Expected Improvement for Contextual Bandits

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Abstract

The expected improvement (EI) is a popular technique to handle the tradeoff between exploration and exploitation under uncertainty. However, compared to other techniques as Upper Confidence Bound (UCB) and Thompson Sampling (TS), the theoretical properties of EI have not been well studied even for non-contextual settings such as standard bandit and Bayesian optimization. In this paper, we introduce and study the EI technique as a new tool for the contextual bandit problem which is a generalization of the standard bandit. We propose two novel EI based algorithms for this problem, one when the reward function is assumed to be linear and the other for more general reward functions. With linear reward function, we demonstrate that our algorithm achieves a near-optimal regret. Our regret improves that of LinTS [3] by a factor $\sqrt{d}$ while avoiding to solve a NP-hard problem at each iteration as in LinUCB [1]. For more general reward functions, we use deep neural networks to model the reward function, and prove that our algorithm achieves a $\tilde{\mathcal{O}}(\tilde{d}\sqrt{T})$ regret, where $\tilde{d}$ is the "effective" dimension of a neural tangent kernel matrix and T is the number of iterations. Finally, we provide an empirical evaluation of the algorithms on various benchmark datasets. Our experiments show that our algorithms work well and consistently outperform existing approaches especially in high dimensions.

1 Introduction

The stochastic contextual bandit problem is an important problem in machine learning ([8, 24]) to optimize the trade-off between exploration and exploitation in sequential decision making, and has been extensively studied in real-world applications such as personalized recommendation [25], advertising [18], robotic control [26], and healthcare [19]. At each round, the agent observes a feature vector (the "context") for each of the K arms, pulls one of them, and in return receives a scalar reward. The goal is to maximize the cumulative reward, or minimize regret (see our definition in Section 2), in a total of T rounds. To do so, the agent must find a trade-off between exploration and exploitation.

There are two standard techniques to solve the trade-off in contextual bandits. The first technique uses the optimism in face of uncertainty which chooses promising actions by maximizing upper-confidence bounds (UCB), and the second one using Thompson Sampling (TS) whose basic idea is to estimate a posterior distribution on the reward, and sample an arm that maximises a random reward drawn from this distribution. A series of work has applied both UCB and TS techniques or their variants to explore in contextual bandits with many forms of reward functions - from linear to nonlinear. In the line of UCB, there are works of [25, 13, 1] for the linear bandits, works of [17, 37] for nonlinear contextual bandits, and very recently [42], which uses neural networks to learn the reward function. In the line of TS, [3, 32] are for linear bandits, [32, 22] for generalized linear functions, and [31, 41] for nonlinear bandits using deep neural networks.

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Besides UCB and TS, the expected improvement (EI) [27] is also one of the oldest and popular techniques to handle the tradeoff between exploration and exploitation under uncertainty. Different from UCB and TS, the EI is a greedy improvement-based heuristic that samples an action offering the greatest expected improvement over an incumbent. Due to its simplicity and ability to handle uncertainty, EI has been widely used in Bayesian optimization [29, 40] - a problem that is closely related to infinite-arm multi-arm bandits. However, *it is yet to be seen whether EI can handle well the trade-off between exploration and exploitation in a contextual bandit problem and further in reinforcement learning which is a generalization of contextual bandits?*

We note that despite its wide use, the theoretical aspects of this technique have not been well studied compared to those of UCB and TS. A notable exception is the work in [10], who provides a convergence rate of EI for BO in the noise-free setting. [39] and [28] consider the regret analysis of EI for BO in the noisy setting. There are also several papers [34, 30] using EI to study the best-arm identification problem (also known as "pure exploration") which is a finite variant of Bayesian optimization. A key challenge of analyzing EI algorithms theoretically comes from its improvement function involving nonlinear, nonconvex term. In contextual bandit problem which is harder than the standard bandit, EI strategy has not been used, let alone an EI algorithm with optimal rate of convergence. Therefore, the design of a provable EI algorithm in contextual bandits is an open problem.

In this work, we study the EI technique for contextual bandits from both theoretical and practical perspectives. Our main contributions in this paper are:

- We introduce and formalize Expected Improvement as a new strategy for contextual bandits creating a parallel to UCB and TS.
- We propose two EI-based algorithms. The first algorithm (LinEI) is designed for the linear bandits whilst the second algorithm (NeuralEI) is designed for more general reward function and we model it by a deep neural network.
- For the linear reward function, our LinEI algorithm is able to achieve $\mathcal{O}(d\sqrt{T\ln^2(T)\ln\frac{T}{\delta}})$ regret t with probability $1-\delta$, which matches the information theoretic lower bound $\Omega(d\sqrt{T})$ for this problem (up to $\ln(T)$). Our regret improves that of LinTS [3] by a factor $\sqrt{d}$ while avoiding to solve a NP-hard problem at each iteration as in LinUCB [1].
- For the general reward function, we prove that, under standard assumptions (see section 4.1), our NeuralEI algorithm is able to achieve $\tilde{\mathcal{O}}(\tilde{d}\sqrt{T})$ regret, where $\tilde{d}$ is the "effective" dimension of a neural tangent kernel matrix and T is the number of rounds.
- Finally, we demonstrate the performance of our proposed EI-based algorithms against UCB and TS based approaches and other baselines on various benchmark datasets. Our experiments show that LinEI outperforms other baselines in the linear setting, and when the reward function is non-linear, NeuralEI outperforms all baselines.

2 Problem Setting

We consider the problem of K-arm contextual bandits. At time $t = 1, 2, ...$, the agent observes K contextual vectors $x_{i,t} \in \mathbb{R}^d$, then selects an arm $a(t)$ and receives a reward $r_{a(t),t}$ which has a general form as follows:

$$r_{a(t),t} = h(x_{a(t),t}) + \xi_{a(t),t},$$

where h is an unknown reward mean function satisfying $0 \leq h(x) \leq 1$ for any $x \in \mathbb{R}^d$, and $\xi_{a(t),t}$ is a zero mean, conditionally R-subGaussian noise with a constant $R \geq 0$, i.e., $\forall\lambda \in \mathbb{R}, \mathbb{E}[e^{\lambda\xi_{a(t),t}}|\{x_{i,t}\}_{i=1}^K] \leq \exp(\frac{\lambda^2R^2}{2})$. In our setting, we assume that these context vectors may be chosen by an adversary in an adaptive manner after observing the arms played and their rewards up to time $t-1$. For the unknown function h, we consider two cases as follows:

- The reward function h is linear, i.e., $h(x_{t,i}) = x_{t,i}^T\theta^*$, where $\theta^* \in \mathbb{R}^d$ are fixed but unknown parameters. Without loss of generality, we here assume that $||x_{i,t}|| \leq 1, ||\theta^*|| \leq 1$.
- The reward function h is modelled by a fully connected neural network with depth $L \geq 2$ defined recursively by

$$f(x;\theta) = \sqrt{m}W_L\sigma(W_{L-1}\sigma(...\sigma(W_1x))),$$

where $\sigma(x) := \max\{x, 0\}$ is the ReLU activation, $\theta = (\text{vec}(W_1); ...; \text{vec}(W_L)) \in \mathbb{R}^p$ is the collection of parameters of the neural network with $p = dm + m^2(L-2) + m$ which is the number of parameters of the network. Without loss of generality, we assume that the width of each hidden layer is the same (i.e., m) for convenience in analysis. We denote the gradient of the neural network function by $g(x;\theta) = \bigtriangledown_\theta f(x;\theta) \in \mathbb{R}^p$.

Performance Measure. Let $a^*(t)$ denote the optimal arm at time t. The objective is to minimize the cumulative regret $R(T) = \sum_{t=1}^{T}(x_{a^*(t),t}^T\theta^* - x_{a(t),t}^T\theta^*)$.

3 The LinEI algorithm for linear bandits

In this section, we design a provable version of EI algorithm for linear bandits. For theoretical guarantees, we make some assumptions on the prior distribution of the reward function, and a form of the expected improvement in context of linear bandits.

Prior and Posterior Distributions. We follow the design for priors of the reward function like TS algorithm [3]. We assume that the reward $r_{i,t}$ of each arm i follows a Gaussian distribution $\mathcal{N}(x_{i,t}^\top\theta^*, v^2)$, where the variance v^2 is a free parameter (possibly time-dependent) that can be set specific to an algorithm. Let $X(t) = \lambda I + \sum_{j=1}^{t-1} x_{a(j),j}x_{a(j),j}^\top$, $\hat{\theta}_t = X(t)^{-1}(\sum_{j=1}^{t-1} x_{a(j),j}r_{a(j),j})$. Then if we assume that the prior for θ^* at time t is given by $\mathcal{N}(\hat{\theta}_t, v^2X^{-1}(t))$, then the posterior distribution of θ^* at time $t+1$ is $\mathcal{N}(\hat{\theta}_{t+1}, v^2X^{-1}(t+1))$ (see the proof in Appendix A.1 in [3]).

Expected Improvement. We now use this posterior distribution update to define the form of the expected improvement of each arm in contextual bandits. We denote $r_t^+ = \max_{i\in\mathcal{K}}\{x_{i,t}^T\hat{\theta}_t\}$ which is the largest mean estimate of reward among all arms at time t. We define the expected improvement of an arm i at time t as

$$\alpha_{i,t}^{EI} = \mathbb{E}_{\mu\sim\mathcal{N}(\hat{\theta}_t, v_t^2X(t)^{-1})}[\max\{0, x_{i,t}^\top\mu - r_t^+\}], \tag{1}$$

The $\alpha_{i,t}^{EI}$ measures the potential of arm i to improve upon the largest posterior reward mean r_t^+ at time t. Here, r_t^+ plays a role as an incumbent. In Bayesian optimization, the incumbent is usually selected as the best reward value so far, or the largest reward mean so far. In our setting with contextual bandits, we choose the latter for convenience in analysis.

The closed form for EI. Since $\mu \sim \mathcal{N}(\hat{\theta}_t, v^2X(t)^{-1})$, the marginal distribution of $x_{i,t}^T\mu$ is Gaussian with mean $x_{i,t}^T\hat{\theta}_t$ and standard deviation $vs_{i,t}$, where we define $s_{i,t} = \sqrt{x_{i,t}^TX(t)^{-1}x_{i,t}}$. Setting $z_{i,t} = \frac{x_{i,t}^\top\hat{\theta}_t - r_t^+}{vs_{i,t}}$, we can express the expected improvement in closed form as follows

$$\alpha_{i,t}^{EI} = vs_{i,t}[z_{i,t}\Phi(z_{i,t}) + \phi(z_{i,t})], \tag{2}$$

where $\Phi(.)$ and $\phi(.)$ are the standard normal cdf and pdf function of the normal distribution respectively.

3.1 Proposed LinEI Algorithm.

We now use the above form of expected improvement to design our algorithm. The algorithm is performed iteratively as follows. At iteration t, it selects the arm suggested by the EI strategy if the expected improvement (measured by $\alpha_{i,t}^{EI}$ of all arms) is higher than a threshold. Otherwise it simply selects the arm suggested by the greedy strategy (corresponding to the arms whose posterior reward mean is r_t^+). The choice of thresholds plays an important role for convergence of our algorithm. We propose to use an adaptive threshold in the form of $\frac{C_0}{t^\beta}$ which is controlled by two parameters C_0, β. A relevant choice of parameters of the threshold comes from our theoretical analysis which will be discussed in the next section. Our algorithm is summarized in Algorithm 1.

We remark that the proposed algorithm can be considered as a variant of EI strategy with a simple modification. This modification comes from our observation that at an iteration, when the EI value is

Algorithm 1 The Linear Expected Improvement Algorithm (LinEI)

Input: Parameters C_0, β

for $t = 1$ to T **do**
  Observe contexts $\{x_{i,t}\}_{i=1}^K$
  Set $\overline{a}(t) := \text{argmax}_{i\in\mathcal{K}} \alpha_{i,t}^{EI}$, $\tilde{a}(t) = \text{argmax}_{i\in\mathcal{K}}\{x_{i,t}^\top \hat{\theta}_t\}$
  if $\alpha_{\overline{a}(t),t}^{EI} \geq \frac{C_0}{t^\beta}$ **then**
    $a(t) = \overline{a}(t)$
  else
    $a(t) = \tilde{a}(t)$
  end if
  Play arm $a(t)$, and observe reward $r_{a(t),t}$
  Update $X(t+1) = \lambda I_d + \sum_{j=1}^t x_{a(j),j} x_{a(j),j}^\top$, $\hat{\theta}_{t+1} = X(t+1)^{-1}(\sum_{j=1}^t x_{a(j),j} r_{a(j),j})$
end for

less than some threshold, using a greedy strategy is better than the EI strategy in the sense that the instantaneous regret is smaller. This is our interesting observation about the relation between the EI and the greedy strategy, and we use this in our algorithm design. Without the modification, a pure EI algorithm can make the cumulative regret become unbounded in our theoretical analysis.

Comparison with LinUCB [1] and LinTS [3]. LinUCB looks for the most optimistic value for an arm in an ellipsoid defined by a level set of the posterior rather than integrating over it, and then chooses an arm that maximizes the optimistic value. LinTS generates a sample μ from the posterior distributions $\mathcal{N}(\hat{\theta}_t, v_t^2 X(t)^{-1})$ of reward and then chooses an arm that maximizes $x_{i,t}^T \mu$. Unlike LinUCB and LinTS, LinEI could choose an arm whose maximum optimistic value is lower and/or choose an arm having lower $x_{i,t}^T \mu$ but for which there are more possibilities for improvement.

3.2 Theoretical Analysis

In this section, we provide the regret bound for the proposed LinEI algorithm.

The EI technique is used so far in BAI and BO problems to seek the best arm with the highest reward mean. In such problems, the reward mean of each arm is fixed in advance. To leverage this property, [30] uses the *allocation matching* technique to allocate enough number of samples to suboptimal arms so that we can eliminate these arm with a high confidence. In BO, [10] uses the monotonicity property of incumbent to derive directly an upper bound for the simple regret. However, in contextual bandits where the best arm does not exist, and the mean reward of any arm can be different in different iterations, the monotonicity property of incumbent disappears, and the allocation technique is also no longer applicable. The proposed LinEI addresses these challenges. Moreover, it selects an arm based on not only EI strategy but also a greedy strategy depending on a threshold function. This makes our regret analysis different from the standard EI technique in [39],[28].

In our proof, we first extend several results in [10] in Bayesian optimization in a non-contextual setting to our setting with contexts and noises. For instance, the following lemma is used to upper bound and lower bound the expected improvement for each arm i.

Lemma 3.1. *Pick* $0 < \delta < 1$. *Set* $I_{i,t} = max\{0, x_{i,t}^T \theta^* - r_t^+\}$. *Then with probability* $1 - \frac{\delta}{t^2}$ *we have*

$$I_{i,t} - \beta_t s_{i,t} \leq \alpha_{i,t}^{EI} \leq I_{i,t} + (\beta_t + v_t) s_{i,t}$$

Here, $\beta_t = R\sqrt{d\ln(\frac{t^3}{\delta})} + 1$, $s_{i,t} = \sqrt{x_{i,t}^\top X(t)^{-1} x_{i,t}}$ and v_t is used instead of v. Then, depending on the arm selection by our LinEI algorithm, we can upper bound the instantaneous regret $r_t = x_{a^*(t),t}^\top \theta^* - x_{a(t),t}^\top \theta^*$ by two different ways. Combining them, we achieve an upper bound for the instantaneous regret $r_t = x_{a^*(t),t}^\top \theta^* - x_{a(t),t}^\top \theta^*$ as in section C of our Supplementary Material:

$$r_t \leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}(2\beta_t + v_t) s_{a(t),t} + \beta_t s_{a(t),t} + \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} \frac{C_0}{t^\beta} + \sqrt{2\ln(Rt^\beta) + 2\sqrt{3C_0^{-2} d\ln(\frac{t}{\delta})}} v_t s_{a(t),t},$$

Algorithm 2 Neural Expected Improvement Algorithm (NeuralEI)

Input: Number of rounds T, exploration variance ν, network width m, regularization parameter λ and parameters C_0, β

Set $U_0 = \lambda I$
for $t = 1$ to T **do**
  Set $\overline{a}(t) := \text{argmax}_{i\in[K]}\alpha_{i,t}^{EI}$, $\tilde{a}(t) = \text{argmax}_{i\in[K]}\{f(x_{i,t};\theta_{t-1})\}$
  if $\alpha_{\overline{a}(t),t}^{EI} \geq \frac{C_0}{t^\beta}$ **then**
    $a(t) = \overline{a}(t)$
  else
    $a(t) = \tilde{a}(t)$
  end if
  Play arm $a(t)$, and observe reward $r_{a(t),t}$
  Set θ_t to be the output of gradient descent for solving Eq(3)
  $U_t = U_{t-1} + g(x_{a(t),t};\theta_t)g^\top(x_{a(t),t};\theta_t)/m$
end for

with probability at least $1-\delta$. The function τ is defined as $\tau(z) = z\Phi(z) + \phi(z)$. Here, we note that parameter v_t plays the role of parameter v at time t we discussed above. In our analysis, v_t is used to eliminate the influence of β_t so that $\frac{\beta_t}{v_t}$ is bounded as t grows.

Finally, by a relevant choice of parameters C_0 and β, we achieve the regret bound for our proposed algorithm as follows:

Theorem 3.2. *Given any $\delta \in (0,1)$. If $v_t = R\sqrt{3dln\frac{t}{\delta}} + 1$, $\sqrt{d} \leq C_0 \leq d$ and $0.5 \leq \beta \leq 3$ then with probability $1-\delta$, the cumulative regret of the LinEI algorithm is bounded as*

$$R(T) = \mathcal{O}(d\sqrt{Tln^2(T)ln\frac{T}{\delta}})$$

4 The NeuralEI algorithm for Neural Contextual Bandits

In this section, we extend our Algorithm 1 to the more general setting where the reward function is modelled by a fully connected neural network. Similar to the Neural Thompson Sampling approach [41], our algorithm maintains a Gaussian distribution for each arm's reward. At time t, the posterior distribution of the reward of arm i is updated as follows. The mean is set to the output of the neural network, denoted by $f(x_{i,t};\theta_{t-1})$, and the variance is defined as $\sigma_{i,t}^2 = \lambda g^\top(x_{i,t};\theta_{t-1})U_{t-1}^{-1}g(x_{i,t};\theta_{t-1})/m$, where the matrix U_t^{-1} is updated as $U_t = U_{t-1} + g(x_{a(t),t};\theta_t)g^\top(x_{a(t),t};\theta_t)/m$ and parameter θ_t is the solution to the following minimization problem:

$$\min_\theta \sum_{i=1}^{t}[f(x_{a(i),i;\theta}) - r_{a(i),i}]^2/2 + m\lambda||\theta-\theta_0||_2^2/2, \tag{3}$$

where θ_0 is randomly initialized network parameter. We can adapt gradient descent algorithms to solve this problem with step size η and total number of iterations J like the gradient descent algorithm of [42].

Expected Improvement for Neural Contextual Bandits. We now define the form of the expected improvement in this setting. At each time step t, we denote $f_t^+ = \max_{i\in[K]}\{f(x_{i,t};\theta_{t-1})\}$ which is the highest mean estimate of $f(x,\theta_{t-1})$ among all arms at time t. We define the expected improvement value of an arm i at time t as

$$\alpha_{i,t}^{EI} = \mathbb{E}_{\widetilde{f}_{i,k}\sim\mathcal{N}(f(x_{i,t};\theta_{t-1}),\nu^2\sigma_{i,t}^2)}[\max\{0, \widetilde{f}_{i,k} - f_t^+\}].$$

Further, by setting $z_{i,t} = \frac{f(x_{i,t};\theta_{t-1})-f_t^+}{\nu\sigma_{i,t}}$, the above expectation can be computed analytically as follows

$$\alpha_{i,t}^{EI} \quad = \quad \nu\sigma_{i,t}[z_{i,t}\Phi(z_{i,t}) + \phi(z_{i,t})] \tag{4}$$

Our NeuralEI algorithm is given in Algorithm 2. It starts by initializing $\theta_0 = (\text{vec}(W_1); ...; \text{vec}(W_L))$, where for each $1 \leq l \leq L-1, W_l = (W, 0; 0, W)$, each entry of W is generated independently from $N(0, 4/m)$; $W_L = (w^\top, -w^\top)$, each entry of w is generated independently from $N(0, 2/m)$. NeuralEI extends our LinEI algorithm to the setting where the reward function h is modelled by a fully connected neural network.

4.1 Regret Analysis

In this section, we provide a regret analysis of the NeuralEI algorithm. We first provide necessary background on the neural tangent kernel (NTK) theory, which plays an important role in our analysis. Following a recent line of research [42, 41], we define the covariance between two data point $x, y \in \mathbb{R}^d$ as follows: $\tilde{H}^{(1)}(x,y) = \sigma^{(1)}(x,y) = x^\top y$, $A^{(l)}(x,y) = \begin{pmatrix} \sigma^{(l)}(x,x) & \sigma^{(l)}(x,y) \\ \sigma^{(l)}(x,y) & \sigma^{(l)}(y,y) \end{pmatrix}$, $\sigma^{l+1}(x,y) = 2\mathbb{E}_{(u,v)\sim N(0,A^{(l)}(x,y))}[\sigma(u)\sigma(v)]$, $\tilde{H}^{(l+1)}(x,y) = 2\tilde{H}^{(l)}(x,y)\mathbb{E}_{(u,v)\sim N(0,A^{(l)}(x,y))}[\sigma'(u)\sigma'(v)] + \sigma^{(l+1)}(x,y)$. Similar to [42, 41], we assume that the number of rounds T is *known* and denote the neural tangent kernel (NTK) matrix $H \in \mathbb{R}^{TK \times TK}$ based on all contextual vectors $\{x_{t,k}\}_{t\in[T],k\in[K]}$. Renumbering $\{x_{t,k}\}_{t\in[T],k\in[K]}$ as $\{x_i\}_{i=1,...,TK}$, then each entry H_{ij} is defined as

$$H_{ij} = (\tilde{H}^{(L)}(x_i, x_j) + \sigma^{(L)}(x_i, x_j))/2, \tag{5}$$

for all $i, j \in [TK]$. Based on the above definition, we impose the following assumption on the contexts generated by the adversary and the corresponding NTK matrix H.

Assumption 4.1. Let H be defined in Eq(5). There exists $\lambda_0 > 0$ such that $H \geq \lambda_0 I$. In addition, for any $t \in [T], k \in [K]$, $||x_{t,k}||_2 = 1$ and $[x_{t,k}]_j = [x_{t,k}]_{j+d/2}$.

Remark 1. Compared to Algorithm 1 for linear bandits, our Algorithm 2 needs an additional Assumption 1 to guarantee the convergence. The assumption that the NTK matrix is positive definite has been considered in prior work on NTK which is a mild condition and also imposed in other related works [4, 15, 42, 41]. The assumption on contexts ensures that $f(x_{i,t}; \theta_0) = 0$ for any $i \in [K], t \in [T]$.

The NTK technique builds a connection between deep neural networks and kernel methods. It enables us to adapt some complexity measures for kernel methods to describe the complexity of the neural network through the notation of the effective dimensions as defined in [42, 41]. The effective dimension $\tilde{d}$ of matrix H with regularization parameter λ is defined as $\tilde{d} = \frac{\log\det(I+H/\lambda)}{\log(1+TK/\lambda)}$.

Using these notations, we are now ready to present the second main result of the paper. Let $a^*(t) = \text{argmax}_{i\in[K]}\mathbb{E}[r_{i,t}]$ be the optimal action at round t that maximizes the expected reward, we define the *expected cumulative regret* after T iterations as $\overline{R}(T) = \mathbb{E}[\sum_{t=1}^{T}(r_{a^*(t),t} - r_{a(t),t})]$. Then, we achieve the following upper regret bound for our Algorithm 2 by combining our EI techniques for LinEI with NTK techniques. A completed proof is provided in Supplementary Material.

Theorem 4.2. *Under Assumption 1, set the parameters in Algorithm 2 as* $\lambda = 1 + 1/T$, $\nu = B + R\sqrt{\tilde{d}log(1+TK/\lambda) + 2 + 2log(1/\delta)}$, *where* $B = max\{1, \sqrt{2h^\top H^{-1}h}\}$ *with* $h = (h(x_1), ..., h(x_{TK}))^\top$. *If* $\sqrt{\tilde{d}} \leq C_0 \leq \tilde{d}$, $\beta \geq 2$, *and the network width* m *satisfies* $m \geq poly(\gamma, T, K, L, log(1/\delta))$, *then with probability at least* $1-\delta$, *the regret of Algorithm 2 is bounded as*

$$\overline{R}(T) \leq \mathcal{O}(\tilde{d}\sqrt{\beta log(1+TK)log(T)T})$$

Remark 2. The regret bound depends on the parameter β. The best choice is $\beta = 2$ that tightens the regret. Theorem 4.2 implies the regret of NeuralEI is on the order of $\tilde{\mathcal{O}}(\tilde{d}\sqrt{T})$. This result matches the regret bound of NeuralUCB ([42]), NeuralTS ([41]), as well as of [12]. The effective dimension $\tilde{d}$ measures how quickly the eigenvalues of H diminish, and only depends on T logarithmically in several special cases ([37]), according to [42]. Furthermore, [41] shows that $\tilde{d}$ can be upper bounded if all contexts are nearly on some low-dimensional subspace of the RKHS space spanned by NTK. Currently, [20] gives an explicit sublinear regret bound for a neural network based UCB algorithm. However, their solution requires that contexts lie on on the d-dimensional hyper-sphere. Compared to these works, our EI based results may be of independent interest.

Remark 3. Similar to most of existing results in neural bandits, our results require a large value of m. This is rooted in the current deep learning theory based on the neural tangent kernel.

4.2 Technical Challenges

While the proof of NeuralEI follows the same lines as that of LinEI, we emphasize several key differences. First, we define filtration $\mathcal{F}_{t-1}$ as the union of history until time $t-1$, and the contexts at time t. Given a time t, we define an event $\mathcal{E}_t^\sigma$ as follows:

$$\mathcal{E}_t^\sigma = \{\omega \in \mathcal{F}_t : \forall i \in [K],\ |\tilde{f}_{i,t} - f(x_{i,t};\theta_{t-1})| \leq c_t \nu \sigma_{i,t}\},$$

where $c_t = \sqrt{4\text{log}t + 2\text{log}K}$.

Similarly, we define an event $\mathcal{E}_t^\mu$ as follows:

$$\mathcal{E}_t^\mu = \{\omega \in \mathcal{F}_t : \forall i \in [K],\ |f(x_{i,t};\theta_{t-1}) - h(x_{t,k})| \leq \nu \sigma_{i,t} + \epsilon(m)\},$$

where $\epsilon(m)$ is defined as in [41].

Based on the definitions of event $\mathcal{E}_t^\sigma$ and $\mathcal{E}_t^\mu$, we achieve two different ways to lower bound and upper bound the expected improvement as follows:

Lemma 4.3. *Assume that the event $\mathcal{E}_t^\mu$ holds. Set $J_{i,t} = max\{0, h(x_{i,t}) - f_t^+\}$. Then for every $i \in [K]$, we have*

$$J_{i,t} - \nu\sigma_{i,t} - \epsilon(m) \leq \alpha_{i,t}^{EI} \leq J_{i,t} + \nu\sigma_{i,t} + \epsilon(m).$$

Lemma 4.4. *Assume that the event $\mathcal{E}_t^\sigma$ holds. Set $I_{i,t} = max\{0, \tilde{f}_{i,t} - f_t^+\}$. Then for every $i \in [K]$, we have*

$$I_{i,t} - c_t\nu\sigma_{i,t} \leq \alpha_{i,t}^{EI} \leq I_{i,t} + \nu(c_t + 1)\sigma_{i,t}.$$

While Lemma 4.3 is an adaptation of Lemma 3.1 to neural contextual bandits, Lemma 4.4 is a novel result compared to the regret analysis in our Section 3.1 for linear bandits. Challenges of analyzing the regret of NeuralEI come from the fact that there exists additionally a factor $\epsilon(m)$ in 4.3. Compared to LinEI, it is hard to analyze directly the regret $h(x_{a^*(t),t}) - h(x_{a(t),t})$. We divide the analysis into two cases: if $\sigma_{a^*(t),t} \leq \epsilon(m)$, we can follow the technique as in LinEI. Otherwise, we use another way to bound the regret using a novel result as we mentioned in the main paper. Please see Lemma D.11 in the appendix for details.

5 Related Works and Discussion

Given the vast literature on bandit algorithms, we restrict our review to linear bandits and neural contextual bandits.

Linear Contextual Bandit. A lower bound of $\Omega(d\sqrt{T})$ for linear bandits was given in [14], when the number of arms is allowed to be infinite. [1] analyze a UCB-style algorithm and provide a regret upper bound $\mathcal{O}(d\text{log}(T)\sqrt{T} + \sqrt{dT\text{log}(T/\delta)})$. Compared to this work, the regret of our proposed LinEI has an additional $\sqrt{\text{ln}T}$, however, it still matches the information theoretic lower bound in this setting. When the number of arms K is finite, [13] achieve a regret bound of $\mathcal{O}(\sqrt{Td\text{ln}^3(KT\text{ln}T)/\delta})$ with probability at least $1-\delta$. [9] provides an algorithm based on exponential weights, with regret of order $\mathcal{O}(d\sqrt{T\text{log}K})$. These algorithms may not be effective when the number of arms K is large. For example, when K is exponential in d, the regret bound of [13] would become $\tilde{\mathcal{O}}(d^2\sqrt{T})$ showing a quadratic growth in d.

The Thompson Sampling algorithm [3] and an alternative given in [2] bear an additional $\sqrt{d}$ in the regret bound. Very recently, [21] improved this regret bound of TS in some cases by integrating a doubly robust estimator with TS. However, this work requires additional significant computations and their setting is limited in independent contexts. In contrast, our EI-based algorithm achieves the optimal order of d even in a general setting where the contexts may be controlled by an adaptive adversary.

Table 1: Characteristics of benchmark datasets used in Section 6.

Dataset	letter	pendigits	covertype	avila	magic	dry bean	statlog
Classes (K)	26	10	7	12	2	7	7
Feature Dimension	17	16	54	10	10	16	8
Dataset size	20000	10992	581012	20867	19020	13611	58000

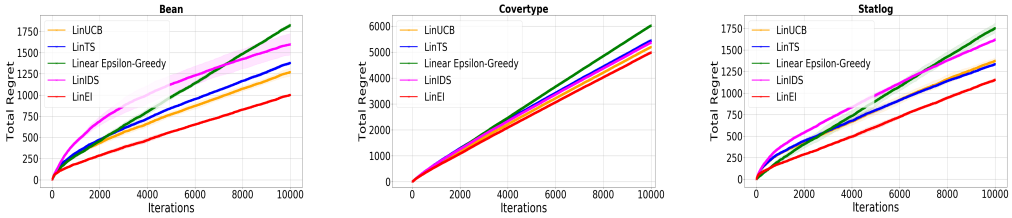

Figure 1: Comparison of our proposed LinEI and baseline algorithms in linear bandits.

Another approach for linear bandits is the Information Directed Sampling (IDS) which was introduced in [33]. It provides an action-selection mechanism by minimizing the information ratio between the squared expected regret and the mutual information between optimal action and the next observation over all action sampling distributions. IDS obtains a performance improvement over TS and UCB algorithms in some cases, but has heavy sampling requirements. It has been shown in their experiments that IDS requires significantly more compute time than Thompson sampling and UCB algorithms. Recently, [5] provided a modification of the arm scoring rule of IDS to reduce computations. However, both [33] and [5] only provide the bounds on *expected regret*. In contrast, our work provides regret bounds in terms of cumulative regret which is tighter than expected regret.

Neural Contextual Bandit. Neural contextual bandits are becoming attractive due to the current advancement in optimization and generalization of deep neural networks [4, 15]. Neural contextual bandits have been considered in both popular techniques UCB [42] and Thompson Sampling [41]. Currently, [6] proposes a novel neural exploration strategy and their solution achieves a sublinear regret on T. Compared to all existing works in this sub-field, our EI based algorithm is new, and may be of independent interest.

Due to space limit, we will add additional related works in Section B of Supplementary Material.

6 Experiments

6.1 Linear Bandits

In this subsection, we assess the performance of our LinEI algorithm on several benchmark datasets including `covertype`, `magic`, `avila`, `dry bean`, `statlog`, `letter`, `pendigits`, all from UCI [16]. See our Table for details. We compare the LinEI with methods designed for linear bandits including: LinTS [3], LinUCB [1], Linear Epsilon Greedy for the linear reward, LinIDS [33] for linear bandits. To transform these classification problems into multi-armed bandits, we adapt the disjoint models to build a context feature vector for each arm: given an input feature $x \in \mathbb{R}^d$ of a k-class classification problem, we build the context feature vector with dimension kd as $x_1 = (x; 0; ...; 0), x_2 = (0; x; ...; 0), ..., x_k = (0; 0...; x)$. The algorithm generates a set of predicted reward and pulls the greedy arm. For these classification problems, if the algorithm selects a correct class by pulling the corresponding arm, it will receive a reward as 1, otherwise 0. The cumulative regret over time horizon T is measured by the total mistakes made by the algorithm.

We set the time horizon of our algorithm to 10000 for all data sets. In the experiments, we shuffle all datasets randomly. For (λ, ν) used in LinUCB and LinTS and our algorithm, we set $\lambda = 1$ following previous works and do a grid search of $\nu \in \{1, 0.1, 0.01\}$ to select the parameter with the best performance. All experiments are repeated 10 times, and the average with standard error are reported. For LinIDS, we use the number of samples $M = 100$. For Linear Epsilon Greedy, we use $\epsilon = 0.1$.

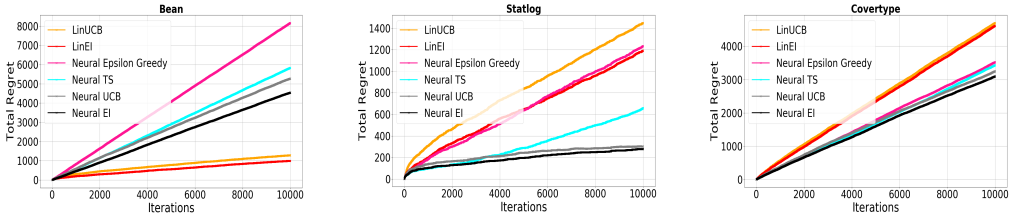

Figure 2: Comparison of NeuralEI and baseline algorithms on real-world datasets.

For our LinEI algorithm, we can choose any value $C_0 \in [\sqrt{d}, d]$ and $\beta \in [0.5, 3]$. For LinEI, we set $C_0 = \sqrt{d}$ and $\beta = 2$.

Figure 1 shows the total regret of all algorithms for datasets `bean`, `covertype` and `statlog`. The Linear Epsilon Greedy performs the worst. While LinUCB, LinTS and LinIDS are competitive, all these methods are significantly outperformed by the proposed algorithm. This difference in performance is because of the strategy used by each method. Due to space limit, the additional results on `magic`, `pendigits`, `letter`, and `avila` are shown in Section A of **Supplementary Material**. Our results on various datasets confirm that the exploration of the expected improvement is effective in practice. This also is widely observed in Bayesian optimization.

6.2 Neural Bandits

We compare the proposed NeuralEI with baselines including: LinUCB [1], our LinEI for linear bandits problem, Neural Epsilon Greedy, NeuralUCB [42], NeuralTS [41]. We do the same classification problems as the experiments in subsection Linear Bandits. For methods using the neural network, we use one-hidden layer neural networks with 100 neurons to model the reward function. During posterior updating, gradient descent is run for 100 iterations with learning rate 0.001. For Neural UCB/Thompson Sampling and Neural EI, we use a grid search on $\lambda \in \{1, 10^1, 10^{-2}, 10^{-3}\}$ and $\nu \in \{10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}\}$ as in [42] and [41]. We consider our algorithm on both synthetic datasets and real-world datasets. Due to space limit, we will provide results on synthetic datasets in Section A of Supplementary Material.

Real-world Datasets. Similar to the subsection Linear Bandit, we build the context feature vector with dimension kd as $x_1 = (x; 0; ...; 0), x_2 = (0; x; ...; 0), ..., x_k = (0; 0...; x)$. We also estimate our algorithm on datasets `bean`, `covertype` and `statlog`. Figure 2 show our results in the case of the neural bandits problem. Neural-based methods perform better because they can capture the nonlinearity of the underlying reward function. In real-datasets, while neural-based methods outperform LinEI and LinUCB for datasets `covertype` and `statlog`, these methods are not sample-efficient for learning the reward function of dataset `bean`. Perhaps, the reward function for dataset `bean` is linear. However, in all cases, our NeuralEI algorithm performs better than other neural-based methods. This suggests that using the expected improvement strategy is effective in both linear bandits and neural contextual bandits.

7 Conclusion

We introduced and formalized Expected Improvement as a new strategy for contextual bandits. We proposed two EI-based algorithms and analyzed them theoretically. The first algorithm assumes the reward function to be linear whilst the second algorithm is designed for the case when the reward function is general and can be modelled by a deep neural network. Our promising empirical results on real-world datasets suggested that our EI-based algorithms work well in practice compared to other approaches especially in high dimensions. We believe our work would be useful for further improvements and extensions. For example, we have used NTK in our work, but the NTK theory assumes overparameterised networks and an extension to narrow networks while maintaining the generalization of the reward function is an interesting open problem.

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Checklist

The checklist follows the references. Please read the checklist guidelines carefully for information on how to answer these questions. For each question, change the default **[TODO]** to [Yes] , [No] , or [N/A] . You are strongly encouraged to include a **justification to your answer**, either by referencing the appropriate section of your paper or providing a brief inline description. For example:

- Did you include the license to the code and datasets? [Yes] See Section **??**.
- Did you include the license to the code and datasets? [No] The code and the data are proprietary.
- Did you include the license to the code and datasets? [N/A]

Please do not modify the questions and only use the provided macros for your answers. Note that the Checklist section does not count towards the page limit. In your paper, please delete this instructions block and only keep the Checklist section heading above along with the questions/answers below.

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]

(b) Did you describe the limitations of your work? [Yes]
(c) Did you discuss any potential negative societal impacts of your work? [N/A]
(d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes]

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes]
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [No]

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [N/A]
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]

5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

Supplementary Material

A Additional Experiments

As mentioned in the main paper, in this section, we provide several additional experiments for linear bandits on datasets: pendigit, avila, magic and letter. Figure 3 also showed that our proposed LinEI

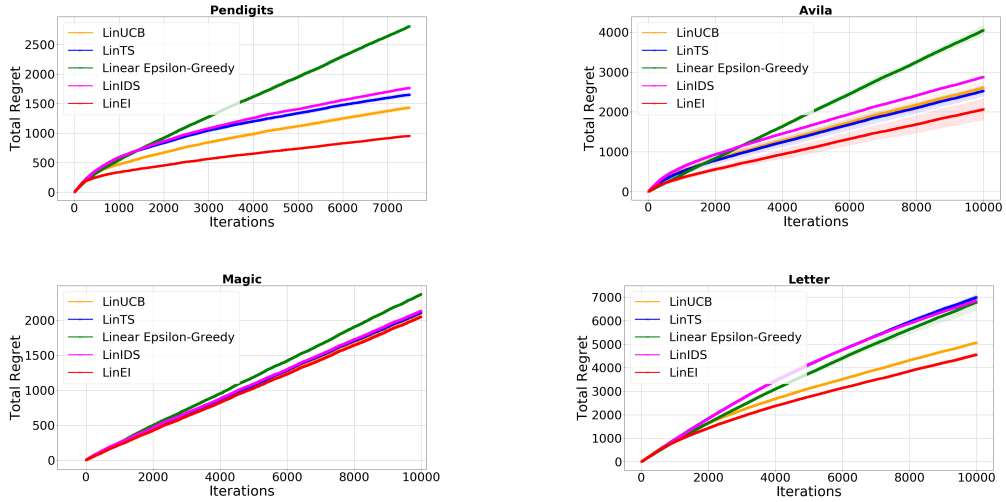

Figure 3: Comparison of LinEI and baseline algorithms on datasets.

algorithm outperforms LinUCB, LinTS and LinIDS and Linear Epsilon Greedy.

A.1 Comparing LinEI with LinUCB and LinTS in terms of dimensions d

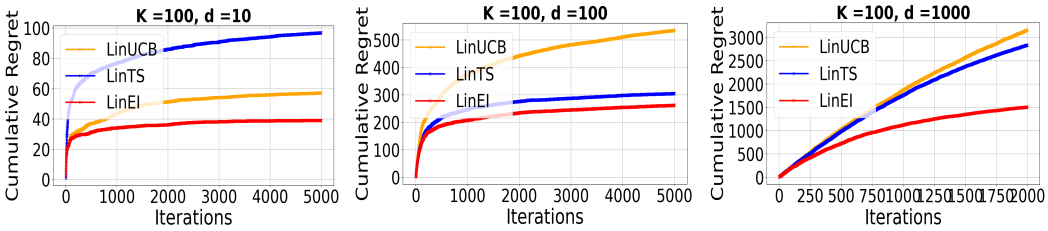

Figure 4: Comparison of our proposed LinEI and baseline algorithms with different dimensions.

Table 2: The average computation time (second)

Dimension	LinUCB	LinTS	LinEI
$d = 10$	0.018	0.015	0.024
$d = 100$	0.46	0.73	0.12
$d = 1000$	1.37	2.32	0.26

To demonstrate that our proposed LinEI scales to higt dimensions better than LinUCB, LinEI, we build a contextual bandit in linear setting as follows. We fix $K = 100$ actions. The context vectors are chosen uniformly at random from the unit ball. The reward function $r = x^T\theta^*$, where θ^* is generated *a priori*. Using this setting, we compared our LinEI with LinUCB and LinTS in a range of dimensions $d = 10, 100$ and 1000. Our results show that

- LinEI scales to high dimensions better than LinUCB and LinTS. This can be explained as the regret of LinEI is better than that of LinTS by a factor $\sqrt{d}$ while LinUCB can be considered as an over-explored strategy in high dimensions. See our Figure 4.

- Concerning the computation time, LinUCB faces a NP-hard problem at each iteration [3], and thus spends more time for optimization especially in high dimensions. LinTS uses a random sampling based heuristic and requires a a multivariate Gaussian sampling step at each iteration. This is a high-dimensional multivariate Gaussian sampling problem [38]. It has computational cost and memory requirements which can rapidly become prohibitive in high dimension. In contrast, our LinEI can avoid both the NP-hard problem and the high-dimensional Gaussian sampling problem. Thus, the computation cost of LinEI is significantly cheaper in high dimensions. See our Table 2.

A.2 Comparing LinEI with LinUCB and LinTS on an Large-scale Multi-Label Dataset

We now compare our proposed LinEI against LinUCB and LinTS on the eurlex-4k dataset which is a large multi-label dataset [7]. It contains data with 5000 features and 3993 labels. It corresponds to a contextual bandit problem with 3993 actions and the dimension of context is $5000 + 3993 = 8993$ when mapped to our setting. This can be considered as a contextual bandit problem with large action space and with very high dimensions. Due to the heavy computation, we run algorithms on only 3000 datapoints from the test set. Our experimental results show that LinEI scales better to high dimensions and to large action space (see our Figure 5). This can be explained as the regret of LinEI is better than that of LinTS by a factor $\sqrt{d}$ while LinUCB is an over- exploration strategy in high dimensions. In terms of required computations, LinEI is significantly cheaper than LinUCB and LinTS. The average-per iteration computation times of LinUCB, LinTS and LinEI are 1055.5s, 1496.2s and 181.3s respectively as shown in Table 3. This is because LinTS faces a high-dimensional multivariate Gaussian sampling problem. LinUCB requires to maximize quadratic forms at every round $1 \leq t \leq T$: argmax $x_{t,i}^T \theta$, where $i \in [K]$, and $\theta \in C_t$, where C_t is the confident set at round t. We note that θ has the same dimension as the input $x_{t,i}$. This is an NP-hard problem as [1] has mentioned in the Related Work section. When the input dimension is high, it is expensive to find a maximum with a limited computational budget. In contrast, the proposed LinEI can avoid this NP-hard problem as long as finding argmax $\alpha_{i,t}^{EI}$, where $i \in [K]$ is solved. We can see that with a not very large value of K, this is no problem.

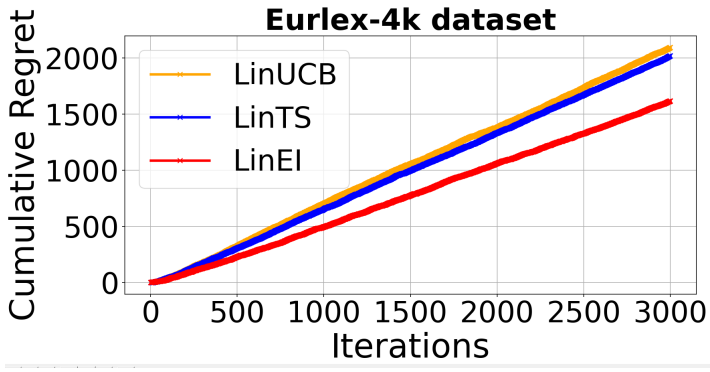

Figure 5: Comparison of our proposed LinEI and baseline algorithms.

Table 3: The average computation time (second)

Dataset	LinUCB	LinTS	LinEI
Eurlex-4k	1055.5	1496.2	181.3

B Additional Related Works

Bayesian optimization. EI has been widely used in Bayesian optimization which is a non-contextual problem. In contextual bandits we consider here, the mean reward of an arm is additionally associated with a context which may be controlled by an adversary. It follows that the mean reward for each arm can be different in each iteration depending on contexts, thus the notion of "best arm" does not exist. Due to this, the framework of EI as in Bayesian optimization does not naturally extend to contextual bandits. Moreover, our proposed algorithm in contextual bandits selects an arm based on not only EI strategy but also a greedy strategy depending on a threshold function. This makes our regret analysis different from the standard EI technique in [39],[28], and [36].

Nonlinear Bandits The works of [37] and [22] extended linear bandits to kernel bandits and generalized linear bandits, respectively. However, they still required fairly restrictive assumptions on the reward function compared to neural contextual bandits. Neural contextual bandits are becoming attractive due to the current advancement in optimization and generalization of deep neural networks [4, 15]. Most of existing algorithms for neural bandits used either UCB technique [42, 20], or Thompson Sampling technique [41]. Currently, [6] proposed a novel neural exploration strategy and their solution achieved a sublinear regret on T. Compared to all existing works in this sub-field, our EI-based algorithm is new, and may be of independent interest.

On the asymptotic regret. In [23], authors analyzed the asymptotic regret for linear bandits. While showing that both optimism principle and Thompson sampling cannot be close to asymptotically optimal in the setting of linear bandits. Currently, the work in [35] analyzed the asymptotic regret for the contextual linear bandit problem which is similar to our setting. In their setting, context x_t are drawn i.i.d. from a context distribution. Different from these settings, we consider contextual linear bandits where contexts may be controlled by an adversary. Further, we also consider the neural contextual bandits which are more general than the linear bandit considered in [23] and [35]. To our knowledge, the analysis of the asymptotic regret for neural contextual bandits is still an open problem.

C Regret Analysis for LinEI Algorithm

C.1 Auxiliary Results

For our theoretical analysis for LinEI, we use following several auxiliary lemmas.

Lemma C.1. *(Upper Bounds of a Hyperharmonic Series, [11]) Given a hyperharmonic series* $p_n = \sum_{t=1}^{n} \frac{1}{t^\beta}$*, where* $n \in \mathbb{N}$*. Then,*

- $p_n < 1 + \frac{n^{1-\beta}-1}{1-\beta}$ *if* $\beta \geq 0$ *and* $\beta \neq 1$*,*
- $p_n < 1 + ln(n)$ *if* $\beta = 1$

Lemma C.2 (Lemma 1 of [3])**.** *For all* t*,* $0 < \delta < 1$*, with probability* $1 - \frac{\delta}{t^2}$*, we have*

$$\forall i : |x_{i,t}^T \hat{\theta}_t - x_{i,t}^T \theta^*| \leq \beta_t s_{i,t},$$

where $\beta_t = R\sqrt{dln(\frac{t^3}{\delta})} + 1$*, and* $s_{i,t} = \sqrt{x_{i,t}^T X(t)^{-1} x_{i,t}}$*.*

Lemma C.3 (Lemma 3 of [13])**.** *For* $T \geq 2$*, we have*

$$\sum_{i=1}^{T} s_{a(t),t} \leq 5\sqrt{dTln(T)}.$$

We note that except that Lemma C.2 and Lemma C.3 are used from the analysis of LinTS and LinUCB, the following results are different from those of LinUCB and LinTS.

To derive the regret for our LinEI algorithm, we will need a lower bound and a upper bound of EI for each arm $i \in [K]$ as follows.

Lemma C.4. *Pick $0 < \delta < 1$. Set $I_{i,t} = max\{0, x_{i,t}^T\theta^* - r_t^+\}$. Then with probability $1 - \frac{\delta}{t^2}$ we have*

$$I_{i,t} - \beta_t s_{i,t} \leq \alpha_{i,t}^{EI} \leq I_{i,t} + (\beta_t + v_t)s_{i,t}.$$

Proof. If $s_i(t) = 0$ then $\alpha_{i,t}^{EI} = I_{i,t}$, which makes the result trivial. We now assume that $s_{i,t} > 0$. Set $q = \frac{x_{i,t}^T\theta^* - r_t^+}{s_{i,t}}$ and $u = \frac{x_{i,t}^T\hat{\theta}_t - r_t^+}{s_{i,t}}$. Set $\tau(z) = z\Phi(z) + \phi(z)$. Then we have that

$$\alpha_{i,t}^{EI} = v_t s_{i,t}\tau(\frac{u}{v_t}).$$

By Lemma C.2, we have that $|u - q| \leq \beta_t$ with probability $1 - \delta$. As $\tau'(z) = \Phi(z) \in [0, 1]$, τ is non-decreasing and $\tau(z) \leq 1 + z$ for $z > 0$. Hence,

$$\begin{aligned}
\alpha_{i,t}^{EI} &\leq v_t s_{i,t}\tau(\frac{\max\{0, q\} + \beta_t}{v_t}) \\
&\leq v_t s_{i,t}(\frac{\max\{0, q\} + \beta_t}{v_t} + 1) \\
&= I_{i,t} + (\beta_t + v_t)s_{i,t}
\end{aligned}$$

If $I_{i,t} = 0$ then the lower bound is trivial as $\alpha_{i,t}^{EI}$ is non-negative. Thus suppose $I_{i,t} > 0$. Since $\alpha_{i,t}^{EI} \geq 0$ and $\tau(z) \geq 0$ for all z, and $\tau(z) = z + \tau(-z) \geq z$. Therefore,

$$\begin{aligned}
\alpha_{i,t}^{EI} &\geq v_t s_{i,t}\tau(\frac{q - \beta_t}{v_t}) \\
&\geq v_t s_{i,t}(\frac{q - \beta_t}{v_t}) \\
&= I_{i,t} - \beta_t s_{i,t}
\end{aligned}$$

□

C.2 Proof for Theorem 3.2

We now derive an upper bound for the cumulative regret $R(T)$. To do this, we upper bound $r_t = x_{a^*(t),t}^T\theta^* - x_{a(t),t}^T\theta^*$ for every $t \in [T]$. We break down r_t into two terms as follows:

$$\begin{aligned}
r_t &= x_{a^*(t),t}^T\theta^* - x_{a(t),t}^T\theta^* \\
&= \underbrace{x_{a^*(t),t}^T\theta^* - r_t^+}_{\text{Term 1}} + \underbrace{r_t^+ - x_{a(t),t}^T\theta^*}_{\text{Term 2}},
\end{aligned}$$

where $r_t^+ = \max_{i\in[K]}\{x_{i,t}^T\hat{\theta}_t\}$. We will upper bound Term 1 and Term 2 according to two different cases of $a(t)$, either $a_t = \text{argmax}_{i\in\mathcal{K}}\alpha_{i,t}^{EI}$, or $a_t = \text{argmax}_{i\in\mathcal{K}}\{x_{i,t}^\top\hat{\theta}_t\}$

C.3 Considering the case $a_t = \textbf{argmax}_{i\in\mathcal{K}}\alpha_{i,t}^{EI}$

We note that this case happens when $\alpha_{\bar{a}(t),t}^{EI} \geq \frac{C_0}{t^\beta}$.

Bounding Term 1

Lemma C.5. *Pick $\delta \in (0, 1)$. Then with probability at least $1 - \frac{\delta}{t^2}$ we have*

$$x_{a^*(t),t}^T\theta^* - r_t^+ \leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}(2\beta_t + v_t)s_{a(t),t}.$$

Proof. First, we consider $s_{a^*(t),t} > 0$. If $x_{a^*(t),t}^T\theta^* < r_t^+$ then the lemma will be trivial. We now consider $x_{a^*(t),t}^T\theta^* \geq r_t^+$. Following the derivation of the acquisition function α^{EI}, we have $\alpha_{a^*(t),t}^{EI} = v_t s_{a^*(t),t}\tau(\frac{x_{a^*(t),t}^T\hat{\theta}_t - r_t^+}{v_t s_{a^*(t),t}})$. Further, we also have $\frac{x_{a^*(t),t}^T\hat{\theta}_t - r_t^+}{v_t s_{a^*(t),t}} \geq \frac{-\beta_t}{v_t}$ with probability $1 - \frac{\delta}{t^2}$. It is because $x_{a^*(t),t}^T\hat{\theta}_t - x_{a^*(t),t}^T\theta^* \geq -\beta_t s_{a^*(t),t}$ with probability $1 - \frac{\delta}{t^2}$ and we are considering the case when $x_{a^*(t),t}^T\theta^* \geq r_t^+$. Therefore, $\alpha_{a^*(t),t}^{EI} \geq v_t\tau(\frac{-\beta_t}{v_t})s_{a^*(t),t}$ with probability $1 - \frac{\delta}{t^2}$.

Now, we combine inequalities $\alpha_{a^*(t),t}^{EI} \geq v_t\tau(\frac{-\beta_t}{v_t})s_{a^*(t),t}$ and $\alpha_{a^*(t),t}^{EI} \geq I_{a^*(t),t} - \beta_t s_{a^*(t),t}$ which is proven in Lemma C.4, we obtain the following inequality:

$$I_{a^*(t),t} \leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}\alpha_{a^*(t),t}^{EI} \tag{6}$$

Here we use the fact $\tau(z) = z + \tau(-z)$ for $z = \frac{\beta_t}{v_t}$. Thus, with probability at least $1 - \frac{\delta}{t^2}$ we achieve

$$\begin{aligned}
x_{a^*(t),t}^T\theta^* - r_t^+ &\leq I_{a^*(t),t} \\
&\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}\alpha_{a^*(t),t}^{EI} \\
&\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}\alpha_{a(t),t}^{EI} \\
&\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}(\max\{0, x_{a(t),t}^T\hat{\theta}_t - r_t^+\} + (\beta_t + v_t)s_{a(t),t}) \\
&\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}(\max\{0, x_{a(t),t}^T\hat{\theta}_t + \beta_t s_{a(t),t} - r_t^+\} + (\beta_t + v_t)s_{a(t),t}) \\
&\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}(\max\{0, \beta_t s_{a(t),t}\} + (\beta_t + v_t)s_{a(t),t}) \\
&= \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}(2\beta_t + v_t)s_{a(t),t},
\end{aligned}$$

where the first inequality holds by the definition of the function I_t. The second one comes from Eq(9). The third one holds by the property of the chosen point $a(t) = \text{argmax}_{i\in[K]}\alpha_{i,t}^{EI}$. The fourth inequality holds due to Lemma C.2. The sixth inequality holds due to the fact that $x_{a(t),t}^T\hat{\theta}_t \leq r_t^+$.

If $s_{a^*(t),t} = 0$ then by definition of $\alpha_{a^*(t),t}^{EI}$, we have $\alpha_{a^*(t),t}^{EI} = I_{a^*(t),t}$. We have $I_{a^*(t),t} = \alpha_{a^*(t),t}^{EI} \leq \alpha_{a(t),t}^{EI}$, where we use the definition $\alpha_{a(t),t}^{EI} = \max_{i\in[K]}\alpha_{i,t}^{EI}$. Similar to the above proof, we obtain $x_{a^*(t),t}^T\theta^* - r_t^+ \leq (2\beta_t + v_t)s_{a(t),t} \leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}(2\beta_t + v_t)s_{a(t),t}$ because $\frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} \geq \frac{\tau(0)}{\tau(0)} = 1$. Thus, the lemma holds. □

Bounding Term 2

Lemma C.6. *Pick a $\delta \in (0,1)$. If $v_t = R\sqrt{3dln(\frac{t}{\delta})} + 1$, then with probability $1 - \frac{\delta}{t^2}$ we have*

$$r_t^+ - x_{a(t),t}^T\theta^* \leq \sqrt{2ln(Rt^\beta) + 2ln(\sqrt{3C_0^{-2}dln(\frac{t}{\delta})} + C_0^{-1}R^{-1})}v_t s_{a(t),t} + \beta_t s_{a(t),t}.$$

Proof. We have

$$\alpha_{a(t),t}^{EI} = (x_{a(t),t}^T\hat{\theta}_t - r_t^+)\Phi(\frac{x_{a(t),t}^T\hat{\theta}_t - r_t^+}{v_t s_{a(t),t}}) + v_t s_{a(t),t}\phi(\frac{x_{a(t),t}^T\hat{\theta}_t - r_t^+}{v_t s_{a(t),t}})$$

$$
\begin{aligned}
&\leq \quad v_t s_{a(t)}(t)\phi(\frac{x_{a(t),t}^T\hat{\theta}_t - r_t^+}{v_t s_{a(t),t}}) \\
&= \quad v_t s_{a(t),t}\frac{1}{2\sqrt{\pi}}\exp(-\frac{1}{2}(\frac{x_{a(t),t}^T\hat{\theta}_t - r_t^+}{v_t s_{a(t),t}})^2),
\end{aligned}
$$

where the first inequality holds due to the definition of action $a(t)$. The second equality holds due to the definition of $\alpha_{a(t),t}^{EI}$. The second inequality comes from the fact that $x_{a(t),t}^T\hat{\theta}_t \leq r_t^+$. The third equality holds due to the definition of function $\phi(.)$.

From the last inequality, we obtain

$$
|x_{a(t),t}^T\hat{\theta}_t - r_t^+| \leq \sqrt{2\ln(\frac{v_t s_{a(t),t}}{\alpha_{a(t),t}^{EI}})}v_t s_{a(t),t}.
$$

By applying the facts $\alpha_{a(t),t}^{EI} \geq \frac{C_0}{t^\beta}$, $s_{a(t),t} \leq 1$, and $v_t = R\sqrt{3d\ln(\frac{t}{\delta})} + 1$ to the above inequality, we have

$$
|x_{a(t),t}^T\hat{\theta}_t - r_t^+| \leq \sqrt{2\ln(\frac{(R\sqrt{3d\ln(\frac{t}{\delta})}+1)t^\beta}{C_0})}v_t s_{a(t),t} = \sqrt{2\ln(Rt^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{t}{\delta})} + C_0^{-1}R^{-1})}v_t s_{a(t),t}.
$$

Finally, we have

$$
\begin{aligned}
r_t^+ - x_{a(t),t}^T\theta^* &= (r_t^+ - x_{a(t),t}^T\hat{\theta}_t) + (x_{a(t),t}^T\hat{\theta}_t - x_{a(t),t}^T\theta^*) \\
&\leq \sqrt{2\ln(Rt^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{t}{\delta})} + C_0^{-1}R^{-1})}v_t s_{a(t),t} + \beta_t s_{a(t),t},
\end{aligned}
$$

where the inequality holds by using Lemma C.2. □

C.4 Considering the case $a(t) = \textbf{argmax}_{i\in[K]}\{x_{i,t}^T\hat{\theta}_t\}$

Bounding Term 1

Lemma C.7. *Pick $\delta \in (0,1)$. Then with probability at least $1 - \frac{\delta}{t^2}$ we have*

$$
x_{a^*(t),t}^T\theta^* - r_t^+ \leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}\frac{C_0}{t^\beta}.
$$

Proof. If $s_{a^*(t),t} = 0$ then by definition of $\alpha_{a^*(t),t}^{EI}$, $\alpha_{a^*(t),t}^{EI} = I_{a^*(t),t}$. We have $I_{a^*(t),t} = \alpha_{a^*(t),t}^{EI} \leq \alpha_{a(t),t}^{EI} \leq \frac{C_0}{t^\beta}$.

We now consider $s_{a^*(t),t} > 0$. If $x_{a^*(t),t}^T\theta^* < r_t^+$ then the lemma will be trivial. We now consider $x_{a^*(t),t}^T\theta^* \geq r_t^+$. Following the derivation of the acquisition function α^{EI}, we have $\alpha_{a^*(t),t}^{EI} = v_t s_{a^*(t),t}\tau(\frac{x_{a^*(t),t}^T\hat{\theta}_t - r_t^+}{v_t s_{a^*(t),t}})$. Further, we also have $\frac{x_{a^*(t),t}^T\hat{\theta}_t - r_t^+}{v_t s_{a^*(t),t}} \geq \frac{-\beta_t}{v_t}$ with probability $1 - \frac{\delta}{t^2}$. It is because $x_{a^*(t),t}^T\hat{\theta}_t - x_{a^*(t),t}^T\theta^* \geq -\beta_t s_{a^*(t),t}$ with probability $1 - \frac{\delta}{t^2}$ and we are considering the case when $x_{a^*(t),t}^T\theta^* \geq r_t^+$. Therefore, $\alpha_{a^*(t),t}^{EI} \geq v_t\tau(\frac{-\beta_t}{v_t})s_{a^*(t),t}$ with probability $1 - \frac{\delta}{t^2}$.

Now, we combine inequalities $\alpha_{a^*(t),t}^{EI} \geq v_t\tau(\frac{-\beta_t}{v_t})s_{a^*(t),t}$ and $\alpha_{a^*(t),t}^{EI} \geq I_{a^*(t),t} - \beta_t s_{a^*(t),t}$ which is proven in Lemma C.4, we obtain the following inequality:

$$
I_{a^*(t),t} \leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}\alpha_{a^*(t),t}^{EI} \tag{7}
$$

Here we use the fact $\tau(z) = z + \tau(-z)$. Finally, with probability at least $1 - \frac{\delta}{t^2}$ we achieve

$$\begin{aligned} x_{a^*(t),t}^T \theta^* - r_t^+ &\leq I_{a^*(t),t} \\ &\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} \alpha_{a^*(t),t}^{EI} \\ &\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} \alpha_{\overline{a}(t),t}^{EI} \\ &\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} \frac{C_0}{t^\beta} \end{aligned}$$

where the first inequality holds by the definition of the function I_t. The second one comes from Eq(7). The third one holds by the definition of $\overline{a}(t)$. The fourth one holds because $\alpha_{\overline{a}(t),t}^{EI} \leq \frac{C_0}{t^\beta}$. □

Bounding Term 2

Lemma C.8. *Pick a $\delta \in (0, 1)$. Then with probability $1 - \frac{\delta}{t^2}$ we have*

$$r_t^+ - x_{a(t),t}^T \theta^* \leq \beta_t s_{a(t),t}.$$

Proof. By definition $a(t) = \text{argmax}_{i \in [K]} \{x_{i,t}^T \hat{\theta}_t\}$, we have $r_t^+ = x_{a(t),t}^T \hat{\theta}_t$. By Lemma C.2, we have $r_t^+ - x_{a(t),t}^T \theta^* \leq \beta_t s_{a(t),t}$. The lemma holds. □

We now are ready to bound $x_{a^*(t),t}^T \theta^* - x_{a(t),t}^T \theta^*$ for both cases of $a(t)$.

Lemma C.9. *For every $1 \leq t \leq T$, with probability $1 - \frac{\delta}{t^2}$ we always have*

$$\begin{aligned} x_{a^*(t),t}^T \theta^* - x_{a(t),t}^T \theta^* &\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} (2\beta_t + v_t) s_{a(t),t} + \sqrt{2ln(Rt^\beta) + 6\sqrt{C_0^{-2} dln(\frac{t+1}{\delta})}} v_t s_{a(t),t} + \\ &\quad + \beta_t s_{a(t),t} + \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} \frac{C_0}{t^\beta} \end{aligned}$$

Proof. Following Algorithm 1, we consider two cases of $a(t)$.

- if $a(t) = \text{argmax}_{i \in \mathcal{K}} \alpha_{i,t}^{EI}$, then by combining Lemma C.5 and C.6 we have

$$\begin{aligned} x_{a^*(t),t}^T \theta^* - x_{a(t),t}^T \theta^* &= (x_{a^*(t),t}^T \theta^* - r_t^+) + (r_t^+ - x_{a(t),t}^T \theta^*) \\ &\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} (2\beta_t + v_t) s_{a(t),t} \\ &\quad + \sqrt{2\ln(Rt^\beta) + 2\ln(\sqrt{3C_0^{-2} d\ln(\frac{t}{\delta})} + C_0^{-1} R^{-1})} v_t s_{a(t),t} + \beta_t s_{a(t),t} \end{aligned}$$

- if $a(t) = \text{argmax}_{i \in [K]} \{x_{i,t}^T \hat{\theta}_t\}$, the by combining Lemma C.7 and C.8 we have

$$\begin{aligned} x_{a^*(t),t}^T \theta^* - x_{a(t),t}^T \theta^* &= (x_{a^*(t),t}^T \theta^* - r_t^+) + (r_t^+ - x_{a(t),t}^T \theta) \\ &\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})} \frac{C_0}{t^\beta} + \beta_t s_{a(t),t} \end{aligned}$$

For both cases of a_t, we always obtain the following upper bound for $x_{a^*(t),t}^T\theta^* - x_{a(t),t}^T\theta^*$ as

$$\begin{aligned} x_{a^*(t),t}^T\theta^* - x_{a(t),t}^T\theta^* &\leq \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}(2\beta_t + v_t)s_{a(t),t} + \sqrt{2\ln(Rt^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{t}{\delta})} + C_0^{-1}R^{-1})}v_t s_{a(t),t} + \\ &\quad + \beta_t s_{a(t),t} + \frac{\tau(\frac{\beta_t}{v_t})}{\tau(-\frac{\beta_t}{v_t})}\frac{C_0}{t^\beta} \end{aligned}$$

Using $v_t = \beta_t = R\sqrt{d\ln(\frac{t^3}{\delta})} + 1$, we obtain

$$\begin{aligned} x_{a^*(t),t}^T\theta^* - x_{a(t),t}^T\theta^* &\leq 3\frac{\tau(1)}{\tau(-1)}\beta_t s_{a(t),t} + \sqrt{2\ln(Rt^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{t}{\delta})} + C_0^{-1}R^{-1})}\beta_t s_{a(t),t} + \\ &\quad + \beta_t s_{a(t),t} + \frac{\tau(1)}{\tau(-1)}\frac{C_0}{t^\beta} \end{aligned}$$

□

We now are ready to prove the correctness of Theorem 3.2.

Theorem C.10. *Given any $\delta \in (0,1)$. If $\sqrt{d} \leq C_0 \leq d$ and $0.5 \leq \beta \leq 3$ then with probability $1-\delta$, the cumulative regret of the Expected Improvement algorithm is bounded as*

$$R(T) = \mathcal{O}(d\sqrt{Tln^2(T)ln\frac{T}{\delta}}).$$

Proof. Using Lemma, for every $1 \leq t \leq T$, we have

$$\begin{aligned} x_{a^*(t),t}^T\theta^* - x_{a(t),t}^T\theta^* &\leq 3\frac{\tau(1)}{\tau(-1)}\beta_t s_{a(t),t} + \sqrt{2\ln(Rt^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{t}{\delta})} + C_0^{-1}R^{-1})}\beta_t s_{a(t),t} + \\ &\quad + \beta_t s_{a(t),t} + \frac{\tau(1)}{\tau(-1)}\frac{C_0}{t^\beta} \end{aligned}$$

Thus,

$$\begin{aligned} R(T) &= \sum_{t=1}^T (x_{a^*(t),t}^T\theta^* - x_{a(t),t}^T\theta^*) \\ &\leq \sum_{t=1}^T [3\frac{\tau(1)}{\tau(-1)}\beta_t s_{a(t),t} + \sqrt{2\ln(Rt^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{t}{\delta})} + C_0^{-1}R^{-1})}\beta_t s_{a(t),t} + \\ &\quad + \beta_t s_{a(t),t} + \frac{\tau(1)}{\tau(-1)}\frac{C_0}{t^\beta}] \\ &= \sum_{t=1}^T [3\frac{\tau(1)}{\tau(-1)} + \sqrt{2\ln(Rt^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{t}{\delta})} + C_0^{-1}R^{-1})} + 1]\beta_t s_{a(t),t} + \sum_{t=1}^T \frac{\tau(1)}{\tau(-1)}\frac{C_0}{t^\beta} \\ &\leq [3\frac{\tau(1)}{\tau(-1)} + \sqrt{2\ln(RT^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{T}{\delta})} + C_0^{-1}R^{-1})} + 1]\beta_T \sum_{t=1}^T s_{a(t),t} + \sum_{t=1}^T \frac{\tau(1)}{\tau(-1)}\frac{C_0}{t^\beta} \\ &\leq 5[3\frac{\tau(1)}{\tau(-1)} + \sqrt{2\ln(RT^\beta) + 2\ln(\sqrt{3C_0^{-2}d\ln(\frac{T}{\delta})} + C_0^{-1}R^{-1})} + 1]\beta_T\sqrt{dT\ln(T)} + \frac{\tau(1)}{\tau(-1)}\sum_{t=1}^T \frac{C_0}{t^\beta}, \end{aligned}$$

where in the second inequality, we use the facts that $\beta_t \leq \beta_T$, $v_t \leq v_T$ as $t \leq T$. In the third inequality, we use Lemma C.3. We consider two cases:

- if $\beta = 1$ then by Lemma C.1, $\sum_{t=1}^{T} \frac{1}{t^\beta} \leq 1 + \ln T$. Hence, using the assumption that $\sqrt{d} \leq C_0 \leq d$, we get that $C_0^{-2} d \leq 1$ and $C_0 \sum_{t=1}^{T} \frac{1}{t^\beta} \leq d(1 + \ln T)$. We recall that $\beta_T = R\sqrt{d \ln(\frac{T^3}{\delta})} + 1$, and $\tau(1), \tau(-1)$ are constant. Thus, $R(T) = \mathcal{O}(d\sqrt{T \ln^2(T) \ln \frac{T}{\delta}})$.

- if $\beta \neq 1$ then by Lemma C.1, $\sum_{t=1}^{T} \frac{1}{t^\beta} \leq 1 + \frac{T^{1-\beta}-1}{1-\beta}$. Combining with the assumption that $1/2 \leq \beta \leq 3$, we consider two cases:
  - if $1/2 \leq \beta < 1$, we have $\sum_{t=1}^{T} \frac{1}{t^\beta} \leq 1 + \frac{T^{1-\beta}-1}{1-\beta} \leq 1 + 2(\sqrt{T} - 1)$. Hence, $C_0 \sum_{t=1}^{T} \frac{1}{t^\beta} \leq d(1 + 2(\sqrt{T} - 1))$. Thus, $R(T) = \mathcal{O}(d\sqrt{T \ln^2(T) \ln \frac{T}{\delta}})$.
  - if $1 < \beta \leq 3$, then $\sum_{t=1}^{T} \frac{1}{t^\beta} \leq 1 + \frac{T^{1-\beta}-1}{1-\beta} \leq 1$ and $T^\beta \leq T^3$. Thus, $R(T) = \mathcal{O}(d\sqrt{T \ln^2(T) \ln \frac{T}{\delta}})$.

□

Remark. We choose $C_0 \in [\sqrt{d}, d]$ to eliminate the term d in the expression $\sqrt{C_0^{-2} d \ln(\frac{T}{\delta})}$ and to ensure that the term $\sum_{i=1}^{T} \frac{C_0}{t^\beta} = \mathcal{O}(d\sqrt{T})$. We choose $\beta \leq 3$ to ensure that the order of $R(T)$ is the same as the case when $1/2 \leq \beta < 1$. For $\beta > 3$, the higher β, the larger the cumulative regret is.

D Regret Analysis for NeuralEI Algorithm

In this section, we provide the regret analysis for the NeuralEI algorithm. We start with the definition of the filtration $\mathcal{F}_{t-1}$ as the union of history until time $t-1$, and the contexts at time t. For any t, we define an event $\mathcal{E}_t^\sigma$ as follows:

$$\mathcal{E}_t^\sigma = \{\omega \in \mathcal{F}_t : \forall i \in [K],\ |\tilde{f}_{i,t} - f(x_{i,t}; \theta_{t-1})| \leq c_t \nu \sigma_{i,t}\},$$

where $c_t = \sqrt{4 \log t + 2 \log K}$.

For any t, we define an event $\mathcal{E}_t^\mu$ as follows:

$$\mathcal{E}_t^\mu = \{\omega \in \mathcal{F}_t : \forall i \in [K],\ |f(x_{i,t}; \theta_{t-1}) - h(x_{t,k})| \leq \nu \sigma_{i,t} + \epsilon(m)\},$$

where $\epsilon(m)$ is defined as in [41]:

$$\begin{aligned}\epsilon(m) = &\bar{C}_1 T^{2/3} m^{-1/6} \lambda^{-2/3} L^3 \sqrt{\log m} + \bar{C}_2 (1 - \eta\, m\lambda)^J \sqrt{TL/\lambda} \\ &+ \bar{C}_3 m^{-1/6} \sqrt{\log m} L^4 T^{5/3} \lambda^{-5/3} (1 + \sqrt{T/\lambda})\end{aligned}$$

Based on these notations, we state the following results from the previous works.

D.1 Auxiliary Lemmas

Lemma D.1 (Lemma 4.2 of [41]). *For any $t \in [T]$, $\mathbb{P}(\mathcal{E}_t^\sigma) \geq 1 - t^{-2}$.*

Lemma D.2 (Lemma 4.3 of [41]). *Set $\eta = C(m\lambda + mLT)^{-1}$, then we have $\mathbb{P}(\mathcal{E}_t^\mu) \geq 1 - \delta$.*

Lemma D.3 (Lemma B.9 of [41]). *For any time $t \in [T]$, $i \in [K]$ and any $\delta \in (0, 1)$, if the network width m satisfies Condition 1, we have with probability at least $1 - \delta$, that $\sigma_{i,t} \leq C_4 \sqrt{L}$, where C_4 is a positive constant.*

Lemma D.4 (Lemma 4.4 of [41]). *For any $t \in [T]$, $i \in [K]$, we have $\mathbb{P}[\tilde{r}_{i,t} + \epsilon(m) > h(x_{i,t}) | \mathcal{F}_t] \geq (4e\sqrt{\pi})^{-1}$.*

Lemma D.5 (Lemma 4.8 of [41]). *Assume that the width of the neural network m satisfies*

$m \geq C max\{\sqrt{\lambda} L^{-3/2} [log(TKL^2/\delta)]^{3/2}, T^6 K^6 L^6 log(TKL/\delta) max\{\lambda_0^{-4}, 1\}\}$

and

$m[log(m)]^{-3} \geq CTL^{12}\lambda^{-1} + CT^7\lambda^{-8}L^{18}(\lambda + LT)^6 + CL^{21}T^7\lambda^{-7}(1 + \sqrt{T/\lambda})^6$*, where C is a positive absolute constant.*

Then $\eta = C_5(m\lambda + mLT)^{-1}$. With high probability $1-\delta$, for every $i \in [K]$ we have

$$\sum_{i=1}^{T} min\{\sigma_{a_t,t}, 1\} \leq \sqrt{2\lambda T(\widetilde{d}log(1+TK)+1)} + C6T^{13/6}\sqrt{logm}m^{-1/6}\lambda^{-2/3}L^{9/2},$$

where C_5, C_6 are absolute constants.

D.2 Proof for Theorem 4.2

We now are ready to derive the regret bound for NeuralEI algorithm. First, we need the following results to lower bound and upper bound the EI acquisition function in the setting of neural contextual bandits. We remark that the following Lemma D.6 is an adaptation of Lemma C.4 (in linear bandits) to neural contextual bandits. The following Lemma D.7 is our novel result. Both Lemma D.6 and Lemma D.7 provide the lower bounds and the upper bounds for the EI acquisition function, but follow the different ways.

Lemma D.6. *Assume that the event $\mathcal{E}_t^\sigma$ holds. Set $I_{i,t} = max\{0, \tilde{f}_{i,t} - f_t^+\}$. Then for every $i \in [K]$, we have*

$$I_{i,t} - c_t\nu\sigma_{i,t} \leq \alpha_{i,t}^{EI} \leq I_{i,t} + \nu(c_t+1)\sigma_{i,t}.$$

Proof. If $\sigma_{i,t} = 0$ then $\alpha_{i,t}^{EI} = I_{i,t}$, which makes the result trivial. We now assume that $\sigma_{i,t} > 0$. Set $q = \frac{\tilde{f}_{i,t} - f_t^+}{\sigma_{i,t}}$ and $u = \frac{f(x_{i,t};\theta_{t-1}) - f_t^+}{\sigma_{i,t}}$. Set $\tau(z) = z\Phi(z) + \phi(z)$. Then we have that

$$\alpha_{i,t}^{EI} = \nu\sigma_{i,t}\tau(\frac{u}{\nu}).$$

By Lemma D.1, we have that $|u - q| \leq c_t\nu$ with probability $1 - t^{-2}$. As $\tau'(z) = \Phi(z) \in [0,1]$, τ is non-decreasing and $\tau(z) \leq 1 + z$ for $z > 0$. Hence,

$$\begin{aligned}
\alpha_{i,t}^{EI} &\leq \nu\sigma_{i,t}\tau(\frac{\max\{0,q\} + c_t\nu}{\nu}) \\
&\leq \nu\sigma_{i,t}(\frac{\max\{0,q\} + c_t\nu}{\nu} + 1) \\
&= I_{i,t} + (c_t\nu + \nu)\sigma_{i,t}
\end{aligned}$$

If $I_{i,t} = 0$ then the lower bound is trivial as $\alpha_{i,t}^{EI}$ is non-negative. Thus suppose $I_{i,t} > 0$. Since $\alpha_{i,t}^{EI} \geq 0$ and $\tau(z) \geq 0$ for all z, and $\tau(z) = z + \tau(-z) \geq z$. Therefore,

$$\begin{aligned}
\alpha_{i,t}^{EI} &\geq \nu\sigma_{i,t}\tau(\frac{q - c_t\nu}{\nu}) \\
&\geq \nu\sigma_{i,t}(\frac{q - c_t\nu}{\nu}) \\
&= I_{i,t} - c_t\nu\sigma_{i,t}
\end{aligned}$$

□

Lemma D.7. *Assume that the event $\mathcal{E}_t^\mu$ holds. Set $J_{i,t} = max\{0, h(x_{i,t}) - f_t^+\}$. Then for every $i \in [K]$, we have*

$$J_{i,t} - \nu\sigma_{i,t} - \epsilon(m) \leq \alpha_{i,t}^{EI} \leq J_{i,t} + \nu\sigma_{i,t} + \epsilon(m).$$

Proof. If $\sigma_{i,t} = 0$ then $\alpha_{i,t}^{EI} = I_{i,t}$, which makes the result trivial. We now assume that $\sigma_{i,t} > 0$. Set $q = \frac{h(x_{i,t}) - f_t^+}{\sigma_{i,t}}$ and $u = \frac{f(x_{i,t};\theta_{t-1}) - f_t^+}{\sigma_{i,t}}$. Set $\tau(z) = z\Phi(z) + \phi(z)$. Then we have that

$$\alpha_{i,t}^{EI} = \nu\sigma_{i,t}\tau(\frac{u}{\nu}).$$

By Lemma D.2, we have that $|u-q| \leq \nu + \frac{\epsilon(m)}{\sigma_{i,t}}$. As $\tau'(z) = \Phi(z) \in [0,1]$, τ is non-decreasing and $\tau(z) \leq 1+z$ for $z > 0$. Hence,

$$\begin{aligned}
\alpha_{i,t}^{EI} &\leq \nu\sigma_{i,t}\tau(\frac{\max\{0,q\}+\nu+\frac{\epsilon(m)}{\sigma_{i,t}}}{\nu}) \\
&\leq \nu\sigma_{i,t}(\frac{\max\{0,q\}+\nu+\frac{\epsilon(m)}{\sigma_{i,t}}}{\nu}+1) \\
&= J_{i,t}+\nu\sigma_{i,t}+\epsilon(m)
\end{aligned}$$

If $I_{i,t} = 0$ then the lower bound is trivial as $\alpha_{i,t}^{EI}$ is non-negative. Thus suppose $I_{i,t} > 0$. Since $\alpha_{i,t}^{EI} \geq 0$ and $\tau(z) \geq 0$ for all z, and $\tau(z) = z + \tau(-z) \geq z$. Therefore,

$$\begin{aligned}
\alpha_{i,t}^{EI} &\geq \nu\sigma_{i,t}\tau(\frac{q-\nu-\frac{\epsilon(m)}{\sigma_{i,t}}}{\nu}) \\
&\geq \nu\sigma_{i,t}(\frac{q-\nu-\frac{\epsilon(m)}{\sigma_{i,t}}}{\nu}) \\
&= J_{i,t}-\nu\sigma_{i,t}-\epsilon(m)
\end{aligned}$$

□

Next, we will use above results to bound $h(x_{a^*(t),t}) - h(x_{a(t),t})$. By NeuralEI algorithm, we will need to bound $h(x_{a^*(t),t}) - h(x_{a(t),t})$ thought different ways depending on the definition of $a(t)$.

D.2.1 Considering the case $a(t) = \overline{a}(t)$

Lemma D.8. *Assume that the event $\mathcal{E}_t^\sigma$ holds. Then for every $i \in [K]$, we have*

$$\tilde{f}_{i,t} - f_t^+ \leq \frac{\tau(c_t)}{\tau(-c_t)}(2c_t+1)\nu\sigma_{a(t),t}.$$

Proof. We provide the proof in Section E □

Lemma D.9. *Assume that the event $\mathcal{E}_t^\mu$ holds. Then for every $i \in [K] : \nu\sigma_{i,t} > \epsilon(m)$, we have*

$$h(x_{i,t}) - f_t^+ \leq (\frac{\tau(2)}{\tau(-2)}+1)(\nu\sigma_{a(t),t}+\epsilon(m)).$$

Proof. We provide the proof in Section E □

Lemma D.10. *Assume that the event $\mathcal{E}_t^\mu$ holds. Pick a $\delta \in (0,1)$. Then with probability $1-\delta$ we have*

$$f_t^+ - h(x_{a(t),t}) \leq (\sqrt{2log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)}+1)\nu\sigma_{a(t),t}+\epsilon(m).$$

Proof. We have

$$\begin{aligned}
\alpha_{a(t),t}^{EI} &= (f(x_{a(t),t};\theta_{t-1})-f_t^+)\Phi(\frac{f(x_{a(t),t};\theta_{t-1})-f_t^+}{\nu\sigma_{a(t),t}})+\nu\sigma_{a(t),t}\phi(\frac{f(x_{a(t),t};\theta_{t-1})-f_t^+}{\nu\sigma_{a(t),t}}) \\
&\leq \nu\sigma_{a(t),t}\phi(\frac{f(x_{a(t),t};\theta_{t-1})-f_t^+}{\nu\sigma_{a(t),t}}) \\
&= \nu\sigma_{a(t),t}\frac{1}{2\sqrt{\pi}}\exp(-\frac{1}{2}(\frac{f(x_{a(t),t};\theta_{t-1})-f_t^+}{\nu\sigma_{a(t),t}})^2)
\end{aligned}$$

where the first inequality holds due to the definition of action $a(t)$. The second equality holds due to the definition of $\alpha^{EI}_{a(t),t}$. The second inequality comes from the fact that $f(x_{a(t),t};\theta_{t-1}) \leq f_t^+$. The third equality holds due to the definition of function $\phi(.)$.

From the last inequality, we obtain

$$|f(x_{a(t),t};\theta_{t-1}) - f_t^+| \leq \sqrt{2\log(\frac{\nu\sigma_{a(t),t}}{\alpha^{EI}_{a(t),t}})}\nu\sigma_{a(t),t}.$$

By using the condition that $\alpha^{EI}_{a(t),t} \geq \frac{C_0}{t^\beta}$ and the fact that $\sigma_{a(t),t} \leq C_1\sqrt{L}$ with probability $1-\delta$, we have

$$|f(x_{a(t),t};\theta_{t-1}) - f_t^+| \leq \sqrt{2\log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)}\nu\sigma_{a(t),t} \tag{8}$$

with probability $1-\delta$.

Finally, with probability $1-\delta$, we have

$$\begin{aligned} f_t^+ - h(x_{a(t),t}) &= f_t^+ - f(x_{a(t),t};\theta_{t-1}) + f(x_{a(t),t};\theta_{t-1}) - h(x_{a(t),t}) \\ &\leq \sqrt{2\log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)}\nu\sigma_{a(t),t} + \nu\sigma_{a(t),t} + \epsilon(m) \\ &= (\sqrt{2\log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)} + 1)\nu\sigma_{a(t),t} + \epsilon(m), \end{aligned}$$

where in the first inequality, we use the inequality Eq(8) and Lemma D.2 □

Lemma D.11. *We assume that both $\mathcal{E}_t^\sigma$ and $\mathcal{E}_t^\mu$ hold. Then,*

- *if $\sigma_{a^*(t),t} > \epsilon(m)$, then*

$$h(x_{a^*(t),t}) - h(x_{a(t),t}) \leq (\frac{\tau(2)}{\tau(-2)}+1)(\nu\sigma_{a(t),t}+\epsilon(m)) + (\sqrt{2log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)}+1)\nu\sigma_{a(t),t}+\epsilon(m)$$

- *if $\sigma_{a^*(t),t} \leq \epsilon(m)$, then*

$$h(x_{a^*(t),t}) - h(x_{a(t),t}) \leq \frac{\tau(c_t)}{\tau(-c_t)}\nu(2c_t+1)\sigma_{a(t),t} + (\sqrt{2log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)}+1)\nu\sigma_{a(t),t} + (\nu+c_t\nu+1)\epsilon(m)$$

Proof. We consider two cases:

- if $\sigma_{a^*(t),t} > \epsilon(m)$. Then, by Lemma D.9, we have

$$h(x_{a^*(t),t}) - f_t^+ \leq (\frac{\tau(2)}{\tau(-2)} + 1)(\nu\sigma_{a(t),t} + \epsilon(m)).$$

  Thus,

$$\begin{aligned} h(x_{a^*(t),t}) - h(x_{a(t),t}) &= [h(x_{a^*(t),t}) - f_t^+] + [f_t^+ - h(x_{a(t),t})] \\ &\leq (\frac{\tau(2)}{\tau(-2)} + 1)(\nu\sigma_{a(t),t} + \epsilon(m)) + (\sqrt{2\log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)} + 1)\nu\sigma_{a(t),t} + \epsilon(m) \end{aligned}$$

- if $\sigma_{a^*(t),t} \leq \epsilon(m)$. We have that $|h(x_{a^*(t),t}) - \tilde{f}_{a^*(t),t}| \leq |h(x_{a^*(t),t}) - f(x_{a^*(t),t};\theta_t)| + |f(x_{a^*(t),t};\theta_t) - \tilde{f}_{a^*(t),t}| \leq \epsilon(m) + (1+c_t)\nu\sigma_{a^*(t),t} \leq (\nu + c_t\nu + 1)\epsilon(m)$. Combining this result with Lemma D.8 and D.9, we have

$$\begin{aligned} h(x_{a^*(t),t}) - h(x_{a(t),t}) &= [h(x_{a^*(t),t}) - \tilde{f}_{a^*(t),t}] + [\tilde{f}_{a^*(t),t} - f_t^+] + [f_t^+ - h(x_{a(t),t})] \\ &\leq (\nu + c_t\nu + 1)\epsilon(m) + \frac{\tau(c_t)}{\tau(-c_t)}\nu(2c_t+1)\sigma_{a(t),t} + \end{aligned}$$

$$
\begin{aligned}
& +(\sqrt{2\log(C_1 C_0^{-1}\sqrt{L}\nu t^{\beta})}+1)\nu\sigma_{a(t),t}+\epsilon(m) \\
= \quad & \frac{\tau(c_t)}{\tau(-c_t)}\nu(2c_t+1)\sigma_{a(t),t}+(\sqrt{2\log(C_1 C_0^{-1}\sqrt{L}\nu t^{\beta})}+1)\nu\sigma_{a(t),t}+ \\
& (\nu+c_t\nu+1)\epsilon(m),
\end{aligned}
$$

where in the above inequality, we apply Lemma D.8 for the arm i_0.

□

D.2.2 Considering the case $a(t) = \textbf{argmax}_{i\in[K]}\{f(x_{i,t};\theta_{t-1})\}$

Lemma D.12. *We assume that both $\mathcal{E}_t^{\sigma}$ holds. Then for $i \in [K]$ we have*

$$
\tilde{f}_{i,t} - f_t^{+} \leq \frac{\tau(c_t)}{\tau(-c_t)}\frac{C_0}{t^{\beta}}.
$$

Proof. The proof is similar to that of Lemma D.8 with a notice that $\alpha^{EI}_{a(t),t} \leq \frac{C_0}{t^{\beta}}$ □

Lemma D.13. *Assume that the event $\mathcal{E}_t^{\mu}$ holds. Then for every $i \in [K] : \nu\sigma_{i,t} > \epsilon(m)$, we have*

$$
h(x_{i,t}) - f_t^{+} \leq (\frac{\tau(2)}{\tau(-2)}+1)\frac{C_0}{t^{\beta}}.
$$

Proof. The proof is similar to that of Lemma D.9 with a notice that $\alpha^{EI}_{a(t),t} \leq \frac{C_0}{t^{\beta}}$ □

Lemma D.14. *We assume that $\mathcal{E}_t^{\mu}$ holds. Then we have*

$$
f_t^{+} - h(x_{a(t),t}) \leq \nu\sigma_{a(t),t} + \epsilon(m).
$$

Proof. By definition, $a(t) = \text{argmax}_{i\in[K]}\{f(x_{i,t};\theta_{t-1})\}$. Hence $f_t^{+} = f(x_{a(t),t};\theta_{t-1})$. By Lemma D.2, we have $f_t^{+} - h(x_{a(t),t}) = f(x_{a(t),t};\theta_{t-1}) - h(x_{a(t),t}) \leq \nu\sigma_{a(t),t} + \epsilon(m)$. The lemma holds. □

By combining the bounds of $h(x_{a^*(t),t}) - h(x_{a(t),t})$ for two cases of $a(t)$, we obtain an unique bound for $h(x_{a^*(t),t}) - h(x_{a(t),t})$ as follows:

Lemma D.15. *We assume that both $\mathcal{E}_t^{\sigma}$ and $\mathcal{E}_t^{\mu}$ hold. Then,*

- *if $\sigma_{a^*(t),t} > \epsilon(m)$, then,*

$$
h(x_{a^*(t),t}) - h(x_{a(t),t}) \leq (\frac{\tau(2)}{\tau(-2)}+1)\frac{C_0}{t^{\beta}} + \nu\sigma_{a(t),t} + \epsilon(m).
$$

- *if $\sigma_{a^*(t),t} \leq \epsilon(m)$, then*

$$
h(x_{a^*(t),t}) - h(x_{a(t),t}) \leq (\nu + c_t\nu + 2)\epsilon(m) + \frac{\tau(c_t)}{\tau(-c_t)}\frac{C_0}{t^{\beta}} + \nu\sigma_{a(t),t}.
$$

Proof. There are two cases:

- if $\sigma_{a^*(t),t} > \epsilon(m)$, then, by Lemma D.13 for action $a^*(t)$, we have

$$h(x_{a^*(t),t}) - f_t^+ \leq (\frac{\tau(2)}{\tau(-2)} + 1)\frac{C_0}{t^\beta}.$$

Combining with Lemma D.14, we have

$$\begin{aligned} h(x_{a^*(t),t}) - h(x_{a(t),t}) &= [h(x_{a^*(t),t}) - f_t^+] + [f_t^+ - h(x_{a(t),t})] \\ &\leq (\frac{\tau(2)}{\tau(-2)} + 1)\frac{C_0}{t^\beta} + \nu\sigma_{a(t),t} + \epsilon(m), \end{aligned}$$

- if $\sigma_{a^*(t),t} \leq \epsilon(m)$, then $|h(x_{a^*(t),t}) - \tilde{f}_{a^*(t),t}| \leq |h(x_{a^*(t),t}) - f(x_{a^*(t),t};\theta_t)| + |f(x_{a^*(t),t};\theta_t) - \tilde{f}_{a^*(t),t}| \leq \epsilon(m) + (1+c_t)\nu\sigma_{a^*(t),t} \leq (\nu + c_t\nu + 1)\epsilon(m)$. Thus, we have Combining with Lemma D.12 and Lemma D.14, we have

$$\begin{aligned} h(x_{a^*(t),t}) - h(x_{a(t),t}) &= [h(x_{a^*(t),t}) - \tilde{f}_{a^*(t),t}] + [\tilde{f}_{a^*(t),t} - f_t^+] + [f_t^+ - h(x_{a(t),t})] \\ &\leq (\nu + c_t\nu + 2)\epsilon(m) + \frac{\tau(c_t)}{\tau(-c_t)}\frac{C_0}{t^\beta} + \nu\sigma_{a(t),t} \end{aligned}$$

.

□

Lemma D.16. *We assume that both $\mathcal{E}_t^\sigma$ and $\mathcal{E}_t^\mu$ hold. Then, there exist constants C_1, C_2, C_3 such that with probability $1-\delta$, we have*

$$h(x_{a^*(t),t}) - h(x_{a(t),t}) \leq C_1(2c_t+1)\nu\sigma_{a(t),t} + (\sqrt{2log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)}+1))\nu\sigma_{a(t),t} + C_2\frac{C_0}{t^\beta} + (\nu + c_t\nu + C_3)\epsilon(m).$$

Proof. This upper bound is obtained by combining the upper bounds of $h(x_{a^*(t),t}) - h(x_{a(t),t})$ from Lemma D.11 and Lemma D.15. We note $\frac{\tau(c_t)}{\tau(-c_t)}$ is bounded by a constant. □

Set $r_t = h(x_{a^*(t),t}) - h(x_{a(t),t})$. We can re-write the above lemma as follows:

Lemma D.17. *With probability $1-\delta$, we have*

$$\begin{aligned} \mathbb{E}[r_t|\mathcal{F}_t, \mathcal{E}_t^\mu] &\leq (C_1(2c_t+1) + (\sqrt{2log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)} + 1)C_1\sqrt{L})\nu\mathbb{E}[min\{\sigma_{a(t),t}, 1\}|\mathcal{F}_t, \mathcal{E}_t^\mu] \\ &\quad + C_2\frac{C_0}{t^\beta} + (\nu + c_t\nu + C_3)\epsilon(m) \end{aligned}$$

Proof. We have

$$\begin{aligned} \mathbb{E}[r_t|\mathcal{F}_t, \mathcal{E}_t^\mu] &= \mathbb{E}[h(x_{a^*(t),t}) - h(x_{a(t),t})|\mathcal{F}_t, \mathcal{E}_t^\mu, \mathcal{E}_t^\sigma]\mathbb{P}(E_t^\sigma) + \\ &\quad + \mathbb{E}[h(x_{a^*(t),t}) - h(x_{a(t),t})|\mathcal{F}_t, \mathcal{E}_t^\mu, \overline{\mathcal{E}}_t^\sigma]\mathbb{P}(\overline{\mathcal{E}}_t^\sigma) \\ &\leq (C_1(2c_t+1) + (\sqrt{2\log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)} + 1))\nu\mathbb{E}[\sigma_{a(t),t}|\mathcal{F}_t, \mathcal{E}_t^\mu] + \\ &\quad + C_2\frac{C_0}{t^\beta} + (\nu + c_t\nu + C_3)\epsilon(m) + \frac{2}{t^2}, \end{aligned}$$

where the first term is bounded by Lemma D.17 and the second term is bounded due to the facts that $h(x_{a^*(t),t}) - h(x_{a(t),t}) \leq |h(x_{a^*(t),t})| + |h(x_{a(t),t})| \leq 2$ and $\mathbb{P}(\overline{\mathcal{E}}_t^\sigma) \leq \frac{1}{t^2}$.

Further, due to $|h(x)| \leq 1$, we obtain an upper bound for $\mathbb{E}[r_t|\mathcal{F}_t, \mathcal{E}_t^\mu]$ as

$$\begin{aligned} \mathbb{E}[r_t|\mathcal{F}_t, \mathcal{E}_t^\mu] &\leq \min\{((C_1(2c_t+1) + (\sqrt{2\log(C_1C_0^{-1}\sqrt{L}\nu t^\beta)} + 1))\nu)\mathbb{E}[\sigma_{a(t),t}|\mathcal{F}_t, \mathcal{E}_t^\mu], 2\} \\ &\quad + C_2\frac{C_0}{t^\beta} + (\nu + c_t\nu + C_3)\epsilon(m) + \frac{2}{t^2} \end{aligned}$$

On the other hand, we have $\nu \geq 1$ by definition, $2c_t + 1 = 2\sqrt{4\log t + 2\log K} + 1 \geq 2$ with $t \geq 2$. The constant C_1 is chosen to be greater than 1. Hence,

$$\begin{aligned}
\mathbb{E}[r_t|\mathcal{F}_t, \mathcal{E}_t^\mu] &\leq ((C_1(2c_t+1) + (\sqrt{2\log(C_1 C_0^{-1}\sqrt{L}\nu t^\beta)} + 1))\nu)\min\{\mathbb{E}[\sigma_{a(t),t}|\mathcal{F}_t, \mathcal{E}_t^\mu], 1\} \\
&\quad + C_2\frac{C_0}{t^\beta} + (\nu + c_t\nu + C_3)\epsilon(m) + \frac{2}{t^2} \\
&\leq ((C_1(2c_t+1) + (\sqrt{2\log(C_1 C_0^{-1}\sqrt{L}\nu t^\beta)} + 1))\nu)C_4\sqrt{L})\mathbb{E}[\min\{\sigma_{a(t),t}, 1\}|\mathcal{F}_t, \mathcal{E}_t^\mu] \\
&\quad + C_2\frac{C_0}{t^\beta} + (\nu + c_t\nu + C_3)\epsilon(m) + \frac{2}{t^2},
\end{aligned}$$

where we use Lemma D.3 with probability $1 - \delta$. □

We now are ready to prove Theorem 4.2.

Theorem D.18. *If the network width m satisfies:*

$$m \geq poly(\gamma, T, K, L, log(1/\delta)),$$

then with probability at least $1 - \delta$, the regret of Algorithm 2 is bounded as

$$R_T \leq C_2(1 + c_T)\nu\sqrt{2\lambda L(\widetilde{d}log(1 + TK) + 1)T} + (4 + C_3(1 + c_T)\nu L)\sqrt{2log(3/\delta)T} + 5.$$

Proof. By Lemma D.2, the event $\mathcal{E}_t^\mu$ holds for all $1 \leq t \leq T$ with probability at least $1 - \delta$. Hence, with probability $1 - \delta$ we have

$$\begin{aligned}
\overline{R}(T) &= \sum_{i=1}^{T} h(x_{a^*(t),t}) - h(x_{a(t),t})\mathbf{1}(\mathcal{E}_t^\mu) \\
&\leq ((C_1(2c_t+1) + (\sqrt{2\log(C_1 C_0^{-1}\sqrt{L}\nu t^\beta)} + 1))\nu)C_4\sqrt{L}\sum_{i=1}^{T}\mathbb{E}[\min\{\sigma_{a(t),t}, 1\}|\mathcal{F}_t, \mathcal{E}_t^\mu] \\
&\quad + \sum_{i=1}^{T} C_2\frac{C_0}{t^\beta} + (\nu + c_t\nu + C_3)\epsilon(m) + \frac{2}{t^2} \\
&\leq MN + C_2 C_0\sum_{i=1}^{T}\frac{1}{t^\beta} + (\nu + c_t\nu + C_3)\epsilon(m)T + \frac{\pi^2}{3},
\end{aligned}$$

where we set $M = ((C_1(2c_t + 1) + (\sqrt{2\log(C_1 C_0^{-1}\sqrt{L}\nu t^\beta)} + 1))\nu)C_4\sqrt{L}$ and $N = (\sqrt{2\lambda T(\widetilde{d}\log(1 + TK) + 1)} + C2T^{13/6}\sqrt{\log m}m^{-1/6}\lambda^{-2/3}L^{9/2})$ which is obtained by Lemma D.5.

With $\beta \geq 2$, $\sum_{i=1}^{T}\frac{1}{t^\beta} < \frac{\pi^2}{6}$. We choose $C_0 \in [\sqrt{\tilde{d}}, \tilde{d}]$ to eliminate the term $\tilde{d}$ in $\sqrt{2\log(C_1 C_0^{-1}\sqrt{L}\nu T^\beta)}$.

By choosing m similar as in [41] such that $C_3(2c_T + 1)C2T^{13/6}\sqrt{\log m}m^{-1/6}\lambda^{-2/3}L^5) \leq \frac{1}{3}$, $(\nu + c_t\nu + C_3)\epsilon(m)T \leq \frac{1}{3}$, we obtain

$$\overline{R}(T) \leq \mathcal{O}(\widetilde{d}\sqrt{\beta\log(1 + TK)\log(T)T})$$

□

E Additional Lemmas

E.0.1 Proof of Lemma D.8

Proof. If $\sigma_{i,t} = 0$ then by definition of $\alpha_{i,t}^{EI}$, we have $\alpha_{i,t}^{EI} = I_{i,t}$. We have

$$I_{i,t} = \alpha_{i,t}^{EI}$$

$$
\begin{aligned}
&\leq \alpha^{EI}_{a(t),t} \\
&\leq I_{a(t),t} + \nu(c_t+1)\sigma_{a(t),t},
\end{aligned}
$$

where in the first inequality, we use the definition $\alpha^{EI}_{a(t),t} = \max_{i\in[K]}\alpha^{EI}_{i,t}$. In the second inequality, we use Lemma D.1. Thus, the lemma holds with probability $1-t^{-2}$.

We now consider $\sigma_{i,t} > 0$. If $\tilde{f}_{i,t} < f^+_t$ then the lemma will be trivial. We now consider $\tilde{f}_{i,t} > f^+_t$. Following the derivation of the acquisition function $\alpha^{EI}_{i,t}$, we have $\alpha^{EI}_{i,t} = \nu\sigma_{i,t}\tau(\frac{f(x_{i,t};\theta_{t-1})-f^+_t}{\nu\sigma_{i,t}})$. Further, we also have $\frac{f(x_{i,t};\theta_{t-1})-f^+_t}{\nu\sigma_{i,t}} \geq \frac{-c_t\nu}{\nu}$. It is because $f(x_{i,t};\theta_{t-1}) - f(x_{i,t}) \geq -c_t\nu\sigma_{i,t}$ and we are considering the case when $\tilde{f}_{i,t} > f^+_t$. Therefore, $\alpha^{EI}_{i,t} \geq \nu\tau(-c_t)\sigma_{i,t}$.

Now, we combine the fact that $\alpha^{EI}_{i,t} \geq \nu\tau(-c_t)\sigma_{i,t}$ with the fact that $\alpha^{EI}_{i,t} \geq I_{i,t} - c_t\nu\sigma_{i,t}$ which is proven in Lemma D.6 to obtain the following inequality:

$$
I_{i,t} \leq \frac{\tau(c_t)}{\tau(-c_t)}\alpha^{EI}_{i,t} \tag{9}
$$

This inequality Eq(9) holds. Finally, we achieve

$$
\begin{aligned}
\tilde{f}_{i,t} - f^+_t &\leq I_{i,t} \\
&\leq \frac{\tau(c_t)}{\tau(-c_t)}\alpha^{EI}_{i,t} \\
&\leq \frac{\tau(c_t)}{\tau(-c_t)}\alpha^{EI}_{a(t),t} \\
&\leq \frac{\tau(c_t)}{\tau(-c_t)}(\max\{0, \tilde{f}_{a(t),t} - f^+_t\} + \nu(c_t+1)\sigma_{a(t),t} \\
&\leq \frac{\tau(c_t)}{\tau(-c_t)}(\max\{0, f(x_{a(t),t};\theta_{t-1}) + c_t\nu\sigma_{a(t),t} - f^+_t\} + \nu(c_t+1)\sigma_{a(t),t} \\
&\leq \frac{\tau(c_t)}{\tau(-c_t)}(\max\{0, c_t\nu\sigma_{a(t),t}\} + \nu(c_t+1)\sigma_{a(t),t} \\
&= \frac{\tau(c_t)}{\tau(-c_t)}(2c_t\nu + \nu)\sigma_{a^(t),t}
\end{aligned}
$$

where the first inequality holds by the definition of the function I_t. The second one comes from Eq(9). The third one holds by the property of the chosen point $a(t) = \text{argmax}_{i\in[K]}\alpha^{EI}_{i,t}$. The final inequality hold due to Lemma D.6. □

E.0.2 Proof of Lemma D.9

Proof. If $\sigma_{i,t} = 0$ then by definition of $\alpha^{EI}_{i,t}$, we have $\alpha^{EI}_{i,t} = I_{i,t}$. We have

$$
\begin{aligned}
I_{i,t} &= \alpha^{EI}_{i,t} \\
&\leq \alpha^{EI}_{a(t),t} \\
&\leq I_{a(t),t} + \nu(c_t+1)\sigma_{a(t),t},
\end{aligned}
$$

where in the first inequality, we use the definition $\alpha^{EI}_{a(t),t} = \max_{i\in[K]}\alpha^{EI}_{i,t}$. In the second inequality, we use Lemma D.2. Thus, the lemma holds with probability $1-t^{-2}$.

We now consider $\sigma_{i,t} > 0$. If $h(x_{i,t}) < f^+_t$ then the lemma will be trivial. We now consider $h(x_{i,t}) > f^+_t$. Following the derivation of the acquisition function $\alpha^{EI}_{i,t}$, we have $\alpha^{EI}_{i,t} = \nu\sigma_{i,t}\tau(\frac{f(x_{i,t};\theta_{t-1})-f^+_t}{\nu\sigma_{i,t}})$. Further, we also have $\frac{f(x_{i,t};\theta_{t-1})-f^+_t}{\nu\sigma_{i,t}} \geq -1 - \frac{\epsilon(m)}{\nu\sigma_{i,t}}$. It is because $f(x_{i,t};\theta_{t-1}) - h(x_{i,t}) \geq -\nu\sigma_{i,t} - \epsilon(m)$ and we are considering the case when $h(x_{i,t}) > f^+_t$. Therefore, $\alpha^{EI}_{i,t} \geq \nu\sigma_{i,t}\tau(-1 - \frac{\epsilon(m)}{\nu\sigma_{i,t}})$.

Now, we combine the fact that $\alpha_{i,t}^{EI} \geq \nu\sigma_{i,t}\tau(-1-\frac{\epsilon(m)}{\nu\sigma_{i,t}})$ with the fact that $\alpha_{i,t}^{EI} \geq J_{i,t} - \nu\sigma_{i,t} - \epsilon(m)$ which is proven in Lemma D.6 to obtain the following inequality:

$$I_{i,t} \leq \frac{\tau(1+\frac{\epsilon(m)}{\nu\sigma_{i,t}})}{\tau(-1-\frac{\epsilon(m)}{\nu\sigma_{i,t}})}\alpha_{i,t}^{EI}.$$

Using the assumption that $\nu\sigma_{i,t} > \epsilon(m)$, we get

$$I_{i,t} \leq \frac{\tau(2)}{\tau(-2)}\alpha_{i,t}^{EI}$$

This inequality Eq(10) holds. Finally, we achieve

$$\begin{aligned}
\tilde{f}_{i,t} - f_t^+ &\leq I_{i,t} \\
&\leq \frac{\tau(2)}{\tau(-2)}\alpha_{i,t}^{EI} \\
&\leq \frac{\tau(2)}{\tau(-2)}\alpha_{a(t),t}^{EI} \\
&\leq \frac{\tau(2)}{\tau(-2)}(\max\{0, h(x_{a(t),t}) - f_t^+\} + \nu\sigma_{a(t),t} + \epsilon(m) \\
&\leq \frac{\tau(2)}{\tau(-2)}(\max\{0, f(x_{a(t),t};\theta_{t-1}) + \nu\sigma_{a(t),t} + \epsilon(m) - f_t^+\} + \nu\sigma_{a(t),t} + \epsilon(m) \\
&\leq \frac{\tau(2)}{\tau(-2)}(\max\{0, \nu\sigma_{a(t),t} + \epsilon(m)\} + \nu\sigma_{a(t),t} + \epsilon(m) \\
&= (\frac{\tau(2)}{\tau(-2)} + 1)(\nu\sigma_{a(t),t} + \epsilon(m))
\end{aligned}$$

where the first inequality holds by the definition of the function I_t. The second one comes from Eq(10). The third one holds by the property of the chosen point $a(t) = \text{argmax}_{i\in[K]}\alpha_{i,t}^{EI}$. The final inequality hold due to Lemma D.6. □