^{(j-2)})) + \left(\frac{2m}{t} + \frac{2}{mt} + \frac{1}{t} \right) \mathbf{k}_e \mathbf{k}_2^2 \quad (\text{by } \mathbf{k}_f(\mathbf{r}_t^{(j)}) \cdot \mathbf{y}_t \mathbf{k}_2^2 \leq 2L_t(\mathbf{r}_t^{(j)})) \\
 = & \quad m (L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-2)})) + \left(\frac{2m}{t} + \frac{2}{mt} + \frac{1}{t} \right) \mathbf{k}_e \mathbf{k}_2^2 \tag{19}
 \end{aligned}$$

For $\mathbf{k}_e \mathbf{k}_2^2$, by Lemma C.7, with probability at least $1 - 2^{-2} (0; 1)$ for some constant C_2 , we have

$$\begin{aligned}
 \mathbf{k}_e \mathbf{k}_2 &= \mathbf{k}_f(\mathbf{r}_t^{(j)}) - \mathbf{f}_t(\mathbf{r}_t^{(j)}) \cdot \mathbf{G}_t^>(\mathbf{r}_t^{(j)}) \mathbf{k}_2 \\
 & \leq \frac{1}{t} \max_{i \in [t]} \mathbf{j}_{\text{GNN}}(\mathbf{G}_i; \mathbf{r}_t^{(j)}) - \mathbf{f}_{\text{GNN}}(\mathbf{G}_i; \mathbf{r}_t^{(j)}) + \mathbf{g}^>(\mathbf{G}_i; \mathbf{r}_t^{(j)}) \\
 & \leq \frac{1}{N} \max_{i \in [t]} \sum_{j \in 2V(\mathbf{G}_i)} \mathbf{j}_{\text{MLP}}(\mathbf{h}_j; \mathbf{r}_t^{(j)}) - \mathbf{f}_{\text{MLP}}(\mathbf{h}_j; \mathbf{r}_t^{(j)}) + \mathbf{g}_{\text{MLP}}(\mathbf{h}_j; \mathbf{r}_t^{(j)}) \\
 & \leq C_2 \frac{4=3L^3}{tm \log(m)} \tag{20}
 \end{aligned}$$

where $V(\mathbf{G})$ as vertex set of a graph \mathbf{G} . Moreover, by Lemma C.4, we have the high probability upper bound for $\frac{1}{t} \mathbf{k}_y \mathbf{k}_2^2$: with probability at least $1 - 3^{-2} (0; 1)$ and some constant C_3 depends on β ,

$$\frac{1}{t} \mathbf{k}_y \mathbf{k}_2^2 \leq \frac{1}{t} (tR^2 + \mathbf{k}_t \mathbf{k}_2^2 + 2 \frac{1}{t} \mathbf{r}_t \mathbf{R} \mathbf{k}_t \mathbf{k}_2) \leq C_3 \left(\frac{\beta}{t} + R^2 \right) \tag{21}$$

Then let $\mathbf{r}_t^{(j)} = \mathbf{r}_t^{(j-1)}$ and plug in $\mathbf{r}_t^{(j+1)}$ and $\mathbf{r}_t^{(j)}$ in (19), by Lemma B.3, with probability at least $1 - 4^{-1}$,

$$\begin{aligned}
 L_t(\mathbf{r}_t^{(j+1)}) - L_t(\mathbf{r}_t^{(j)}) & \leq (1 - m = 2)(L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-1)})) + \frac{m}{2} L_t(\mathbf{r}_t^{(j-1)}) + \left(\frac{2m}{t} + \frac{2}{mt} + \frac{1}{t} \right) \mathbf{k}_e \mathbf{k}_2^2 \\
 & \leq (1 - m = 2)(L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-1)})) + \frac{m}{2} \left(\frac{1}{t} \mathbf{k}_y \mathbf{k}_2^2 + m \mathbf{k}_o \mathbf{k}_2^2 \right) \\
 & \quad + (2m + 2 = m + 1) C_2^2 \frac{8=3L^6}{tm \log(m)} \quad (\text{by (21)}) \\
 & \leq (1 - m = 2)(L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-1)})) + \frac{m}{2} (C_3 \left(\frac{\beta}{t} + R^2 \right) + m \mathbf{k}_o \mathbf{k}_2^2) \\
 & \quad + \frac{5}{m} C_2^2 \frac{8=3L^6}{tm \log(m)} \quad (\text{by (20) and } m \geq 1) \\
 & \leq (1 - m = 2)(L_t(\mathbf{r}_t^{(j)}) - L_t(\mathbf{r}_t^{(j-1)})) + C_4 m \left(\frac{\beta}{t} + R^2 \right) + \frac{5}{m} C_2^2 \frac{8=3L^6}{tm \log(m)} \\
 & \quad (\text{by Lemma B.3})
 \end{aligned}$$

Now we further set $\eta = \frac{C}{m} \frac{r}{\sqrt{\frac{\sigma^2 + R^2}{m}}}$ and the upper bound for $L_t(\theta^{(j+1)}) - L_t(\theta^0)$ is

$$\begin{aligned} L_t(\theta^{(j+1)}) - L_t(\theta^0) &\leq (1 - \eta)(L_t(\theta^{(j)}) - L_t(\theta^0)) + C_4 \eta m (\frac{\sigma^2}{m} + R^2) + \frac{5}{m} C^2 C_2^2 (\frac{\sigma^2}{m} + R^2)^{2=3} \leq L^6 \log(m) \\ &\quad \text{(by } \eta = \frac{C}{m} \frac{r}{\sqrt{\frac{\sigma^2 + R^2}{m}}}) \\ &\leq (1 - \eta)(L_t(\theta^{(j)}) - L_t(\theta^0)) + C_4 \eta m (\frac{\sigma^2}{m} + R^2) + C_5 \eta m (\frac{\sigma^2}{m} + R^2) \\ &\quad \text{(by choice of } \eta \text{ in Lemma C.7)} \end{aligned}$$

where C_4 is a constant depends on σ and R and C_5 depends on σ , σ and R . Then by recursion,

$$L_t(\theta^{(j+1)}) - L_t(\theta^0) \leq \frac{C_6 m (\frac{\sigma^2}{m} + R^2)}{m = 2} = C_6 (\frac{\sigma^2}{m} + R^2)$$

where $C_6 = C_4 + C_5$ and $C_6 = 2C_6$. Recall that $\frac{1}{2t} \sum_{i=1}^t \langle \nabla f_t(\theta), y_i \rangle^2 = 2tL_t(\theta) - \frac{m}{2} k_2^2 - 2tL_t(\theta)$, with some constant C_7 derived from C_6 and C_4 , then we have

$$\begin{aligned} \frac{1}{2t} \sum_{i=1}^t \langle \nabla f_t(\theta), y_i \rangle^2 - 2tL_t(\theta) &\leq 2tC_6 (\frac{\sigma^2}{m} + R^2) + 2tL_t(\theta) \\ &= 2tC_6 (\frac{\sigma^2}{m} + R^2) + 2t(\frac{1}{2t} \sum_{i=1}^t \langle \nabla f_t(\theta), y_i \rangle^2 + \frac{m}{2} k_2^2) \\ &\leq C_7 t (\frac{\sigma^2}{m} + R^2) \quad \text{(by Lemma B.3)} \end{aligned}$$

which implies our result by setting $\eta = \frac{1}{2} = \frac{1}{2} = \frac{1}{2} = \frac{1}{2} = \frac{1}{2}$ where $\epsilon > 0$ is arbitrary small. □

Lemma B.3 (Parameter Bound for Proximal Optimization). Let $\{\theta_t^{(j)}\}_{j=1}^J$ be the gradient descent update sequence of parameters of the following optimization,

$$\min_{\theta} \frac{1}{2t} \sum_{i=1}^t (\langle \nabla f_i(\theta); \theta \rangle - \langle \nabla f_i(\theta); y_i \rangle)^2 + \frac{m}{2} k_2^2$$

Then if $m = \text{poly}(L, \frac{1}{\epsilon}; \log(N = \frac{1}{\epsilon}))$ and learning rate $\eta = \frac{C}{mL + m} \frac{1}{\epsilon}$ for some constant C . Then for some constant C and for any $\delta > 0$ and $J > 0$, with probability at least $1 - \delta$ (0; 1),

$$\begin{aligned} \|\theta_t^{(j)} - \theta^*\|_2 &\leq C \frac{r}{m} \sqrt{\frac{\sigma^2 + R^2}{m}} \\ \|\theta_t^{(j)} - \theta^*\|_2 &\leq C \frac{r}{m} \sqrt{\frac{\sigma^2 + R^2}{m}} \\ \|\theta_t^{(j)} - \theta^*\|_2 &\leq C (2 - m)^j \frac{r}{m} \sqrt{\frac{\sigma^2 + R^2}{m}} \end{aligned}$$

for some constant C which is independent of m and t .

Proof. Denote $L_t(\theta) := \frac{1}{2t} \sum_{i=1}^t (\langle \nabla f_i(\theta); \theta \rangle - \langle \nabla f_i(\theta); y_i \rangle)^2 + \frac{m}{2} k_2^2$ as the loss function in our proximal optimization. By Lemma B.4, with probability at least $1 - \delta$ (0; 1) the Hessian of $L_t(\theta)$ satisfies:

$$0 \preceq \nabla^2 L_t = \nabla^2 G_t \succeq \frac{1}{4} (kG_t k_F^2 \succeq \frac{1}{4} (C_1^2 mL + m))$$

which reveals that L_t is strongly convex and $(C_1^2 mL + m)$ -smooth. Thus if $\eta = \frac{1}{(C_1^2 mL + m)}$, L_t is a monotonically decreasing function:

$$\frac{1}{2t} \sum_{i=1}^t \langle \nabla f_i(\theta), y_i \rangle^2 - 2tL_t(\theta) \leq \frac{1}{2t} \sum_{i=1}^t \langle \nabla f_i(\theta), y_i \rangle^2 + \frac{m}{2} k_2^2 - 2tL_t(\theta)$$

which indicates

$$k_t^{(j)} k_2^2 = \frac{1}{tm} ky_t k_2^2 + k_0 k_2^2$$

$$\frac{1}{tm} (k_t k_2^2 + k_t k_2^2 + 2k_t k_2 k_t k_2) + k_0 k_2^2$$

Note that the proximal optimization is optimization for ridge regression which has the closed form solution:

$$= \beta_0 + U_t^{-1} G_t y_t = m$$

and $\tilde{k}_t^{(j)}$ converges to k_2 with the following rate:

$$k_t^{(j+1)} k_2^2 = k_t^{(j)} k_2^2 - rL(\tilde{k}_t^{(j)}) k_2^2$$

$$= k_t^{(j)} k_2^2 + 2krL(\tilde{k}_t^{(j)}) k_2^2 - 2(\tilde{k}_t^{(j)})^2 > rL(\tilde{k}_t^{(j)})$$

$$k_t^{(j)} k_2^2 + 2(C_1^2 mL + m)^2 k_t^{(j)} k_2^2 - 2(\tilde{k}_t^{(j)})^2 > rL(\tilde{k}_t^{(j)}) \quad (\text{by smoothness})$$

$$k_t^{(j)} k_2^2 + 2(C_1^2 mL + m)^2 k_t^{(j)} k_2^2 + 2(L(\cdot) - L(\tilde{k}_t^{(j)})) \quad (\text{by convexity})$$

$$2k_t^{(j)} k_2^2 + 2(L(\cdot) - L(\tilde{k}_t^{(j)})) \quad (\text{by } (C_1^2 mL + m)^{-1})$$

$$2k_t^{(j)} k_2^2 - m k_t^{(j)} k_2^2 \quad (\text{by } m\text{-strongly convexity})$$

$$= (2 - m) k_t^{(j)} k_2^2$$

Therefore,

$$k_t^{(j+1)} k_2^2 = (2 - m)^j k_0 k_2^2$$

$$(2 - m)^j \frac{2}{m} (L(\beta_0) - L(\cdot)) \quad (\text{by } m\text{-strongly convexity})$$

$$(2 - m)^j \frac{2}{m} L(\beta_0)$$

$$= (2 - m)^j \frac{1}{tm} ky_t k_2^2 + k_0 k_2^2$$

Then combine with Lemma C.4 and $k_t k_2 \stackrel{P}{\leq} tk_{H_1} \stackrel{P}{\leq} tR$, we have that with probability at least $1 - 2^{-2} (0; 1)$,

$$\frac{1}{tm} ky_t k_2^2 = \frac{1}{tm} (tR^2 + k_t k_2^2 + 2 \stackrel{P}{\leq} tR k_t k_2) \leq C_1 (\beta^2 + R^2) = m$$

where C_1 is some constant depends on β . Therefore, for any $\beta \in (0; 1)$, set $\beta_1 = \beta_2 = \beta = 2$, with probability at least $1 - \beta$,

$$k_t^{(j)} k_2 \leq C_2 \frac{\beta^2 + R^2}{m}$$

$$k_t^{(j)} \leq k_2 \leq C_2 \frac{\beta^2 + R^2}{m}$$

and

$$k_t^{(j)} \beta_0 + U_t^{-1} G_t y_t = m k_2 \leq (2 - m)^j C_2 \frac{\beta^2 + R^2}{m}$$

where C_2 is some constant depends on β and $k_0 k_2$.

□

Lemma B.4 (Gradient Descent Norm Bound). Define $G_t^{(j)} := [g(G_1; \tilde{k}_t^{(j)}); \dots; g(G_t; \tilde{k}_t^{(j)})] \in \mathbb{R}^p$ for the gradients in the j -th updates in GNN training (optimization of (6)) at round t . Also define $f_{\text{gnn},t}^{(j)} := [f_{\text{GNN}}(G_1; \tilde{k}_t^{(j)}); \dots; f_{\text{GNN}}(G_t; \tilde{k}_t^{(j)})] \in \mathbb{R}^t$. Assume β is set such that $k_t^{(j)} \leq k_2$

for all t and $\forall j \leq J$. Suppose $m \geq \text{poly}(L, \lambda^{-1}, \log(N/\delta))$ where $\delta \in (0, 1)$, then with probability at least $1 - \delta$,

$$\begin{aligned}\|\bar{\mathbf{G}}_t\|_F &\leq C_1 \sqrt{tmL} \\ \|\mathbf{G}_t^{(j)}\|_F &\leq C_1 \sqrt{tmL} \\ \|\bar{\mathbf{G}}_t - \mathbf{G}_t^{(j)}\|_F &\leq C_2 \tau^{1/3} L^{7/2} \sqrt{tm \log(m)} \\ \|\mathbf{f}_{gnn,t}^{(j)} - \binom{(j)}{t} \bar{\mathbf{G}}_t\|_2 &\leq C_3 \tau^{4/3} L^3 \sqrt{tm \log(m)}\end{aligned}$$

for some constant C_1, C_2, C_3 which does not depend on m and t .

Proof. From Lemma C.7, we can bounding the $\|\mathbf{g}(G_i; \mathbf{0})\|_2$ with probability at least $1 - \delta \in (0, 1)$, which provides the high probability upper bound for the Frobenius norm of $\bar{\mathbf{G}}_t$:

$$\|\bar{\mathbf{G}}_t\|_F \leq \sqrt{t} \max_i \|\mathbf{g}(G_i; \mathbf{0})\|_2 \leq \frac{\sqrt{t}}{N} \max_{i \in [t]} \max_{j \in \mathcal{V}(G_i)} \|\mathbf{g}_{\text{MLP}}(\mathbf{h}_j; \mathbf{0})\|_2 \leq C_1 \sqrt{tmL}$$

and the high probability upper bound for the Frobenius norm of $\mathbf{G}_t^{(j)}$:

$$\|\mathbf{G}_t^{(j)}\|_F \leq \sqrt{t} \max_i \|\mathbf{g}(G_i; \binom{(j)}{t})\|_2 \leq \frac{\sqrt{t}}{N} \max_{i \in [t]} \max_{j \in \mathcal{V}(G_i)} \|\mathbf{g}_{\text{MLP}}(\mathbf{h}_j; \binom{(j)}{t})\|_2 \leq C_1 \sqrt{tmL}$$

For the gradients difference, by Lemma C.7, with probability at least $1 - \delta$,

$$\begin{aligned}\|\bar{\mathbf{G}}_t - \mathbf{G}_t^{(j)}\|_F &\leq \sqrt{t} \max_i \|\mathbf{g}(G_i; \mathbf{0}) - \mathbf{g}(G_i; \binom{(j)}{t})\|_2 \\ &\leq \frac{\sqrt{t}}{N} \max_{i \in [t]} \max_{j \in \mathcal{V}(G_i)} \|\mathbf{g}_{\text{MLP}}(\mathbf{h}_j; \mathbf{0}) - \mathbf{g}_{\text{MLP}}(\mathbf{h}_j; \binom{(j)}{t})\|_2 \\ &\leq C_2 \tau^{1/3} L^{7/2} \sqrt{tm \log(m)}\end{aligned}$$

The last norm for difference between the GNN prediction and linearized prediction is bounded due to Lemma C.7, with probability at least $1 - \delta$,

$$\begin{aligned}\|\mathbf{f}_{gnn,t}^{(j)} - \binom{(j)}{t} \bar{\mathbf{G}}_t\|_2 &\leq \sqrt{t} \max_i |f_{\text{GNN}}(G_i; \binom{(j)}{t}) - \binom{(j)}{t} \mathbf{g}(G_i; \mathbf{0})| \\ &\leq \frac{\sqrt{t}}{N} \max_{i \in [t]} \max_{j \in \mathcal{V}(G_i)} |f_{\text{MLP}}(\mathbf{h}_j; \binom{(j)}{t}) - \binom{(j)}{t} \mathbf{g}_{\text{MLP}}(\mathbf{h}_j; \mathbf{0})| \\ &\leq C_3 \tau^{4/3} L^3 \sqrt{tm \log(m)}\end{aligned}$$

□

B.4 Lemmas for GNTK

Lemma B.5 (Approximation from GNTK). *Set $\delta \in (0, 1)$ and*

$$m = \Omega(L^{10} T^4 |\mathcal{G}|^6 \rho_{\min}^{-4} \log(LN^2 |\mathcal{G}|^2 / \delta)).$$

Then with probability at least $1 - \delta$,

(i) (Approximate Linearized Neural Network) \exists such that, for $\forall G \in \mathcal{G}$

$$\begin{aligned}\mu(G) &= \langle \mathbf{g}(G; \mathbf{0}), \cdot \rangle \\ \sqrt{m} \|\cdot\|_2 &\leq \sqrt{2} R\end{aligned}$$

(ii) (Spectral Bound for Uncertainty Matrix $\bar{\mathbf{U}}_t$ by GNTK)

$$\begin{aligned}\lambda_{\max}(\bar{\mathbf{U}}_t) &\leq \lambda + \frac{3}{2} \rho_{\max} \\ \log \det(\lambda^{-1} \bar{\mathbf{U}}_t) &\leq \log \det(\mathbf{I}_{|G|} + \lambda^{-1} t \mathbf{K}) + 1\end{aligned}$$

Proof. In this proof, set $\delta_1 = \delta_2 = \delta/2$ where $\delta \in (0, 1)$ is an arbitrary real value. Recall the definition of the true reward function $\mu : \mathcal{G} \rightarrow \mathbb{R}$ and the GNTK matrix $\mathbf{K} \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$. We further define the vector of function values $\boldsymbol{\mu} \in \mathbb{R}^{|\mathcal{G}| \times 1}$ as well as the gradient matrix $\bar{\mathbf{G}} \in \mathbb{R}^{p \times |\mathcal{G}|}$ on initialization $\mathbf{0}$.

$$\begin{aligned} [\mathbf{K}]_{ij} &= k(G^i, G^j) \quad \forall G^i, G^j \in \mathcal{G} \\ [\boldsymbol{\mu}]_i &= \mu(G^i) \quad \forall G^i \in \mathcal{G} \\ \bar{\mathbf{G}}_i &= \mathbf{g}(G^i; \mathbf{0}) \end{aligned}$$

Proof for (i): By the connection between GNTK and NTK,

$$\begin{aligned} \|\mathbf{K} - \bar{\mathbf{G}} \bar{\mathbf{G}}/m\|_F &= \frac{\sum_{i=1}^{|\mathcal{G}|} \sum_{j=1}^{|\mathcal{G}|} (k(G^i, G^j) - \mathbf{g}(G^i; \mathbf{0})\mathbf{g}(G^j; \mathbf{0})/m)^2}{|\mathcal{G}| \cdot |\mathcal{G}|} \\ &= \frac{\sum_{i=1}^{|\mathcal{G}|} \sum_{j=1}^{|\mathcal{G}|} \frac{1}{N^2} (k_{\text{MLP}}(\mathbf{h}_u^{G^i}, \mathbf{h}_v^{G^j}) - \mathbf{g}_{\text{MLP}}(\mathbf{h}_u^{G^i}; \mathbf{0})\mathbf{g}_{\text{MLP}}(\mathbf{h}_v^{G^j}; \mathbf{0})/m)^2}{|\mathcal{G}| \cdot |\mathcal{G}|} \\ &\leq \frac{\sum_{i=1}^{|\mathcal{G}|} \sum_{j=1}^{|\mathcal{G}|} (k_{\text{MLP}}(\mathbf{h}_u^{G^i}, \mathbf{h}_v^{G^j}) - \mathbf{g}_{\text{MLP}}(\mathbf{h}_u^{G^i}; \mathbf{0})\mathbf{g}_{\text{MLP}}(\mathbf{h}_v^{G^j}; \mathbf{0})/m)^2}{|\mathcal{G}| \cdot |\mathcal{G}|} \end{aligned} \quad 2$$

where \mathcal{V}_G denotes the vertex set of a graph G . By Lemma C.6, when $m = \Omega(L^{10}N^4|\mathcal{G}|^4\rho_{\min}^{-4}\log(LN^2|\mathcal{G}|^2/\delta_1))$, then with probability at least $1 - \delta_1/(N^2|\mathcal{G}|^2)$, $|k_{\text{MLP}}(\mathbf{h}_u^{G^i}, \mathbf{h}_v^{G^j}) - \mathbf{g}_{\text{MLP}}(\mathbf{h}_u^{G^i}; \mathbf{0})\mathbf{g}_{\text{MLP}}(\mathbf{h}_v^{G^j}; \mathbf{0})/m| \leq \frac{\rho_{\min}}{2N|\mathcal{G}|}$. Then apply union bound over all pairs $(\mathbf{h}_u^{G^i}, \mathbf{h}_v^{G^j})$, the following holds with probability at least $1 - \delta_1$,

$$\|\mathbf{K} - \bar{\mathbf{G}} \bar{\mathbf{G}}/m\|_F \leq \rho_{\min}/2$$

which shows that

$$\begin{aligned} \bar{\mathbf{G}} \bar{\mathbf{G}}/m &< \mathbf{K} - \|\mathbf{K} - \bar{\mathbf{G}} \bar{\mathbf{G}}/m\|_2 \mathbf{I}_{|\mathcal{G}|} \\ &< \mathbf{K} - \|\mathbf{K} - \bar{\mathbf{G}} \bar{\mathbf{G}}/m\|_F \mathbf{I}_{|\mathcal{G}|} \\ &< \mathbf{K} - \frac{\rho_{\min}}{2} \mathbf{I}_{|\mathcal{G}|} \\ &< \mathbf{K}/2 \succ \mathbf{0} \end{aligned} \quad (22)$$

Suppose $\bar{\mathbf{G}} = \mathbf{P}\boldsymbol{\Lambda}\mathbf{Q}$ is the decomposition of $\bar{\mathbf{G}}$ where $\mathbf{P} \in \mathbb{R}^{p \times |\mathcal{G}|}$, $\mathbf{Q} \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$ are unitary and $\boldsymbol{\Lambda} \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$. By (22), we know $\boldsymbol{\Lambda} \succ \mathbf{0}$ with probability at least $1 - \delta_1$. Now denote $\boldsymbol{\mu} = \mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{Q} \boldsymbol{\mu}$ and it satisfies

$$\begin{aligned} \bar{\mathbf{G}} &= \mathbf{Q}\boldsymbol{\Lambda}\mathbf{P} \quad \mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{Q} \boldsymbol{\mu} = \boldsymbol{\mu} \\ \Rightarrow \mu(G) &= \langle \mathbf{g}(G; \mathbf{0}), \boldsymbol{\mu} \rangle \quad \forall G \in \mathcal{G} \end{aligned}$$

Moreover, the norm of $\boldsymbol{\mu}$ is also bounded:

$$\|\boldsymbol{\mu}\|_2^2 = \boldsymbol{\mu} \mathbf{Q}\boldsymbol{\Lambda}^{-2}\mathbf{Q} \boldsymbol{\mu} = \boldsymbol{\mu} (\bar{\mathbf{G}} \bar{\mathbf{G}})^{-1} \boldsymbol{\mu} \leq \frac{2}{m} \boldsymbol{\mu} \mathbf{K}^{-1} \boldsymbol{\mu} \leq \frac{2R^2}{m}$$

which completes our proof for (i).

Proof for (ii): From the definition of $\bar{\mathbf{G}}_t$, we have

$$\begin{aligned}
 \log \det(\mathbf{I}_{|G|} + \lambda^{-1} \bar{\mathbf{G}}_t \bar{\mathbf{G}}_t/m) &= \log \det \left(\mathbf{I}_{|G|} + \sum_{i=1}^t \mathbf{g}(G_i; \mathbf{0}) \mathbf{g}(G_i; \mathbf{0}) / (m\lambda) \right) \\
 &\leq \log \det \left(\mathbf{I}_{|G|} + t \sum_{G \in \mathcal{G}} \mathbf{g}(G; \mathbf{0}) \mathbf{g}(G; \mathbf{0}) / (m\lambda) \right) \\
 &\leq \log \det \left(\mathbf{I}_{|G|} + t \sum_{G \in \mathcal{G}} \mathbf{g}(G; \mathbf{0}) \mathbf{g}(G; \mathbf{0}) / (m\lambda) \right) \quad (\text{by } \mathcal{G}_t \in \mathcal{G} \text{ for } \forall t \in [T]) \\
 &= \log \det(\mathbf{I}_{|G|} + t \bar{\mathbf{G}} \bar{\mathbf{G}} / (m\lambda)) \\
 &= \log \det(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda + t(\bar{\mathbf{G}} \bar{\mathbf{G}} / m - \mathbf{K}) / \lambda) \\
 (\text{by concavity of } \log \det(\cdot)) &\leq \log \det(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda) + \langle (\mathbf{I} + t \mathbf{K} / \lambda)^{-1}, t(\bar{\mathbf{G}} \bar{\mathbf{G}} / m - \mathbf{K}) / \lambda \rangle_F \\
 &\leq \log \det(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda) + \|(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda)^{-1}\|_F \|t(\bar{\mathbf{G}} \bar{\mathbf{G}} / m - \mathbf{K}) / \lambda\|_F \\
 &\leq \log \det(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda) + t \|\bar{\mathcal{G}}\| \|(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda)^{-1}\|_2 \|\bar{\mathbf{G}} \bar{\mathbf{G}} / m - \mathbf{K}\|_F / \lambda \\
 &= \log \det(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda) + \|\bar{\mathcal{G}}\| (\lambda/t + \rho_{\min})^{-1} \|\bar{\mathbf{G}} \bar{\mathbf{G}} / m - \mathbf{K}\|_F
 \end{aligned}$$

By Lemma C.6, when $m = \Omega(L^{10} N^4 |\mathcal{G}|^6 \rho_{\min}^{-4} \log(LN^2 |\mathcal{G}|^2 / \delta_2))$, then with probability at least $1 - \delta_2 / (N^2 |\mathcal{G}|^2)$, $|k_{\text{MLP}}(\mathbf{h}_u^{G^i}, \mathbf{h}_v^{G^j}) - \mathbf{g}_{\text{MLP}}(\mathbf{h}_u^{G^i}; \mathbf{0}) \mathbf{g}_{\text{MLP}}(\mathbf{h}_v^{G^j}; \mathbf{0}) / m| \leq \frac{\rho_{\min}}{N |\mathcal{G}|^{3/2}}$. Then apply union bound over all pairs $(\mathbf{h}_u^{G^i}, \mathbf{h}_v^{G^j})$, with probability at least $1 - \delta_2$, $\|\bar{\mathbf{G}} \bar{\mathbf{G}} / m - \mathbf{K}\|_F \leq \frac{\rho_{\min}}{\sqrt{|\mathcal{G}|}}$, which indicates that

$$\begin{aligned}
 \log \det(\mathbf{I}_{|G|} + \lambda^{-1} \bar{\mathbf{G}}_t \bar{\mathbf{G}}_t/m) &\leq \log \det(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda) + \|\bar{\mathcal{G}}\| (\lambda/t + \rho_{\min})^{-1} \|\bar{\mathbf{G}} \bar{\mathbf{G}} / m - \mathbf{K}\|_F \\
 &\leq \log \det(\mathbf{I}_{|G|} + t \mathbf{K} / \lambda) + 1
 \end{aligned}$$

Finally, with probability at least $1 - \delta_1$,

$$\bar{\mathbf{G}} \bar{\mathbf{G}} / m \leq 4 \mathbf{K} + \|\mathbf{K} - \bar{\mathbf{G}} \bar{\mathbf{G}} / m\|_2 \mathbf{I}_{|G|} \leq 4 \mathbf{K} + \frac{\rho_{\max}}{2} \mathbf{I}_{|G|} \leq \frac{3}{2} \rho_{\max} \mathbf{I}_{|G|}$$

which indicates that $\lambda_{\max}(\bar{\mathbf{U}}_t) \leq \lambda + \frac{3}{2} \rho_{\max}$. \square

Lemma B.6. Fix $\delta \in (0, 1)$. Then, for $m = \Omega(L^{10} |\mathcal{G}|^4 \varepsilon^{-4} \log(L/\delta))$, with probability at least $1 - \delta$,

$$|\rho_{\max} - \hat{\rho}_{\max}| \leq \varepsilon.$$

Proof. Let m be as in Lemma C.6. Recall that $\|\mathbf{h}_u^{G^i}\| = 1$ for all $u \in \mathcal{V}(G)$ and $G \in \mathcal{G}$, by construction. Let $N_i := |\mathcal{V}(G^i)|$. Then, we have, with probability at least $1 - \delta$,

$$\begin{aligned}
 &|k(G^i, G^j) - \hat{k}(G^i, G^j)| \\
 &\leq \frac{1}{N_i N_j} \sum_{\substack{u \in \mathcal{V}(G^i) \\ v \in \mathcal{V}(G^j)}} k_{\text{MLP}}(\mathbf{h}_u^{G^i}, \mathbf{h}_v^{G^j}) - \mathbf{g}_{\text{MLP}}(\mathbf{h}_u^{G^i}; \mathbf{0}) \mathbf{g}_{\text{MLP}}(\mathbf{h}_v^{G^j}; \mathbf{0}) / m \leq \varepsilon
 \end{aligned}$$

by Lemma C.6. Then

$$\|\mathbf{K} - \hat{\mathbf{K}}\|_{\text{op}} \leq \|\mathbf{K} - \hat{\mathbf{K}}\|_F \leq |\mathcal{G}| \varepsilon.$$

Then, from Weyl's inequality, $|\rho_{\max} - \hat{\rho}_{\max}| \leq |\mathcal{G}| \varepsilon$. Replacing ε with $\varepsilon / |\mathcal{G}|$ the result follows. \square

C Supporting Lemmas

Lemma C.1. Suppose \mathbf{a}, \mathbf{b} are vectors and \mathbf{A} is a matrix. c is assumed to be positive scalar. Then we have the following results: (i) $|\mathbf{a} \mathbf{A} \mathbf{b}| \leq \sqrt{\mathbf{a} \mathbf{A} \mathbf{a}} \sqrt{\mathbf{b} \mathbf{A} \mathbf{b}}$. (ii) $\mathbf{a} \mathbf{b} + c \|\mathbf{a}\|_2^2 \geq -\|\mathbf{b}\|_2^2 / 4c$.

Lemma C.2. Suppose $X \sim \mathcal{N}(\mu, \sigma^2)$ and $\beta > 0$, then

$$\mathbb{P}(|X - \mu| \leq \beta\sigma) \geq 1 - e^{-\beta^2/2}$$

Lemma C.3. Suppose $X \sim \mathcal{N}(\mu, \sigma^2)$ and $\beta > 0$, then

$$\mathbb{P}(X - \mu > \beta\sigma) \geq \frac{e^{-\beta^2}}{4\beta\sqrt{\pi}}$$

Lemma C.4. Suppose $\mathbf{x} \in \mathbb{R}^t$ is a subgaussian random vector with subgaussian constant σ^2 , then

$$\mathbb{E}[\|\mathbf{x}\|_2] \leq 4\sigma\sqrt{t}$$

and with probability at least $1 - \delta$ for $\delta \in (0, 1)$,

$$\|\mathbf{x}\|_2 \leq C\sigma\sqrt{t}.$$

where C is some constant depending on δ .

Lemma C.5. (Theorem 1 (Chowdhury and Gopalan, 2017)) Let $\{\mathbf{x}_t\}_{t=1}$ be an \mathbb{R}^d -valued discrete time stochastic process that is predictable with respect to the filtration $\{\mathcal{F}_t\}_{t=1}$. Let $\{\varepsilon_t\}_{t=1}$ be a real-valued stochastic process and for any $\forall t$, ε_t is \mathcal{F}_t -measurable and subgaussian with constant R conditionally on \mathcal{F}_{t-1} . Let $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ be a symmetric positive-definite kernel. Then for any $\eta > 0$, $\delta \in (0, 1)$, with probability at least $1 - \delta$,

$$\| \mathbf{t} \|_{((\mathbf{K}_{t+\eta} / t)^{-1} + \mathbf{I}_t)^{-1}} \leq R^2 \log \det((1 + \eta)\mathbf{I}_t + \mathbf{K}_t) + 2R^2 \log(1/\delta)$$

where $\mathbf{t} := (\varepsilon_1, \dots, \varepsilon_t) \in \mathbb{R}^t$ and $\mathbf{K}_t \in \mathbb{R}^{t \times t}$ is a matrix with $[\mathbf{K}_t]_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$, $1 \leq i, j \leq t$.

Lemma C.6 (Theorem 3.1 (Arora et al., 2019)). Fix $\varepsilon > 0$ and $\delta \in (0, 1)$. Suppose a MLP $f_{\text{MLP}}(\cdot; \theta)$ with ReLU activation has L layers and width $m = \Omega(L^{10}\varepsilon^{-4} \log(L/\delta))$. Then for any input \mathbf{x} , \mathbf{x}' such that $\|\mathbf{x}\|_2 \leq 1$, $\|\mathbf{x}'\|_2 \leq 1$, with probability at least $1 - \delta$,

$$|k_{\text{MLP}}(\mathbf{x}, \mathbf{x}') - \mathbf{g}_{\text{MLP}}(\mathbf{x}; \theta) \cdot \mathbf{g}_{\text{MLP}}(\mathbf{x}'; \theta) / m| \leq \varepsilon$$

where k_{MLP} is the neural tangent kernel associated with f_{MLP} and $\mathbf{g}_{\text{MLP}}(\cdot; \theta) = \nabla f_{\text{MLP}}(\cdot; \theta)$.

Lemma C.7 (Lemma B.4/Lemma B.5/Lemma B.6 (Zhou et al., 2020) / Lemma C.4 (Zhang et al., 2020)). Suppose θ is parameters for a MLP $f_{\text{MLP}}(\cdot; \theta)$ with L layers and width m and this neural network $f_{\text{MLP}}(\cdot; \theta)$ is trained via gradient descent with initialization θ_0 , learning rate η and ℓ_2 regularization constant λ in a mean squared loss. The input feature set is denoted as $\mathcal{X} = \{\mathbf{x}_i\}_{i=1}^T$. Then there are positive constants $\{C_i\}_{i=1}^7$ such that for $\forall \delta \in (0, 1)$, if τ satisfies

$$\begin{aligned} \tau &\geq C_1 m^{-3/2} L^{-3/2} \max((\log(TL^2/\delta))^{3/2}, (\log(m))^{-3/2}) \\ \tau &\leq \min(C_2 L^{-6} (\log(m))^{-3/2}, C_3 L^{-9/2} (\log(m))^{-3}, C_4 m^3 \lambda^{9/2} \eta^3 L^{-9} (\log(m))^{-3/2}) \end{aligned} \quad (23)$$

then with probability at least $1 - \delta$, for $\|\mathbf{x} - \mathbf{x}'\|_2 \leq \tau$ and $\|\mathbf{x}\|_2 \leq \tau$, for $\forall \mathbf{x} \in \mathcal{X}$, we have

$$\|\mathbf{g}_{\text{MLP}}(\mathbf{x}; \theta) - \mathbf{g}_{\text{MLP}}(\mathbf{x}'; \theta)\|_2 \leq C_5 \sqrt{\log(m)} \tau^{1/3} L^3 \|\mathbf{g}_{\text{MLP}}(\mathbf{x}; \theta)\|_2$$

and

$$|f_{\text{MLP}}(\mathbf{x}; \theta) - f_{\text{MLP}}(\mathbf{x}'; \theta) - \langle \mathbf{g}_{\text{MLP}}(\mathbf{x}; \theta), \mathbf{x} - \mathbf{x}' \rangle| \leq C_6 \tau^{4/3} L^3 \sqrt{m \log(m)}$$

and

$$\|\mathbf{g}_{\text{MLP}}(\mathbf{x}; \theta)\|_2 \leq C_7 \sqrt{mL}.$$

D Supplement to Experiments

D.1 Data Generation

We use synthetic data environments for our experiments. The datasets are generated from two different random graph models and three different reward function generating models. The random graph models are Erdős–Rényi random graph model and random dot product graph model. We use a linear model, Gaussian process with GNTK model, Gaussian process with representation kernel to generate our reward function. In all data environments, the feature dimension is set as $d = 10$. For any synthetic graph, all entries of the associated feature matrix $\{\mathbf{X}_{ji}\}_{j \in [N], i \in [d]}$ are i.i.d from a standard Gaussian distribution. The noisy reward is assumed to have standard deviation $\sigma_\varepsilon = 0.01$. All performance curves in our empirical studies show an average of over 10 repetitions with a standard deviation of the corresponding bandit problem with horizon $T = 1000$. Our experiment assumes the graph domain is fully observable, $\mathcal{G}_t = \mathcal{G}$ for all $t \in [T]$. We experiment four graph size $|\mathcal{G}| \in \{10, 50, 100, 200\}$ in the random dot product graphs with $N = 100$ and representation kernel.

D.1.1 Random Graph

Erdős–Rényi Random Graphs. Erdős–Rényi random graphs are generated by edge probability p and number of nodes N . Set the graph has N nodes and for any node pair $(i, j) \in [N]^2$, there is an edge linking i and j with probability p . We investigate $p \in \{0.2, 0.4, 0.6, 0.8\}$ and $N \in \{10, 50, 100, 500\}$ in our experiment. Including 3 types of reward function generating and 4 sizes of graph space \mathcal{G} , there are 192 combinations of datasets of Erdős–Rényi random graph environments.

Random Dot Product Graphs. Random dot product graphs are generated by modeling the expected edge probabilities as the function of the inner product of features. In our experiment, we set the latent embeddings observed as features, i.e. X_i is the latent embedding of node i . Formally, the edge probability for node i and j is generated by $p_{ij} = \text{sigmoid}(\mathbf{X}_i \cdot \mathbf{X}_j)$. We also investigate $N \in \{10, 50, 100, 500\}$. Including 3 types of reward function generating and 4 sizes of graph space \mathcal{G} , there are 48 combinations of datasets of random dot product graph environments.

D.1.2 Reward Function Generation

Linear Model. We generate a true parameter $\mu \in \mathbb{R}^d$ whose elements are i.i.d standard Gaussian. Then the true reward mean is

$$\mu(G) = \langle \mu, \bar{\mathbf{h}}^G \rangle$$

where $\bar{\mathbf{h}}^G = \frac{1}{N} \sum_{i=1}^N \mathbf{h}_i^G$.

Gaussian Process with GNTK. We also use Gaussian process and Graph Neural Tangent Kernel (GNTK) as introduced from experiment in (Kassraie et al., 2022). We approximately construct the GNTK matrix \mathbf{K} by the empirical GNTK matrix $\hat{\mathbf{K}} \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$ whose entries are $\hat{K}_{ij} = \frac{1}{m} \langle \mathbf{g}(G^i; \mathbf{0}), \mathbf{g}(G^j; \mathbf{0}) \rangle$ for any $G^i, G^j \in \mathcal{G}$. We use this empirical GNTK matrix $\hat{\mathbf{K}}$ as the covariance matrix of prior, i.e. $\mathcal{N}(0, \mathbf{K}^{gntk})$ and use $\{(G, y_G)\}_{G \in \mathcal{G}}$ where $\{y_G\}_{G \in \mathcal{G}}$ are i.i.d from $\mathcal{N}(0, 1)$ as our training data. To train this Gaussian process model, we use negative log-likelihood loss with Adam optimizer with learning rate 0.01 and 30 epochs. The true reward means are sampled from the posterior in this Gaussian process.

Gaussian Process with Representation Kernel. For the Gaussian process with representation kernel, we trained a GNN for a graph property prediction task and used the mean pooling over all nodes of the last layer representations as the graph representation. In our experiment, we utilize the average degree prediction as our task. That is, suppose outcome is $d_G = \frac{1}{N} \sum_{j=1}^N \text{deg}(j)$ and train GNN in (2) to predict this outcome. Then denote the last layer representation as $\bar{\mathbf{h}}_{\text{rep}}^G = \frac{1}{N} \sum_{j=1}^N f^{(L-1)}(\mathbf{h}_j^G)$. Then we define the representation kernel as the inner product of the graph representations

$$k_{\text{rep}}(G, G) := \langle \bar{\mathbf{h}}_{\text{rep}}^G, \bar{\mathbf{h}}_{\text{rep}}^G \rangle.$$

The associated kernel matrix is denoted as $\mathbf{K}^{rep} \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$ with entries $\{k^{rep}(G, G)\}_{G, G \in \mathcal{G}}$. In this Gaussian process, we sample the true reward means by $\{\mu(G)\}_{G \in \mathcal{G}} \sim \mathcal{N}(\mathbf{0}, \mathbf{K}^{rep})$. To train this

Gaussian process model, we use MSE loss with Adam optimizer with learning rate 0.01 mini-batch size 2 and 30 epochs.

D.2 Algorithms Set Up

We provide the practical details and set up on our proposed algorithms and baseline algorithms.

Algorithms. We investigate 3 GNN-based bandit algorithms (GNN-TS, GNN-UCB and GNN-PE) and 3 corresponding NN-based bandit algorithms (NN-TS, NN-UCB and NN-PE). All algorithms in our work use the loss function (6) which is different from previous work. All gradients used for in our experiments are $\mathbf{g}(G; t)$ not $\mathbf{g}(G; 0)$ unless special stated. In addition, in order to show the benefit of considering the graph structure, we include NN-UCB, NN-TS, NN-PE as our baselines. For this NN-based algorithm, we ignore the adjacency matrix for a graph (assume $\mathbf{A} = \mathbf{I}$), and pass through the model in (1) and (2) by $\mathbf{h}_i^G = \mathbf{X}_i$. For GNN-TS, we tuned the exploration scale with grid search on $\nu \in \{0.01, 0.1, 1.0, 10.0\}$ and NN-TS follows the same value. For GNN-UCB, we tuned the hyperparameter with grid search on $\beta \in \{0.01, 0.1, 1.0, 10.0\}$ and NN-UCB follows the same value. For GNN-PE, we tuned the hyperparameter with grid search on $\beta \in \{0.01, 0.1, 1.0, 10.0\}$ and NN-PE follows the same value. All the hyperparameter tuning is performed in Erdős–Rényi random graphs with $p = 0.4$, $N = 50$, $|\mathcal{G}| = 100$ and Gaussian process with GNTK for all the Erdős–Rényi random graphs settings and random dot product graphs with 50 nodes and $|\mathcal{G}| = 100$ and Gaussian process with GNTK for all the random dot product graphs settings.

Neural Networks. The MLPs in our experiments have 2 layers ($L = 2$) and width $m = 512$. We use SGD optimizer with mini-batch size 5 and 30 epochs. Learning rates (η) we tuned from and the regularization hyperparameters λ we tuned from $\{10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}\}$. Initialization for the trainable GNN parameter satisfies the condition $f_{\text{GNN}}(G; 0) = 0$ for all $G \in \mathcal{G}$, which is handle by the treatment in Kassraie and Krause (2022). Suppose the initialization is θ_0 . The matrix inversion in the algorithms is approximated by diagonal inversion across all policy algorithms.

D.3 Experiments on Scalability ($|\mathcal{G}|$)

We set the size of the graph domain to $|\mathcal{G}| = 100$ in Figure 1 and we experiment across different sizes $|\mathcal{G}| \in \{10, 50, 100, 200\}$ to check the scalability of the algorithms. Figure 2 shows that given a fixed horizon length, larger $|\mathcal{G}|$ leads to a harder bandit problem. It also shows that GNN-TS can achieve top performance across all algorithms in all scales of the graph space. This empirical observation shows that GNN-TS is robust to the scalability of the action space, supporting our theoretical justification in Section 4.

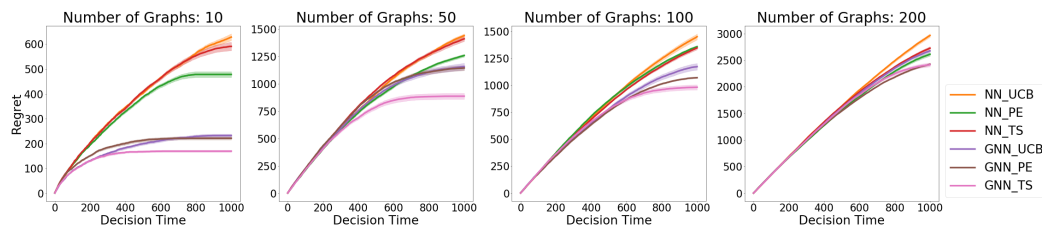


Figure 2: Competitive performance of GNN-TS is consistent across different sizes of graph space.

D.4 Effect of m and Initial Gradients

Our regret analysis depends on the assumption that the width of the neural network m must be large enough. We conduct an experiment to observe the effect from the width which is chosen from $\{32, 128, 512, 2048\}$. As some previous works on Neural bandit use the gradients at initialization ($\mathbf{g}(G_t; 0)$) for uncertainty calculation (Zhou et al., 2020; Kassraie et al., 2022) while some works use $\mathbf{g}(G_t; t-1)$ which aligns with ours (Zhang et al., 2020). Formally, instead of the update of

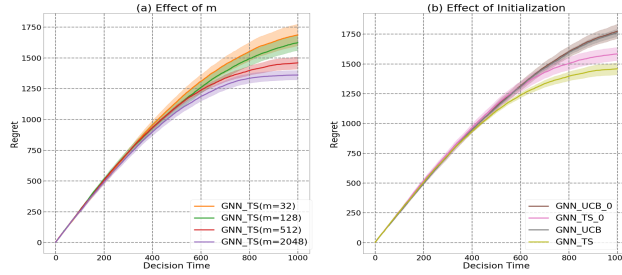


Figure 3: Increasing m can improve the performance of GNN-TS and no improvement of using $g(G_t; \bar{U}_t)$.

uncertainty estimate in (5), using initial gradient means performing the following

$$\bar{\sigma}_t^2(G) = \frac{1}{m} \|g(G; \bar{U}_t)\|_{\bar{U}_t}^2, \quad \bar{U}_t = \bar{U}_{t-1} + g(G_t; \bar{U}_t)g(G_t; \bar{U}_t) / m.$$

Part (a) of Figure 3 reflects that the wider MLP has better performance which matches our expectation. Moreover, part (b) of Figure 3 reflects that there are no benefits from setting gradients used in algorithms to be the initial gradients for all $t \in [T]$. One small final observation is that the effects of m and initialization are not strong.

D.5 Additional Figures and Tables

D.5.1 Results for Erdős–Rényi Random Graphs.

For better visualization of the 192 synthetic data environments using Erdős–Rényi random graphs, we summarised the result in Table 1. The metrics are relative regret and top rate, which are defined based on regret as follow. The relative regret of one algorithm in one data environment is defined as

$$\text{Relative Regret: } \tilde{R}^{\text{alg, env}} = \frac{R_T^{\text{alg, env}}}{\max_{\text{alg}} R_T^{\text{alg, env}}}$$

where $R_T^{\text{alg, env}}$ is the cumulative regret of algorithm alg, and data environment env.

We define the top rate for the policy in algorithm as the number of times such that the policy achieve the least two cumulative regret R_T . The denomnator is the number of total trails, which is the 1920, the 10 repetition and 192 combinations of ER environments. The top rate of one algorithm is defined as

$$\text{Top Rate: } \alpha_{\text{alg}} = \frac{\# \text{ times alg achieves "Top 2"}}{\# \text{ trails}}.$$

	NN-UCB	NN-PE	NN-TS	GNN-UCB	GNN-PE	GNN-TS
Top Rate (α_{alg})	0.0%	1.6%	0.0%	9.4%	90.6%	98.4 %
Relative Regret ($\tilde{R}^{\text{alg, env}}$)	0.994(0.02)	0.891(0.06)	0.943(0.05)	0.762(0.15)	0.690(0.14)	0.595(0.16)

Table 1: Results on Erdős–Rényi random graphs. 192 data environments with 10 repetitions.

D.5.2 Results for Random Dot Product Graphs

We provide the experiment results for regret on all random dot product graph settings. In thee plots, different rows represents different sizes of the graph space ($|\mathcal{G}|$) and columns represents the choices of the number of nodes in the graph (N).

