Distributed Thompson Sampling under constrained communication (with appendix)

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***Abstract*— In Bayesian optimization, a black-box function is maximized via the use of a surrogate model. We apply distributed Thompson sampling, using a Gaussian process as a surrogate model, to approach the multi-agent Bayesian optimization problem. In our distributed Thompson Sampling implementation, each agent receives sampled points from neighbors, where the communication network is encoded in a graph; each agent utilizes a Gaussian process to model the objective function. We demonstrate a theoretical bound on Bayesian Simple Regret, where the bound depends on the size of the largest complete subgraph of the communication graph. Unlike in batch Bayesian optimization, this bound is applicable in cases where the communication graph amongst agents is constrained. When compared to sequential Thompson sampling, our bound guarantees faster convergence with respect to time as long as there is a fully connected subgraph of at least two agents. We confirm the efficacy of our algorithm with numerical simulations on traditional optimization test functions, illustrating the significance of graph connectivity on improving regret convergence.**

***Index Terms*— Bayesian optimization, Thompson sampling, Gaussian process, Distributed optimization, Multi-agent systems**

A. Introduction

Bayesian optimization (BO) [1], [2] is a technique used to optimize a black-box objective function, where the function is unknown and expensive to evaluate. BO is particularly useful in applications where sampling the objective function involves significant computational resources, such as robotics [3], [4], hyperparameter tuning in machine learning [5], [6], and simulation-based optimization [7]. In BO, a surrogate model is used to approximate the unknown objective function - a Gaussian process (GP) [8] is commonly used for this task. An acquisition function based on this surrogate model is used to determine which points should be queried next. Using the acquisition function, query points can be chosen to incorporate a tradeoff between exploration and exploitation by balancing uncertainty reduction in the model and sampling near the current optimum.

Acquisition functions govern the query selection process, which is critical for ensuring efficient optimization. A popular acquisition function is expected improvement (EI), within which the next query point is selected as one which maximizes the expected improvement over the current best-known value [2]. Alternatively, an upper confidence bound (UCB) can be used to select the next query point by selecting a point which maximizes an upper bound on the predicted value [9]. In entropy search (ES), the query points are selected such that the mutual information between the query points and the location of the global optimum is maximized [10], [11]. In Thompson sampling, the next query point is selected as one which maximizes a realization sampled from the posterior of the surrogate model [12]. Thompson sampling is of particular interest to us, as it lends itself well to multi-agent settings [13].

Evaluation of the efficacy of an implementation of Bayesian optimization is multifaceted. Standard performance metrics for Bayesian optimization include time complexity, sample complexity, and regret. Time complexity describes the number of iterations the algorithm requires to converge to a sufficiently optimal solution [14]. Sample complexity refers to the quantity of samples required for the algorithm to reach an approximately optimal solution [15]. To evaluate the quality of the selection of query points, *regret* is often used, which quantifies the gap between sampled points and the global optimum [16]. Regret can take many forms, including simple regret, which considers the performance of the best queried point [17], and cumulative regret, which considers performance of all prior sampled points [18].

Bayesian optimization can be used in a multi-agent setting, in which multiple agents can sample the objective function at a single timestep. This is advantageous because in multi-agent settings, the extrema of the objective function can be determined in fewer timesteps than in a single-agent setting - however, additional complexity is introduced, because in order to fully realize this advantage, the agents must engage in collaboration. To facilitate collaboration, existing literature has been focused on batch Bayesian optimization, a centralized setting in which a central coordinator has access to each agents' acquired information [19], [13]. It then processes and computes the sampling decisions for all agents, which are in turn communicated to each agent. These decisions are often disseminated in batches, allowing multiple agents to simultaneously sample points and consequently parallelizing the optimization process [20], [21].

Centralized approaches are inapplicable in distributed cases, in which there is no centralized coordinator and each agent must possess a local instance of the optimization algorithm [22]. Additionally, they often do not scale well, as they require a central coordinator to manage the processing of all agents' data. Distributed networks are prevalent in real-world applications, such as in multi-robot source seeking and sensor networks [19], [23]. It may not be the case that

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all agents have access to all prior sampled points as in the batch setting - communication may be constrained, where some agents are only able to communicate with specific other agents [24]. These constraints may be due to limited communication capacity or computational capacity of the agents, or due to physical proximity constraints. In this work, we study the distributed multi-agent case, where the communication network of agents is given by a static graph.

Our contribution: we propose a distributed Thompson sampling algorithm to approach the multi-agent Bayesian optimization problem. Unlike in batch cases, in which all agents query points based on a posterior distribution which depends on all previously sampled points, our algorithm is applicable in cases with constrained communication. Prior literature providing theoretical guarantees on distributed Thompson sampling algorithms require fully connected communication graphs, even in asynchronous cases [13], [25], and thus are inapplicable in settings with constrained communication. We establish a theoretical bound on regret that is dependent on the size of the largest complete subgraph of the communication graph - we are the first to demonstrate a distributed BO algorithm with probable guarantees in the constrained communication case. Additionally, we establish the efficacy of our performance and confirm the feasibility of our theoretical bound with numerical simulations on standard optimization test functions.

B. Problem Formulation and Preliminaries

A. Problem Formulation

For a compact set $\mathcal{X} \subset \mathbb{R}^d$, consider an unknown continuous function $f : \mathcal{X} \to \mathbb{R}$, with optimizer x^*. In the BO setting, we wish to find the maximum of this function, where we are only able to sample f through expensive and noisy evaluations. We assume any of M agents can query f at any point and receive a noisy value $y = f(x) + \epsilon$, with $\epsilon \sim \mathcal{N}(0, \sigma_\epsilon^2)$. Agents query f throughout a total of T iterations. For agent $i \in \{1, \dots, M\}$ and iteration $t \in \{1, \dots, T\}$, $x_{t,i}$ is the query point, and $y_{t,i}$ is the corresponding evaluation. Define $X_{t,i} = \{x_{1,i}, \dots, x_{t,i}\}$, $Y_{t,i} = \{y_{1,i}, \dots, y_{t,i}\}$ to be the queries and evaluations made by agent i up to time t. The communication network of M agents is described by graph $G = (V, E)$, where $|V| = M$, and $E \subset \{\{i, j\} : i, j \in V, i \neq j\}$. An unordered pair $\{i, j\} \in E$ if agents i and j are able to communicate with each other. Additionally, we denote the set of neighbors of agent i as $N(i) = \{j : \{i, j\} \in E\}$. The data accessible to agent i at time t is $D_{t,i} = \{(x_{\tau,j}, y_{\tau,j})\}_{j \in N(i) \cup i, \tau < t}$. The set $D_{t,i}$ contains all sampled points by agent i and its neighbors.

B. Gaussian Process

We will use a Gaussian process (GP) to model our unknown objective function f in our BO setting. Recall the unknown continuous objective function $f : \mathcal{X} \to \mathbb{R}$. Let $\mathbf{X}_{D_t} = \{x_1, x_2, \cdots, x_t\}$, where x_j is the jth evaluated point. Let $k : \mathcal{X}^2 \to \mathbb{R}$ be a kernel function selected based on prior beliefs about f. Define

$$\mu_{D_t}(x) = \mathbf{k}_t(x)^\intercal (\mathbf{K}_{D_t} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{y}_{D_t}$$
$$k_{D_t}(x, x') = k(x, x') - \mathbf{k}_{D_t}(x)^\intercal (\mathbf{K}_{D_t} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{k}_{D_t}(x'),$$

where $\mathbf{K}_{D_t} := [k(x', x'')]_{x', x'' \in \mathbf{X}_{D_t}}$, $\mathbf{k}_{D_t}(x) := [k(x', x)]_{x' \in \mathbf{X}_{D_t}}$ and $\mathbf{y}_{D_t} = \{f(x') + \epsilon'\}_{x' \in \mathbf{X}_{D_t}}$, where $\epsilon' \sim \mathcal{N}(0, \sigma_\epsilon^2)$. Thus we can define our GP, in which we denote $f | \mathcal{F}_{D_t} \sim GP(\mu_{D_t}(x), k_{D_t}(x, x'))$. Note that due to the nature of the GP, it is the case that for any $x \in \mathcal{X}$, $f(x) | \mathcal{F}_{D_t} \sim N(\mu_{D_t}(x), \sigma^2_{D_t}(x))$, where $\sigma^2_{D_t}(x) = k_{D_t}(x, x)$ [8]. Furthermore, recall the distributed multi-agent setting, where each of M agents have access to queried points in set $D_{t,i}$, where $D_{t,i}$ and $D_{t,j}$ may not be equal for distinct agents i and j. In our distributed setting, we equip each agent with a unique GP model of f, and thus we write $f_i(x) | \mathcal{F}_{t,i} \sim \mathcal{N}(\mu_{D_{t,i}}(x), \sigma^2_{D_{t,i}}(x))$

C. Regret

Our metric for algorithm performance is regret, which is an assessment of the quality of sampled points. Specifically, we consider the simple regret, which is the difference between the optimal value of the true function and the best value achieved amongst the previous queried points. This definition of regret is useful because optimization settings focus on locating the extrema of a function, and the simple regret tracks the smallest gap between the value at a sampled point and the optimal value. To account for randomness of f in our regret expression, we take expectation of simple regret to yield the following expression, which is called Bayesian Simple Regret:

$$R_{SB}(t) = \min_{i \in \{1, 2, \cdots, M\}, \tau \in \{1, 2, \cdots, t\}} \mathbb{E}[f(x^*) - f(x_{\tau,i})] \quad (1)$$

In our theoretical analysis, we provide a bound on Bayesian Simple Regret.

D. Thompson Sampling

Thompson sampling is an algorithm for sequential decision making that can be utilized in this context for determining the next point of the objective function to query [12]. When using Thompson sampling in our Bayesian optimization framework, a function is sampled from the posterior distribution of the Gaussian process. The maximizer of this function is the next query point at which the black-box objective function is sampled. The Gaussian process is then updated with new information from this sample, and the process repeats for the duration of the experiment.

In sequential Thompson sampling, each subsequent query point is determined based on a model updated on all prior sampled points. Alternative implementations of Thompson sampling include batch Thompson sampling, in which multiple query points are determined as a set at each round, and query the objective function in parallel [13], [21]. Batch Thompson sampling is advantageous in systems capable of parallelizing, e.g. multi-agent systems, because it allows for convergence in fewer number of rounds than sequential Thompson sampling.

In the context of multi-agent systems, Batch Thompson sampling can be thought of as a centralized network, where all agents are simultaneously sampling the objective function at different query points, and all agents have access to the same information. However, this may not be realistic in real-world situations, where communication between agents may be more constrained due to bandwidth limitations, computational constrictions, or privacy concerns. In these cases, agents may only have access to the sampled points by some subset of the other agents, and thus each agent will have may have different models of the objective function across their unique GPs. We propose a Thompson Sampling algorithm for this constrained communication case, and provide theoretical guarantees for the algorithm.

C. Algorithm: Distributed Thompson Sampling

In our implementation of distributed Thompson sampling, each of M agents have distinct Gaussian processes $\mathcal{GP}_i$ for modeling the objective function. At each time step t, all agents update their GPs with the data history available to them. The agent then queries the objective function at $x_{t,i}$, which is the maximizer of the acquisition function sampled from the posterior GP, $\hat{f}_{t,i} \sim \mathcal{GP}_{t,i}$. Each agent then communicates its sampled point to its neighbors, receives the points sampled by their neighbors, and updates their data history accordingly. The collection of data received by neighbors of agent i at time t is denoted as $C_{t,i} = \{(x_{t,j}, y_{t,j})\}_{j \in N(i)}$. Our method is shown in Algorithm 1.

Algorithm 1 Distributed Thompson Sampling

```
Place GP prior on f
for i= 1, ..., M do
    Initial data D_{1,i}
    GP_{0,i} ← GP
end for
for t = 1, ..., T do
    for i= 1, ..., M do
        Update posterior GP_{t,i} conditioned on D_{t,i}
        Sample f̂_{t,i} ~ GP_{t,i}
        Choose next query point
                x_{t,i} ← arg max_x f̂_{t,i}(x)
        Observe y_{t,i}
        Broadcast y_{t,i} to neighbors N(i);
        Collect evaluations C_{t,i} from neighbors N(i)
        Update data history D_{t+1,i} ← D_{t,i} ∪ C_{t,i} ∪ {(x_{t,i}, y_{t,i})}
    end for
end for
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A. Theoretical Result

We analyze the performance of the Distributed Thompson Sampling algorithm on the Bayesian Simple Regret metric. Our regret bound depends on the number of timesteps T and the structure of the agent communication graph G. As in prior work, we utilize notions from information theory in our regret bound [26].

Our regret bound involves the Maximum Information Gain (MIG), which is a constant that captures the difficulty of the objective function. MIG has been shown to be bounded for several kernel functions commonly used with GPs, including Squared Exponential and Matérn kernels, the latter of which was used in our numerical implementation [9].

Let $D = \{x_1, \ldots, x_t\} \subset \mathcal{X}$, and define $y_D = \{(x, f(x) + \epsilon) : x \in D\}$. The MIG is denoted as

$$\Psi_t = \max_{D \subset \mathcal{X}, |D| = t} I(f; y_D), \tag{2}$$

where I is the Shannon Mutual Information. The MIG Ψ_t represents the largest mutual information gain from f by sampling t points. Additionally, for any positive integer n, we define the constant ξ_n, which bounds the information gain of the current round of evaluations [13]. Suppose $|D| = t$ points were already sampled, and i points are being queried in the current round of evaluations, with $i < n$; denote these points in set A, where $A \subset \mathcal{X}$, and $y_A = \{(x, f(x) + \epsilon) : x \in A\}$. Then for $i \geq 1$, ξ_n satisfies

$$\max_{A \subset \mathcal{X}, |A| < n} I(f; y_A | y_D) \leq \frac{1}{2} \log(\xi_n). \tag{3}$$

In the following theorem, we provide a bound for Bayesian Simple Regret for an M agent system with communication graph G. After proving Theorem 3.1, we will introduce and discuss its implication, Corollary 3.2, which is our main convergence result.

Theorem 3.1. *Suppose $k(x, x') \leq 1$ for all x, x'. Let $G_s = (V_s, E_s)$ be a complete subgraph of G. Then the Bayesian Simple Regret after t timesteps satisfies $R_{SB}(t) \leq \frac{C_1}{t|V_s|} + \sqrt{\frac{C_2 \xi_{|V_s|} \beta_t \Psi_{t|V_s|}}{t|V_s|}}$, where $\beta_t = 2\log(t^2 |V_s||\mathcal{X}|)$, $C_1 = \frac{\sqrt{2}\pi^{3/2}}{12}$, and $C_2 = \frac{2}{\log(1+\sigma_\epsilon^{-2})}$.*

Proof. The structure of our proof follows techniques from Kandasamy et al. [13]. We aim to provide a bound on Bayesian Simple Regret. Our proof begins by noting that we can bound Bayesian Simple Regret the average expected regret of any subset of agents. We then decompose this into three sums, each of which utilize a confidence function $U_{t,i}(\cdot)$. We bound each of these sums by incorporating notions from information theory, which allows us to use information gain constants introduced in Equations 3 and 2 to analyze the efficacy of the Gaussian process.

Recall from equation 1 that $R_{SB}(t) = \min_{i \in \{1,2,\cdots,M\}, \tau \in \{1,2,\cdots,t\}} \mathbb{E}[f_i(x^*) - f_i(x_{\tau,i})]$. Define $U_{t,i}(x) = \mu_{D_{t,i}}(x) + \beta_t^{1/2} \sigma_{D_{t,i}}(x)$. Note that, since $R_{SB}(t)$ represents a minimum value of the expression $\mathbb{E}[f_i(x^*) - f_i(x_{\tau,i})]$, it is upper bounded by the average of this expression across any subset of agents. Enumerate the agents in the complete graph $G_s = (V_s, E_s)$ as $\{1, 2, \cdots, |V_s|\}$, and thus we reindex the M agents such that agents $i \in \{1, 2, \cdots, |V_s|\} \in V_s$ and agents $j \in \{|V_s| + 1, \cdots, M\} \in V \backslash V_s$. Thus we can write that

$$R_{SB}(t) \leq \frac{1}{t|V_s|} \sum_{\tau=1}^{t} \sum_{i=1}^{|V_s|} \mathbb{E}[f_i(x^*) - f_i(x_{\tau,i})].$$

We will then focus on upper bounding the expression $\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[f_i(x^*)-f_i(x_{\tau,i})]$.

$$\begin{aligned}
&\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[f_i(x^*)-f_i(x_{\tau,i})]\\
&=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[f_i(x^*)-U_{\tau,i}(x^*)+U_{\tau,i}(x^*)-U_{\tau,i}(x_{\tau,i})\\
&\qquad\qquad+U_{\tau,i}(x_{\tau,i})-f_i(x_{\tau,i})]\\
&=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\underbrace{\mathbb{E}[f_i(x^*)-U_{\tau,i}(x^*)]}_{S1}+\underbrace{\mathbb{E}[U_{\tau,i}(x^*)-U_{\tau,i}(x_{\tau,i})]}_{S2}\\
&\qquad\qquad+\underbrace{\mathbb{E}[U_{\tau,i}(x_{\tau,i})-f_i(x_{\tau,i})]}_{S3}
\end{aligned}$$

We will now bound each of these sums.

S1. Let's begin by upper bounding the sum $S1=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[f_i(x^*)-U_{\tau,i}(x^*)]$.

$$S1=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[f_i(x^*)-U_{\tau,i}(x^*)] \tag{4}$$

$$\leq\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[\mathbb{I}\{f_i(x^*)>U_{\tau,i}(x^*)\}\left(f_i(x^*)-U_{\tau,i}(x^*)\right)] \tag{5}$$

$$\leq\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\sum_{x\in\mathcal{X}}\frac{e^{-\beta_\tau/2}}{\sqrt{2\pi}} \tag{6}$$

$$\leq\sum_{\tau=1}^{t}\frac{1}{\tau^2\sqrt{2\pi}}\leq\frac{\sqrt{2}\pi^{3/2}}{12} \tag{7}$$

Line (5) upper bounds $S1$ by positive terms, Line (6) utilizes Lemma I.1 in Appendix I to bound the expectation of positive terms in a normal distribution. Line (7) results from substituting for β_τ, and the fact that $\sum_{j=1}^{\infty}\frac{1}{j^2}=\frac{\pi^2}{6}$. Therefore, we have established an upper bound for $S1$.

S2. Let's evaluate the expression $S2=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[U_{\tau,i}(x^*)-U_{\tau,i}(x_{\tau,i})]$. First let's focus on the interior of the summation, $\mathbb{E}[U_{\tau,i}(x^*)-U_{\tau,i}(x_{\tau,i})]$. We will proceed to show that this expression evaluates to 0.

By the law of total expectation, $\mathbb{E}[U_{\tau,i}(x^*)-U_{\tau,i}(x_{\tau,i})]=\mathbb{E}[\mathbb{E}[U_{\tau,i}(x^*)-U_{\tau,i}(x_{\tau,i})]|D_{t,i}]$. Because $x_{t,i}$ is sampled from the posterior distribution of $x^*|D_{t,i}$, we must have that $x_{t,i}$ and x^* have the same distribution after conditioning on the acquired data, and thus $x_{t,i}|D_{t,i}\sim x^*|D_{t,i}$. We also notice that $U_{t,i}$ is deterministic when conditioned on $D_{t,i}$. Thus we have that $\mathbb{E}[\mathbb{E}[U_{\tau,i}(x^*)-U_{\tau,i}(x_{\tau,i})]|D_{t,i}]=0$, and consequently $S2=0$.

S3. Lastly, we bound $S3=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[U_{\tau,i}(x_{\tau,i})-f_i(x_{\tau,i})]$. For the evaluation of this sum, we will introduce some additional notation. Denote $\bar{D}_t=\{(x_{\tau,j},y_{\tau,j})\}_{j\in V_s,\tau<t}$. We can think of $\bar{D}_t$ as representing the data acquired by round t in a batch setting exclusively by agents in V_s. Additionally, define $\sigma_{t,i}(x):=\sigma(x)\mid\bar{D}_t\cup\{(x_{t,j},y_{t,j})\}_{j\in V_s,j<i}$. We pick to define $\sigma_{t,i}(\cdot)$ in this way to impose an ordering of the acquired data; in this sense, $\sigma_{t,i}(\cdot)$ depends on $(t-1)|V_s|+i-1$ previously sampled points. With this additional notation, we are well-equipped to upper bound $S3$.

$$S3=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[U_{\tau,i}(x_{\tau,i})-f_i(x_{\tau,i})] \tag{8}$$

$$=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[\mathbb{E}[\mu_{D_{\tau,i}}(x_{\tau,i})+\beta_\tau^{1/2}\sigma_{D_{\tau,i}}(x_{\tau,i})-f_i(x_{\tau,i})]|D_{\tau,i}]] \tag{9}$$

$$=\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[\beta_\tau^{1/2}\sigma_{D_{\tau,i}}(x_{\tau,i})] \tag{10}$$

$$\leq\beta_t^{1/2}\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[\sigma_{D_{\tau,i}}(x_{\tau,i})] \tag{11}$$

$$\leq\beta_t^{1/2}\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[\sigma_{\bar{D}_\tau}(x_{\tau,i})] \tag{12}$$

$$\leq\beta_t^{1/2}\mathbb{E}\left[\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\sigma_{\tau,i}(x_{\tau,i})\exp(I(f;\{y_{\tau,j}\}_{j<i}|y_{\bar{D}_\tau})\right] \tag{13}$$

$$\leq\beta_t^{1/2}\mathbb{E}\left[\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\sigma_{\tau,i}(x_{\tau,i})\xi_i^{1/2}\right] \tag{14}$$

$$\leq\beta_t^{1/2}\xi_{|V_s|}^{1/2}\mathbb{E}\left[\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\sigma_{\tau,i}(x_{\tau,i})\right] \tag{15}$$

$$\leq\beta_t^{1/2}\xi_{|V_s|}^{1/2}\mathbb{E}\left[\left(t|V_s|\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\sigma_{\tau,i}^2(x_{\tau,i})\right)^{1/2}\right] \tag{16}$$

$$\leq\beta_t^{1/2}\xi_{|V_s|}^{1/2}\sqrt{\frac{2t|V_s|\Psi_{t|V_s|}}{\log(1+\sigma_\epsilon^{-2})}} \tag{17}$$

$$\leq\sqrt{\frac{2\xi_{|V_s|}t|V_s|\beta_t\Psi_{t|V_s|}}{\log(1+\sigma_\epsilon^{-2})}} \tag{18}$$

Lines (10) and (11) follow by the law of total expectation. Line (12) follows by noting that β_τ is increasing with τ. Recall that because G_s is a subgraph of G, for all agents $i\in V_s$, $V_s\subset(N(i)\cup i)$. Therefore, $\bar{D}_\tau$ is contained in $D_{\tau,i}$ for all agents $i\in V_s$. In essence, $\bar{D}_\tau\subset D_{\tau,i}\implies\sigma_{\bar{D}_\tau}\geq\sigma_{D_{\tau,i}}$. Line (13) applies this property. Line (14) follows from Lemma I.4 in Appendix I, which introduces ξ_i to bound the information gain of the current set of evaluations. Line (15) follows from the definition of ξ_i, which was stated in Equation 3. Line (16) is a consequence of the fact that ξ_i is increasing with i, and Line (17) follows from application of the Cauchy-Schwarz inequality. Finally, Line (18) is a consequence of Lemma I.3, which bounds the sums of the posterior variances by the MIG term.

Recall that $\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[f_i(x^*)-f_i(x_{\tau,i})]=S1+S2+S3$. Thus, we have shown that

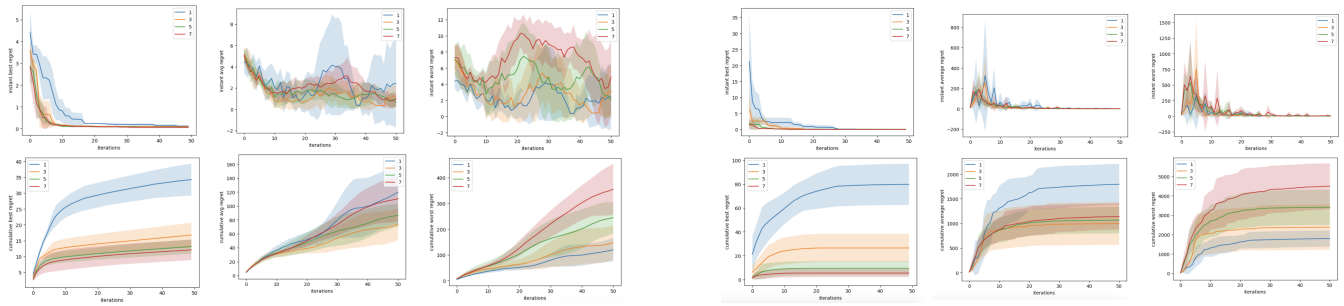

Fig. 1: Simulations of regret analysis with varying agent quantity on star graph configuration, on Ackley (left) and Rosenbrock (right) objective functions.

$\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[f_i(x^*) - f_i(x_{\tau,i})] \leq \frac{\sqrt{2}\pi^{3/2}}{12} + \sqrt{\frac{2\xi_{|V_s|}t|V_s|\beta_t\Psi_{t|V_s|}}{\log(1+\sigma_\epsilon^{-2})}}$. However, we wish to bound $R_{SB}(t)$. Since $R_{SB}(t) \leq \frac{1}{t|V_s|}\sum_{\tau=1}^{t}\sum_{i=1}^{|V_s|}\mathbb{E}[f_i(x^*) - f_i(x_{\tau,i})]$, it directly follows that $R_{SB}(t) \leq \frac{\sqrt{2}\pi^{3/2}}{12t|V_s|} + \sqrt{\frac{2\xi_{|V_s|}\beta_t\Psi_{t|V_s|}}{t|V_s|\log(1+\sigma_\epsilon^{-2})}}$, thus concluding our proof. □

Picking G_s to be the largest complete subgraph of the communication network G yields the following corollary.

Corollary 3.2. *Suppose $k(x,x') \leq 1$ for all x, x'. Let $G_{max} = (V_{max}, E_{max})$ be the largest complete subgraph of G. Then the Bayesian Simple Regret after t timesteps satisfies $R_{SB}(t) \leq \frac{C_1}{t|V_{max}|} + \sqrt{\frac{C_2\xi_{|V_{max}|}\beta_t\Psi_{t|V_{max}|}}{t|V_{max}|}}$, where $\beta_t = 2\log(t^2|V_s||\mathcal{X}|)$, $C_1 = \frac{\sqrt{2}\pi^{3/2}}{12}$, and $C_2 = \frac{2}{\log(1+\sigma_\epsilon^{-2})}$.*

From the corollary, we see that $R_{SB}(t) = \tilde{O}\left(\sqrt{\frac{\xi_{|V_{max}|}\Psi_{t|V_{max}|}}{t|V_{max}|}}\right)$. We note that the term $\Psi_{t|V_{max}|}$ corresponds to the maximal mutual information gain from $t|V_{max}|$ observations, and that this quantity depends only logarithmically on $t|V_{max}|$ for standard kernels such as the squared exponential kernel. For more details, we refer to Appendix II. We note that the term $\xi_{|V_{max}|}$ is the price we pay for the delay in communication within the subgraph G_{max}, and is a standard term that arises in non-sequential Bayesian Optimization. By an appropriately designed initialization phase, this term can actually be reduced to $\tilde{O}(1)$ (see Appendix B.3 in [21] for more details). Thus, compared to the sequential case with t rounds which has simple regret $\tilde{O}\left(\sqrt{\frac{1}{t}}\right)$ [9], our algorithm satisfies a regret of $\tilde{O}\left(\sqrt{\frac{1}{t|V_{max}|}}\right)$, i.e. an improvement of $\sqrt{\frac{1}{|V_{max}|}}$, demonstrating the benefit of the network structure.

D. Numerical Experiments

A. Simulation

In the numerical implementation, performance was assessed utilizing the following regret metrics."Instant best regret" R_B is the best regret achieved by any agent at any time step $\tau \leq t$, and we define its sum to be $\overline{R_B}$:

$$R_B(t) = f^* - \max_{\substack{i\in\{1,2,\dots M\}\\ x_{t,i}\in X_{t,i}}} f(\mathbf{x}_t^i), \quad \overline{R_B}(t) = \sum_{\tau=1}^{t} R_B(\tau),$$

where $f^* = \max_{x\in\mathcal{X}} f(x)$. "Instant worst regret" R_W is the regret of the worst performing agent at time step t, and we define its sum to be the quantity $\overline{R_W}$:

$$R_W(t) = f^* - \min_{i\in\{1,2,\dots M\}} f(x_{t,i}), \quad \overline{R_W}(t) = \sum_{\tau=1}^{t} R_W(\tau).$$

"Instant average regret" R_A is the average of the regrets of all agents at time step t, and we define its sum to be $\overline{R_A}$:

$$R_A(t) = \frac{1}{M}\sum_{i=1}^{M}\left(f^* - f(x_{t,i})\right), \quad \overline{R_A}(t) = \sum_{\tau=1}^{t} R_A(\tau).$$

Numerical results were constructed in a Python implementation built upon the BOTorch package [27]. The code used to generate the simulation and corresponding Figure 1 is available at https://github.com/sabzer/distributed-bo. The Gaussian processes utilized the Matérn kernel with parameter $\nu = \frac{5}{2}$. The numerical simulations were run over $T = 100$ timesteps. Simulations were run based on two test functions for the objective function: Ackley, which has many local maxima and one global minima in the origin, and Rosenbrock, which contains a large valley in which the global minima is situated. The equations of the aforementioned objective functions and their plots are available in Appendix III. Since we were solving a maximization problem, we multiplied the canonical definitions of these functions by -1 for the purpose of our simulation. For the communication networks in our simulations, we used a "star" graph; in a case of N agents, the star graph possesses a central agent that communicates to all other agents, and the other $N-1$ agents can only connect to the central node. We can define this graph for N agents as $G_{star} = (V, E)$, $V = \{1, 2, \dots, N\}$, and $E = \{\{1, j\} : j \in V, j \neq 1\}$. We chose the star graph to model the communication network because our theoretical result bounds instant best regret by the performance of the largest complete subset of agents, and in the star configuration, the largest complete subset of agents remains constant regardless of the number of agents.

B. Discussion

Our Distributed Thompson Sampling algorithm was able to achieve the extrema of the Ackley and Rosenbrock objective functions, and thus is effective at the Bayesian optimization task. Our theoretical result bounds expectation

of Bayesian Simple Regret, $R_{SB}(t)$, with the bound dependent on the size of the largest complete subgraph of the communication network between agents. In the star graph configuration, the largest complete subgraph contained 2 vertices for any star graph containing at least 2 vertices. Interestingly, in Figure 1, we see similar performance in the $3, 5$, and 7 agent cases, with significantly worse performance in the single agent case. This matches intuition motivated by our theoretical result, as the $3, 5$, and 7 agent cases all have largest complete subgraph size of 2, as opposed to the single agent case, where the largest complete subgraph is of size 1.

E. Conclusion

In this paper, we proposed a Distributed Thompson Sampling algorithm to address the multi-agent Bayesian optimization problem under constrained communication. We develop a bound on Bayesian Simple Regret for this approach, where the bound is dependent on properties of the largest complete subgraph of the graph encoding communication structure between agents. With our bound, we show that in multi-agent communication networks, Bayesian Simple Regret will converge faster than in the sequential case (with the same number of rounds). Additionally, we demonstrate the efficacy of our algorithm with regret analysis on optimization test functions, illustrating faster convergence with graphs possessing larger connected subgraphs. Future work will focus on giving a tighter regret bound, and developing adjustments for the Distributed Thompson Sampling algorithm to better control the exploration/exploitation tradeoff.

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APPENDIX I
ADDITIONAL ANALYSIS

Lemma I.1. *([13][26]) At step j, for all $x \in \mathcal{A}$, $\mathbb{E}[\mathbb{I}\{f(x) > U_j(x)\} \cdot (f(x) - U_j(x))] \leq \frac{1}{\sqrt{2\pi}} e^{-\beta_j/2}$.*

Proof. Since f is a GP, we know $f(x)|D_j \sim \mathcal{N}(\mu_j(x), \sigma_j^2(x))$. Recall that $U_j(\cdot) = \mu_j(\cdot) + \beta_j^{1/2}\sigma_j(\cdot)$. Thus, we know that $f(x) - U_j(x)|D_j \sim \mathcal{N}(-\beta_j^{1/2}\sigma_j(x), \sigma_j^2(x))$. For a normal distribution $Z \sim \mathcal{N}(\mu, \sigma^2)$, with $\mu \leq 0$, we have that $\mathbb{E}[Z\mathbb{I}(Z > 0)] \leq \frac{\sigma}{\sqrt{2\pi}} e^{-\mu^2/(2\sigma^2)}$. Thus, we can apply this fact to our setting, yielding:

$$\begin{aligned}
\mathbb{E}[\mathbb{I}\{f(x) > U_j(x)\} \cdot (f(x) - U_j(x))] &\leq \frac{\sigma_j(x)}{\sqrt{2\pi}} e^{-\beta_j/2} && \text{(Aforementioned property of } \mathcal{N}) \\
&\leq \frac{1}{\sqrt{2\pi}} e^{-\beta_j/2} && (\sigma_j(x) \leq \kappa(x,x) \leq 1)
\end{aligned}$$

□

Lemma I.2. *[9] The information gain for selected points can be expressed in terms of the predictive variances. if $f_{[n]} = (f(x_n)) \in \mathbb{R}^n$:*

$$I(y_{[n]}; f_{[n]}) = \frac{1}{2} \sum_{j=1}^{n} \log(1 + \sigma_\epsilon^{-2} \sigma_{j-1}^2(x_n))$$

Proof.

$$\begin{aligned}
I(y_{[n]}; f_{[n]}) &= H(y_{[n]}) + H(y_{[n]}|f_{[n]}) && \text{(Def of information)} \\
&= H(y_{[n]}) - \frac{1}{2} \log |2\pi e \sigma_\epsilon^2 \mathbf{I}| && \text{(Gaussian entropy: } H(N(\mu, \Sigma)) = \frac{1}{2} \log |2\pi e \Sigma|)
\end{aligned}$$

Now let's develop an expression for $H(y_{[n]})$:

$$H(y_{[n]}) = H(y_{[n-1]}) + H(y_n|y_{[n-1]}) \qquad \text{(Entropy chain rule: } H(A,B) = H(A) + H(B|A))$$

$$= H(y_{[n-1]}) + \frac{1}{2} \log(2\pi e(\sigma_\epsilon^2 + \sigma_{n-1}^2(x_n))/2 \quad (y_n|y_{[n-1]} = f(x_n) + \epsilon_n, y_n|y_{[n-1]} \sim N(\mu_{n-1}(x_n), \sigma_{n-1}^2(x_n) + \sigma_\epsilon^2)$$

We now have developed a recursive relation for $H(y_{[n]})$; we can inductively show that $H(y_{[n]}) = \sum_{j=1}^{n} \frac{1}{2} \log(2\pi e(\sigma_\epsilon^2 + \sigma_{j-1}^2(x_n))/2$. Utilizing this expression, we can return to our mutual information expression:

$$\begin{aligned}
I(y_{[n]}; f_{[n]}) &= H(y_{[n]}) - \frac{1}{2} \log |2\pi e \sigma_\epsilon^2 \mathbf{I}| && \text{(Previously shown)} \\
&= \sum_{j=1}^{n} \frac{1}{2} \log(2\pi e(\sigma_\epsilon^2 + \sigma_{j-1}^2(x_n))/2 - \frac{1}{2} \log |2\pi e \sigma_\epsilon^2 \mathbf{I}| && \text{(Substituting developed } H(y_{[n]} \text{ expression)} \\
&= \frac{1}{2} \sum_{j=1}^{n} \log(1 + \sigma_{j-1}^2(x_n) \sigma_\epsilon^{-2}) && \text{(Simplifying log subtraction)}
\end{aligned}$$

□

Lemma I.3. *[13] Let $f \sim GP(0, \kappa), f : \mathcal{X} \to \mathbb{R}$ and each time we query $x \in \mathbb{X}$ we observe $y = f(x) + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \sigma_n^2)$. Let $\{x_1, \ldots, x_t\}$ be an arbitrary set of t evaluations to f where $x_j \in \mathcal{X}$ for all j. Let σ_j^2 denote the posterior variance conditioned on the first j of these queries, $\{x_1, \ldots, x_j\}$. Then, $\sum_{j=1}^{n} \sigma_{j-1}^2(x_j) \leq \frac{2\Psi_n}{\log(1+\sigma_\epsilon^{-2})}$.*

Proof.

$$\begin{aligned}
\Psi_n &\geq I(y_{[n]}; f_{[n]}) && \text{(Definition of } \Psi_n) \\
&\geq \frac{1}{2} \sum_{j=1}^{n} \log(1 + \sigma_\epsilon^{-2} \sigma_{j-1}^2(x_j)) && \text{(Lemma I.2)}
\end{aligned}$$

Note that the function $\frac{x}{1+\log(x)}$ increases with x. Also note that $0 \leq \sigma_\epsilon^2, \sigma_j^2(x_j) \leq 1$ by assumption, and thus $\sigma_\epsilon^{-2}\sigma_j^2(x_j) \leq \sigma_\epsilon^{-2}$. Therefore,

$$\frac{\sigma_\epsilon^{-2}\sigma_{j-1}^2(x_j)}{\log(1 + \sigma_\epsilon^{-2}\sigma_{j-1}^2(x_j))} \leq \frac{\sigma_\epsilon^{-2}}{\log(1 + \sigma_\epsilon^{-2})} \implies \sigma_{j-1}^2(x_j) \log(1 + \sigma_\epsilon^{-2}) \leq \log(1 + \sigma_\epsilon^{-2}\sigma_{j-1}^2(x_j)).$$

Now we can revisit our earlier Ψ_n expression:

$$\begin{aligned}\Psi_n &\geq \frac{1}{2}\sum_{j=1}^{n}\log(1+\sigma_\epsilon^{-2}\sigma_{j-1}^2(x_j)) && \text{(Lemma I.2)}\\ &\geq \frac{1}{2}\log(1+\sigma_\epsilon^{-2})\sum_{j=1}^{n}\sigma_{j-1}^2(x_j) && \text{(Previously shown)}\end{aligned}$$

With algebraic manipulation, the last expression is equivalent to $\sum_{j=1}^{n}\sigma_{j-1}^2(x_j) \leq \frac{2\Psi_n}{\log(1+\sigma_\epsilon^{-2})}$, our desired statement. □

Lemma I.4. *Let $f \sim GP(0,\kappa)$, and let A, B be finite subsets of $\mathcal{X}$. Let $y_A \in \mathbb{R}^{|A|}$ and $y_B \in \mathbb{R}^{|B|}$ denote the observations when we evaluate f at A and B. Let $\sigma_A, \sigma_{A\cup B} : \mathcal{X} \to \mathbb{R}$ denote the posterior standard deviation of the GP when conditioned on A and $A \cup B$, respectively. Then*

$$\forall x \in \mathcal{X}, \qquad \frac{\sigma_A(x)}{\sigma_{A\cup B}(x)} = exp(I(f; y_B|y_A))$$

Proof.

$$\begin{aligned}I(f; y_B|y_A) &= H(f|y_A) - H(f|y_{A\cup B}) && \text{(Mutual information with conditional entropy)}\\ &= \frac{1}{2}\log|2\pi e\sigma_A^2| - \frac{1}{2}\log|2\pi e\sigma_{A\cup B}^2| && \text{(Entropy for GP)}\\ &= \log\left(\frac{\sigma_A}{\sigma_{A\cup B}}\right)\end{aligned}$$

Thus, $\frac{\sigma_A}{\sigma_{A\cup B}} = exp(I(f; y_B|y_A))$ □

APPENDIX II
BOUNDS FOR THE INFORMATION GAIN QUANTITY Ψ_τ FOR DIFFERENT KERNELS

We note that following a known result in [9], Ψ_τ in fact satisfies sublinear growth for three well-known classes of kernels, namely the linear, exponential and Matern kernels.

Lemma II.1 (cf. Theorem 5 in [9])**.** *For any $\tau > 0$, the maximal information gain Ψ_τ can be bounded as follows for the following kernels.*

1) *(Linear kernel): If $k(x,x') = x^\top x'$, then*
$$\Psi_\tau = O(d\log(\tau)).$$
2) *(Squared exponential kernel): If $k(x,x') = \exp(-\|x-x'\|^2/2)$, then*
$$\Psi_\tau = O((\log(\tau))^{d+1}).$$
3) *(Matern kernel with $\nu > 1$): If $k(x,x') = \frac{1}{\Gamma(\nu)2^{\nu-1}}\left(\frac{\sqrt{2\nu}}{d}\|x-x'\|\right)^v K_v\left(\frac{\sqrt{2v}}{d}\|x-x'\|\right)$, where $K_v(\cdot)$ is a modified Bessel function, and $\Gamma(\cdot)$ denotes the gamma function, then*
$$\Psi_\tau = O((\tau)^{\frac{d(d+1)}{2\nu+d(d+1)}}\log(\tau))$$

APPENDIX III
OBJECTIVE FUNCTIONS

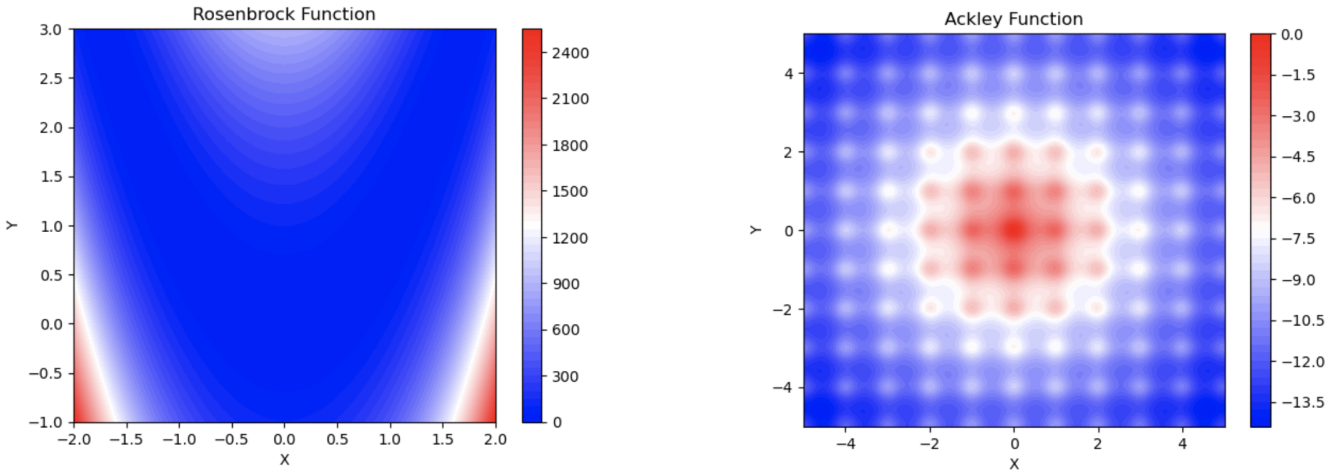
The test objective functions used in our simulations were the Rosenbrock and Ackley functions. The equations of those functions are as follows:

Rosenbrock:

$$f(x,y) = (1-x)^2 + 100(y-x^2)^2 \tag{19}$$

Ackley:

$$f(x,y) = -20\exp\left(-0.2\sqrt{\frac{x^2+y^2}{2}}\right) - \exp\left(\frac{1}{2}(\cos(2\pi x)+\cos(2\pi y))\right) + 20 + \exp(1) \tag{20}$$



(a) Plot of Rosenbrock Function.

(b) Plot of Ackley Function.

Fig. 2: Plots of test objective functions.