On the Structure and Computation of Random Walk Times in Finite Graphs

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Abstract

We consider random walks in which the walk originates in one set of nodes and then continues until it reaches one or more nodes in a target set. The time required for the walk to reach the target set is of interest in understanding the convergence of Markov processes, as well as applications in control, machine learning, and social sciences. In this paper, we investigate the computational structure of the random walk times as a function of the set of target nodes, and find that the commute, hitting, and cover times all exhibit submodular structure, even in non-stationary random walks. We provide a unifying proof of this structure by considering each of these times as special cases of stopping times. We generalize our framework to walks in which the transition probabilities and target sets are jointly chosen to minimize the travel times, leading to polynomial-time approximation algorithms for choosing target sets. Our results are validated through numerical study.

I. INTRODUCTION

A random walk is a stochastic process over a graph, in which each node transitions to one of its neighbors at each time step according to a (possibly non-stationary) probability distribution [1], [2]. Random walks on graphs are used to model and design a variety of stochastic systems. Opinion propagation in social networks, as well as gossip and consensus algorithms in communications and networked control systems, are modeled and analyzed via random walks [3].
Random walks also serve as distance metrics in clustering, image segmentation, and other machine learning applications. The behavior of physical processes, such as heat diffusion and electrical networks, can also be characterized through equivalent random walks.

One aspect of random walks that has achieved significant research attention is the expected time for the walk to reach a given node or set of nodes. Relevant metrics include the hitting time, defined as the expected time for a random walk to reach any node in a given set, the commute time, defined as the expected time for the walk to reach any node in a given set and then return to the origin of the walk, and the cover time, which is the time for the walk to reach all nodes in a desired set. These times give rise to bounds on the rate at which the walk converges to a stationary distribution, and also provide metrics for quantifying the centrality or distance between nodes.

The times of a random walk are related to system performance in a diverse set of network applications. The convergence rate of gossip and consensus algorithms is determined by the hitting time to a desired set of leader or anchor nodes. The effective resistance of an electrical network is captured by its commute time to the set of grounded nodes. The performance of random-walk query processing algorithms is captured by the cover time of the set of nodes needed to answer the query. Optimal control problems such as motion planning and traffic analysis are described by the probability of reaching a target set or the resource cost per cycle of reaching a target set infinitely often.

In each of these application domains, a set of nodes is selected in order to optimize one or more random walk metrics. The optimization problem will depend on whether the distribution of the random walk is affected by the choice of input nodes. Some systems will have a fixed walk distribution, determined by physical laws (such as heat diffusion or social influence propagation), for any set of input nodes. In other applications, the distribution can be selected during the design stage, and hence the distribution of the walk and the set to be reached can be jointly optimized, as in Markov decision processes. In both cases, however, the number of possible sets of nodes is exponential in the network size, making the optimization problem computationally intractable in the worst case, requiring additional structure of the random walk times. At present however, computational structures of random walks have received little attention by the research community.

In this paper, we investigate the hitting, commute, cover, and cycle times, as well as the
reachability probability, of a random walk as functions of a set of nodes. We show that these metrics exhibit a submodular structure, and give a unifying proof of submodularity for the different metrics. We consider both fixed distributions and the case where the set and distribution are jointly selected. We make the following specific contributions:

- We formulate the problem of jointly selecting a set and a control policy in order to maximize the probability of reaching the set from any initial state, as well as the average (per cycle) cost of reaching the set infinitely often.
- We prove that each problem can be approximated in polynomial time with provable optimality bounds using submodular optimization techniques. Our approach is to relate the existence of a probability distribution that satisfies a given cycle cost to the volume of a linear polytope, which is a submodular function of the desired set. We extend our approach to joint optimization of reachability and cycle cost, which we prove is equivalent to a matroid optimization problem.
- In the case where the probability distribution is fixed, we develop a unifying framework, based on the submodularity of selecting subsets of stopping times, which includes proofs of the supermodularity of hitting and commute times and the submodularity of the cover time as special cases. Since the cover time is itself NP-hard to compute, we study and prove submodularity of standard upper bounds for the cover time.
- We evaluate our results through numerical study, and show that the submodular structure of the system enables improvement over other heuristics such as greedy and centrality-based algorithms.

This paper is organized as follows. In Section II, we review the related work. In Section III, we present our system model and background on submodularity. In Section IV, we demonstrate submodularity of random walk times when the walk distribution is chosen to optimize the times. In Section V, we study submodularity of random walk times with fixed distribution. In Section VI, we present numerical results. In Section VII, we conclude the paper.

II. RELATED WORK

Commute, cover, and hitting times have been studied extensively, dating to classical bounds on the mixing time [20], [1]. Generalizations to these times have been proposed in [21], [22]. Connections between random walk times and electrical resistor networks were described in [17]. These classical works, however, do not consider the submodularity of the random walk times.
Submodularity of random walk times has been investigated based on connections between the hitting and commute times of random walks, and the performance of linear networked systems \cite{16,23}. The supermodularity of the commute time was shown in \cite{16}. The supermodularity of the hitting time was shown in \cite{23} and further studied in \cite{15}. These works assumed a fixed, stationary transition probability distribution, and also did not consider submodularity of the cover time. Our framework derives these existing results as special cases of a more general result, while also considering non-stationary transition probability distributions.

Random walk times have been used for image segmentation and clustering applications. In these settings, the distance between two locations in an image is quantified via the commute time of a random walk with a probability distribution determined by a heat kernel \cite{8}. Clustering algorithms were then proposed based on minimizing the commute time between two sets \cite{24}.

This work is related to the problem of selecting an optimal control policy for a Markov decision process \cite{25}. Prior work has investigated selecting a control policy in order to maximize the probability of reaching a desired target set \cite{26,27}, or to minimize the cost per cycle of reaching the target set \cite{28}. These works assume that the target set is given. In this paper, we consider the dual problem of selecting a target set in order to optimize these metrics.

### III. Background and Preliminaries

This section gives background on random walk times, Markov decision processes, and submodularity. Notations used throughout the paper are introduced.

#### A. Random Walk Times

Let $G = (V, E)$ denote a graph with vertex set $V$ and edge set $E$. A random walk is a discrete-time random process $X_k$ with state space $V$. The distribution of the walk is defined by a set of maps $P_k : V^k \rightarrow \Pi^V$, where $V^k = V \times \cdots \times V$ and $\Pi^V$ is the simplex of probability distributions over $V$. We have that

$$
Pr(X_k = v_k | X_1 = v_1, \ldots, X_{k-1} = v_{k-1}) = P_k(v_1, \ldots, v_k).
$$

The random walk is stationary if there exists a stochastic matrix $P$ such that $Pr(X_k = v_k | X_1 = v_1, \ldots, X_{k-1} = v_{k-1}) = P(v_{k-1}, v_k)$. Matrix $P$ is denoted as the transition matrix. A walk is \textit{ergodic} if there exists a probability distribution $\pi$ such that $\lim_{k \rightarrow \infty} P^k = \pi^T$, implying that
the distribution of the walk will eventually converge to \( \pi \) regardless of the initial distribution.

Throughout the paper, we let \( \mathbb{E}(\cdot) \) denote the expectation of a random variable.

Let \( S \subseteq V \) be a subset of nodes in the graph. The hitting, commute, and cover time of \( S \) are defined as follows.

**Definition 1:** First define the following functions:

\[
\begin{align*}
\nu(S) &= \min \left\{ k : X_k \in S \right\} \\
\kappa(S, u) &= \min \left\{ k : X_k = u, X_j \in S \text{ for some } j < k \right\} \\
\phi(S) &= \min \left\{ k : \forall s \in S, \exists j \leq k \text{ s.t. } X_j = s \right\}
\end{align*}
\]

The hitting time of \( S \) from a given node \( v \) is equal to \( H(S, v) \triangleq \mathbb{E}(\nu(S)|X_1 = v) \). The commute time of \( S \) from node \( v \) is equal to \( K(S, v) = \mathbb{E}(\kappa(S, v)|X_1 = v) \). The cover time of \( S \) from node \( v \) is equal to \( C(S, v) = \mathbb{E}(\phi(S)|X_1 = v) \).

Intuitively, the hitting time is the expected time for the random walk to reach the set \( S \), the commute time is the expected time for a walk starting at a node \( v \) to reach any node in \( S \) and return to \( v \), and the cover time is the expected time for the walk to reach all nodes in the set \( S \). If \( \pi \) is a probability distribution, we can further generalize the above definitions to \( H(S, \pi) \), \( K(S, \pi) \), and \( C(S, \pi) \), which are the expected hitting, commute, and cover times when the initial state is chosen from distribution \( \pi \). The times described above are all special cases of stopping times of a stochastic process.

**Definition 2:** Let \( Z = \{Z_k : k \geq 0\} \) be a discrete-time stochastic process. A stopping time with respect to \( Z \) is a random variable \( \tau \) taking values in \( \{1, 2, 3, \ldots\} \) such that the event \( \{\tau = n\} \) is determined completely by \( Z \).

The hitting time is a stopping time where \( \tau = \min \left\{ k : X_k \in S \right\} \). The cover time is a stopping time with

\[
\tau = \min \left\{ k : \forall i \in S, \exists l \leq k \text{ s.t. } X_l = i \right\},
\]

while the commute time is a stopping time with

\[
\tau = \min \left\{ k : x_k = u, x_l \in S \text{ for some } l < k \right\}.
\]

### B. Markov Decision Processes

A Markov Decision Process (MDP) is a generalization of a Markov chain, defined as follows.
**Definition 3:** An MDP $\mathcal{M}$ is a tuple $\mathcal{M} = (V, \{A_i : i \in V\}, P)$, where $V$ is a set of states, $A_i$ is a set of actions at state $i$, and $P$ is a transition probability function defined by

$$P(i, a, j) = Pr(X_{k+1} = j \mid X_k = i, \text{action } a \text{ chosen at step } k).$$

Define $A = \bigcup_{i=1}^n A_i$ and $A = |A|$. In the specific case where the action set is empty or consists of a single element at each node, the MDP reduces to a Markov chain. The set of actions at each node corresponds to the possible control inputs that can be supplied to the chain at that node. A control policy is a function that takes as input a sequence of states $X_1, \ldots, X_k$ and gives as output an action $u_k \in A_{X_k}$. A stationary control policy is a control policy $\mu$ that depends only on the current state, and hence can be characterized by a function $\mu : V \rightarrow A$. We let $\mathcal{P}$ denote the set of valid policies.

The control policy $\mu$ is selected in order to achieve a design goal of the system. Such goals are quantified via specifications on the random process $X_k$. Two relevant specifications are safety and liveness constraints. A safety constraint specifies that a set of states $R$ should never be reached by the walk. A liveness constraint specifies that a given set of states $S$ must be reached infinitely often. In an MDP, two optimization problems arise in order to satisfy such constraints, namely, the reachability and average-cost-per-cycle problems.

The reachability problem consists of selecting a policy in order to maximize the probability that a desired set of nodes $S$ is reached by the Markov process while the unsafe set $R$ is not reached. The average-cost-per-cycle (ACPC) problem is defined via the following metric.

**Definition 4:** The average cost per cycle metric from state $s_0$ under policy $\mu$ is defined by

$$J(s_0) = \limsup_{N \to \infty} E \left\{ \frac{\sum_{k=0}^N g(X_k, \mu_k(X_k))}{C(\mu, N)} \right\},$$

where $g(X_k, \mu_k(X_k))$ is the cost of taking an action $\mu_k(X_k)$ at state $X_k$, and $C$ is the number of cycles up to time $N$. In the special case where $g(X_k, \mu_k(X_k)) = 1$ for all states and actions, the average cost per cycle is the number of steps in between times when the set $S$ is reached.

The average cost per cycle can be viewed as the average number of steps in between times when the set $S$ is reached. The ACPC problem consists of choosing the set $S$ and policy $\mu$ in order to minimize $J(s_0)$. Applications of this problem include motion planning, in which the goal of a robot is to reach a desired state infinitely often while minimizing energy consumption.
C. Submodularity

Submodularity is a property of set functions $f : 2^W \to \mathbb{R}$, where $W$ is a finite set. A function is submodular if, for any sets $S$ and $T$ with $S \subseteq T \subseteq W$ and any $v \notin T$,

$$f(S \cup \{v\}) - f(S) \geq f(T \cup \{v\}) - f(T).$$

A function is supermodular if $-f$ is submodular, while a function is modular if it is both submodular and supermodular. For any modular function, a set of coefficients $\{c_i : i \in W\}$ can be defined such that

$$f(S) = \sum_{i \in S} c_i.$$

Furthermore, for any set of coefficients $\{c_i : i \in W\}$, the function $f(S) = \max \{c_i : i \in S\}$ is increasing and submodular, while the function $\min \{c_i : i \in S\}$ is decreasing and supermodular. Any nonnegative weighted sum of submodular (resp. supermodular) functions is submodular (resp. supermodular).

A matroid is defined as follows.

**Definition 5:** A matroid $\mathcal{M} = (V, \mathcal{I})$ is defined by a set $V$ and a collection of subsets $\mathcal{I}$. The set $\mathcal{I}$ satisfies the following conditions: (i) $\emptyset \in \mathcal{I}$, (ii) $B \in \mathcal{I}$ and $A \subseteq B$ implies that $A \in \mathcal{I}$, and (iii) If $|A| < |B|$ and $A, B \in \mathcal{I}$, then there exists $v \in B \setminus A$ such that $(A \cup \{v\}) \in \mathcal{I}$. The collection of sets $\mathcal{I}$ is denoted as the independent sets of the matroid. A **basis** is a maximal independent set. The uniform matroid $\mathcal{M}_k$ is defined by $A \in \mathcal{I}$ iff $|A| \leq k$. A **partition matroid** is defined as follows.

**Definition 6:** Let $V = V_1 \cup \cdots \cup V_m$ with $V_i \cap V_j = \emptyset$ for $i \neq j$ be a partition of a set $V$. The partition matroid $\mathcal{M} = (V, \mathcal{I})$ is defined by $A \in \mathcal{I}$ if $|A \cap V_i| \leq 1$ for all $i = 1, \ldots, m$.

Finally, the union of matroids $\mathcal{M} = \mathcal{M}_1 \vee \mathcal{M}_2$ is defined by $A \in \mathcal{I}$ iff $A = A_1 \cup A_2$ for $A_1 \in \mathcal{I}_1$ and $A_2 \in \mathcal{I}_2$.

IV. RANDOM WALKS WITH OPTIMAL DISTRIBUTIONS

In this section, we consider the problem of selecting a set $S$ of states for an MDP to reach in order to optimize a performance metric. We consider two problems, namely, the problem of selecting a set of states $S$ in order to maximize the reachability probability to $S$ while minimizing the probability of reaching an unsafe set $R$, and the problem of selecting a set of states $S$ in order to minimize the ACPC. A motivating scenario is a setting where an unmanned vehicle
must reach a refueling station or transit depot infinitely often, and the goal is to place the set of stations in order to maximize the probability of reaching one or minimize the cost of reaching.

A. Reachability Problem Formulation

The problem of selecting a set $S$ with at most $k$ nodes in order to maximize the probability of reaching $S$ under the optimal policy $\mu$ is considered as follows. Let $Z(S)$ denote the event that the walk reaches $S$ at some finite time and does not reach the unsafe state $R$ at any time. The problem formulation is given by

$$\maximize_{S \subseteq V} \max_{\mu \in \mathcal{P}} Pr(Z(S)|\mu)$$

subject to $|S| \leq k$ \hspace{1cm} (2)

This formulation is equivalent to

$$\maximize_{\mu} \max_{S, |S| \leq k} Pr(Z(S)|\mu)$$

The following known result gives a linear programming approach to maximizing the probability of reachability for a fixed set $S$.

**Lemma 1 ([29], Theorem 10.105):** The optimal value of $\max \{Pr(Z(S)|\mu) : \mu \in \mathcal{P}\}$ is equal to

$$\min \quad 1^T x$$

subject to $x \in \mathbb{R}^n$

$$x_i \in [0, 1] \ \forall i$$

$$x_i = 1 \ \forall i \in S, x_i = 0 \ \forall i \in R$$

$$x_i \geq \sum_{j=1}^{n} P(i, u_j)x_j \ \forall i \in V, u \in U_i$$ \hspace{1cm} (4)

In addition to giving the optimal value of the maximal reachability problem, Eq. (4) can also be used to compute the optimal policy. In order for $x$ to be the solution to (4), for each $i \in V \setminus (R \cup S)$, there must be an action $u^*_i$ such that

$$x_i = \sum_{j=1}^{n} P(i, u^*_i, j)x_j.$$ 

Otherwise, it would be possible to decrease $x_i$ and hence the objective function of (4). Hence the optimal policy $\mu$ is given by $\mu(i) = u^*_i$.

Based on Lemma 1 we formulate an equivalent problem to (2). Define a vector $\vec{x} \in \mathbb{R}^{n2^n}$, with elements indexed as $\vec{x}_i^S$. The element $\vec{x}_i^S$ can be viewed as the probability that the reachability
condition is satisfied starting from node \( i \) when the set of states to be reached is \( S \). The following lemma gives an optimization problem that generalizes Lemma 1 to the case where \( S \) can also be optimized.

**Lemma 2:** The value of the optimization problem (3) is equal to the value of

\[
\min_X \max_{S:|S|\leq k} \sum_{i\in V} x_i^S
\]

s.t.

\[
\begin{align*}
x_i^S &= 1 \quad \forall i \in S \\
x_i^S &= 0 \quad \forall i \in R \\
x_i^S &\geq \sum_{j=1}^{n} P(i, u, j)x_j^S \quad \forall i, u \in A_i
\end{align*}
\]

Letting \( \mathbf{x}^* \) denote the solution to (5), the set \( S^* = \arg \max_S \{ \sum_{i=1}^{n} x_i^S \} \) is the solution to (2).

**Proof:** By Lemma 1 for each \( S \), \( \{ x_i^S : i = 1, \ldots, n \} \) defines the optimal reachability probabilities for each node. Hence \( \max_{S:|S|\leq k} \{ \sum_{i\in V} x_i^S \} \) is the maximum reachability probability over all sets \( S \).

While Eq. (5) gives the maximum reachability, the number of optimization variables is exponential in the number of nodes, making the problem computationally intractable. In what follows, we formulate a relaxed problem that can be solved in polynomial time. Define a matrix \( \mathbf{P} \) with dimensions \( nA2^n \times n2^n \). The rows of \( \mathbf{P} \) are indexed \( \{(S, i, u) : S \subseteq \{1, \ldots, n\}, i = 1, \ldots, n, u \in A\} \).

\[
\mathbf{P}_{(S,i,u),(T,j)} = \begin{cases} P(i, u, j), & S = T, u \in U_i \\ 0, & \text{else} \end{cases}
\]

Let

\[
\pi = \{ x_i^S : x_i^S = 0 \quad \forall i \in R, \mathbf{P}\mathbf{x} \leq \mathbf{x} \}.
\]

As a first step, we have the following relaxation of (5)

\[
\min_{\mathbf{x}} \max_{S:|S|\leq k} \{ \sum_{i\in V} x_i^S + \rho \left( \sum_S \sum_{i\in S} (1 - x_i^S) \right) \}
\]

s.t.

\[
\mathbf{x} \in \pi
\]

for some \( \rho > 0 \). The following lemma leads to a tractable equivalent formulation to (6).

**Lemma 3:** The solution to (6) is equivalent to the solution to

\[
\min_{\mathbf{x}} \max_{S} \left( \sum_{i=1}^{N} x_i - \rho \sum_{i\in S} x_i \right)
\]

s.t.

\[
\mathbf{x} \in \Pi
\]
Proof: The solution to (6) is equal to a constant plus the solution to
\[
\begin{align*}
\text{minimize} & \quad \max_{S:|S|\leq k} \left( \sum_{i=1}^{n} x_i^S - \rho \sum_{i\in S} x_i^S \right) \\
\text{s.t.} & \quad \mathbf{x} \in \Pi
\end{align*}
\]

By choosing \( \{x_i^S : i = 1, \ldots, n\} \) as the solution to (4) with desired set \( S \), the last term of the objective function can be set to zero. Hence the variables \( \{x_i^S : S \neq S_{\text{max}}\} \) have no impact on the solution to the optimization problem, and the problem reduces to (7).

The objective function of (7) is a pointwise maximum of convex functions and is therefore convex. A subgradient of the objective function at any point \( x_0 \), denoted \( v(x_0) \), is given by
\[
v(x_0)_i = \begin{cases} 
1 - \lambda, & i \in S_{\text{max}}(x_0) \\
1, & \text{else}
\end{cases}
\]

where
\[
S_{\text{max}}(x_0) = \arg \min \left\{ \sum_{i \in S} (x_0)_i : |S| \leq k \right\}.
\]

Computing this subgradient is a modular optimization problem, and hence can be performed in linear time in \( S \). A polynomial-time algorithm for solving (7) can be obtained using interior-point methods, as shown in Algorithm [1].

The interior-point approach of Algorithm [1] thus gives an efficient algorithm for maximizing the optimal reachability problem by choosing the set. We further observe that more general constraints than \(|S| \leq k\) can be constructed. One possible constraint is to ensure that, for some partition \( V_1, \ldots, V_m \), we have \(|S \cap V_i| \geq 1\) for each \( i = 1, \ldots, m\). Intuitively, this constraint implies that there must be at least one state to be reached in each partition set \( V_i \). This constraint is equivalent to the constraint \( S \in \mathcal{M}_k \), where \( \mathcal{M}_k \) is the union of the partition matroid and the uniform matroid of rank \( k - m \). The calculation of \( S_{\text{max}}(x_0) \) then becomes
\[
S_{\text{max}}(x_0) = \arg \min \left\{ \sum_{i \in S} (x_0)_i : S \in \mathcal{M}_k \right\}.
\]

This problem can also be solved in polynomial time due to the matroid structure of \( \mathcal{M}_k \) using a greedy algorithm.
**Algorithm 1** Algorithm for selecting a set of states $S$ to maximize probability of reachability.

1: **procedure** MAX_REACH($G = (V, E), U, P, R, k, \epsilon, \delta$)
2: **Input:** Graph $G = (V, E)$, set of actions $U_i$ at each node $i$, probability distribution $P$, unsafe nodes $R$, number of states $k$, convergence parameters $\epsilon$ and $\delta$.
3: **Output:** Set of nodes $S$
4: $\Phi \leftarrow$ barrier function for polytope $\Pi$
5: $x \leftarrow 0$
6: $x' \leftarrow 1$
7: while $||x - x'||_2 > \epsilon$ do
8:   $S \leftarrow \arg\max\{\sum_{i \in S} x_i : |S| \leq k\}$
9:   $v \leftarrow 1$
10:  $v_i \leftarrow (1 - \rho) \; \forall i \in S$
11:  $w \leftarrow \nabla_x \Phi(x)$
12:  $x' \leftarrow x$
13:  $x \leftarrow x + \delta(v + w)$
14: end while
15: $S \leftarrow \arg\max\{\sum_{i \in S} x_i : |S| \leq k\}$
16: **return** $S$
17: **end procedure**

**B. Minimizing the Average Cost Per Cycle**

In order to interpret the minimum ACPC problem, we introduce the notions of gain and bias as follows. The gain-bias pair $(J_\mu, h_\mu)$ is defined by $J_\mu = P_\mu J_\mu$, $h_\mu = 1 + P_\mu h_\mu + \bar{P}_\mu J_\mu$, and $(I - \bar{P}_\mu)h_\mu + v_\mu = P_\mu v_\mu$, where $P_\mu$ is the transition matrix induced by policy $\mu$. The gain can be interpreted as the average cost per cycle across all nodes in the network, while the bias is the deviation of each node’s cost per cycle from the average. The following result relates the gain-bias pair to the optimal ACPC policy.

**Theorem 1 ([30]):** Suppose that there exists a policy $\mu$ and $\rho \in \mathbb{R}$ such that the gain-bias pair $(J, h)$, where $J = \lambda 1$, satisfies

$$\lambda + h(i) = \min_{u \in U_i} \left[ 1 + \sum_{j=1}^{n} P(i, u, j)h(j) + \lambda \sum_{j \notin S} P(i, u, j) \right].$$  \hspace{1cm} (8)
Then $\lambda$ is the minimum value of the ACPC problem.

Based on Theorem 1 in order to ensure that the minimum ACPC is no more than $\lambda$, it suffices to show that there is no $h$ satisfying (8) for the chosen set $S$. Note that this condition is sufficient but not necessary. Hence the following optimization problem gives a lower bound on the ACPC

$$\text{minimize} \quad \max \lambda$$

subject to

$$\lambda + h(i) \leq 1 + \sum_{j=1}^{n} P(i, u, j)h(j)$$
$$+ \lambda \sum_{j \notin S} P(i, u, j) \forall i, u \in U_i$$

(9)

The following theorem gives a sufficient condition for the minimum ACPC.

**Theorem 2:** Suppose that, for any $h$, there exists $u$ and $i$ such that

$$\lambda 1\{i \in S\} + h(i) - \sum_{j=1}^{n} P(i, u, j)h(j) > 1.$$  

(10)

Then the ACPC is bounded above by $\lambda$.

In order to prove Theorem 2, we introduce an augmented graph that will have the same ACPC cost. Define the graph $\overline{G} = (\overline{V}, \overline{E})$ as follows. Let

$$\overline{V} = \{i_l : i \in V, l = 0, 1\},$$

$$\overline{E} = \{(i_0, i_0) : i \in V\} \cup \{(i_0, j) : (i, j) \in E\}.$$

The sets of actions satisfy $U_{i_0} = \overline{U}_{i_1} = U_i$. The transition probabilities are given by

$$\overline{P}(i_1, u, i_0) = 1, \quad \overline{P}(i_0, u, j_1) = P(i, j).$$

Finally, the set $\overline{S}$ for $\overline{G}$ is constructed from the set $S$ for $G$ via

$$\overline{S} = \{i_0 : i \in S\}.$$

The following result establishes the equivalence between the graph formulations.

**Proposition 1:** The minimum ACPC of $G$ with set $S$ is equal to the minimum ACPC of $\overline{G}$ with set $\overline{S}$.

**Proof:** There is a one-to-one correspondence between policies on $G$ and policies on $\overline{G}$. Indeed, any policy $\mu$ on $G$ can be extended to a policy $\overline{\mu}$ on $\overline{G}$ by setting $\overline{\mu}_{i_0} = \mu_i$ and $\overline{\mu}_{i_1} = 1$ for all $i$. Furthermore, by construction, the ACPC for $G$ with policy $\mu$ will be equal to the ACPC with policy $\overline{\mu}$. In particular, the cost per cycle of the minimum-cost policies will be equal.

We are now ready to prove Theorem 2.
Proof of Theorem 2: For the augmented graph, the constraint of Eq. (9) is equivalent to
\[
\lambda 1\{i \in S\} + h(i_1) \leq h(i_0)
\]
(11)

\[
h(i_0) - \sum_{j=1}^{n} P(i, u, j) h(j_1) \leq 1
\]
(12)
for all \(i, j,\) and \(u\). Hence, in order for the minimum cost per cycle to be less than \(\lambda\), at least one of (11) or (12) must fail for each \(h \in \mathbb{R}^{2N}\). For each \(h\), let \(S_h = \{i : \lambda + h(i_1) > h(i_0)\}\), so that the condition that the ACPC is less than \(\lambda\) is equivalent to
\[S_h \cap S \neq \emptyset \quad \forall h \in \mathbb{R}^{2N}.
\]
Furthermore, we can combine Eq. (11) and (12) to obtain
\[
\lambda 1\{i \in S\} + h(i_1) \leq 1 + \sum_{j=1}^{n} P(i, u, j) h(j_1).
\]
We can then remove the subscripts to obtain
\[
\lambda 1\{i \in S\} + h(i) \leq 1 + \sum_{j=1}^{n} P(i, u, j) h(j)
\]
as a necessary and sufficient condition for the ACPC to be at least \(\lambda\). This is equivalent to (10).

The following result maps the minimum ACPC problem to submodular optimization via Theorem 2.

Proposition 2: Let \(\mathcal{P}(\lambda, S)\) denote the polytope
\[
\mathcal{P}(\lambda, S) = \{h : \mathbf{A}h \leq 1 - \lambda 1\{i \in S\} \} \cap \{||h||_\infty \leq \zeta\}.
\]
Then the function \(r_\lambda(S) = \text{vol}(\mathcal{P}(\lambda, S))\) is decreasing and supermodular as a function of \(S\). Furthermore, if \(r_\lambda(S) = 0\), then the ACPC is bounded above by \(\lambda\).

Proof: Define a sequence of functions \(r_\lambda^N(S)\) as follows. For each \(N\), partition the set \(\mathcal{P}(0, \emptyset) = \{h : \mathbf{A}h \leq 1\}\) into \(N\) equally-sized regions with center \(x_1, \ldots, x_N\) and volume \(\delta_N\). Define
\[
r_\lambda^N(S) = \sum_{i=1}^{N} \delta_N 1\{x_i \in \mathcal{P}(\lambda, S)\}.
\]
Since \(\mathcal{P}(\lambda, S) \subseteq \mathcal{P}(0, \emptyset)\) for all \(S\) and \(\lambda\), we have that
\[
\text{vol}(\mathcal{P}(\lambda, S)) \approx r_\lambda^N(S)
\]
and
\[ \lim_{N \to \infty} r_N^\lambda(S) = r_\lambda(S). \]

The term \( 1\{x_i \in P(\lambda, S)\} \) is equal to the decreasing supermodular function
\[ 1\{S_{x_i} \cap S = \emptyset\}. \]

Hence \( r_N^\lambda(S) \) is a decreasing supermodular function, and \( r_\lambda(S) \) is a limit of decreasing supermodular functions and is therefore decreasing supermodular. Finally, we have that if \( r_\lambda(S) = \emptyset \), then for any \( \epsilon > 0 \), there is no \( h \) satisfying \( A'h \leq 1 - (\lambda + \epsilon)1\{i \in S\} \).

In Proposition 2, the constraint \( ||h||_\infty \leq \zeta \) is added to ensure that the polytope is compact.

Proposition 2 implies that ensuring that the ACPC is bounded above by \( \lambda \) is equivalent to the submodular constraint \( r_\lambda(S) = 0 \). This motivates a bijection-based algorithm for solving the minimum ACPC problem (Algorithm 2).

The following theorem describes the optimality bounds and complexity of the algorithm.

**Theorem 3:** Algorithm 2 terminates in \( O(kn^6 \log \lambda_{\text{max}}) \) time. For any \( \lambda \) such that there exists a set \( S \) of size \( k \) satisfying \( r_\lambda(S) = 0 \), Algorithm 2 returns a set \( \hat{S} \) with
\[ \frac{|\hat{S}|}{|S|} \leq 1 + \log \left\{ \min_v \left\{ \frac{r_\lambda(\emptyset)}{r_\lambda(S \setminus \{v\})} \right\} \right\}. \]

**Proof:** The number of rounds in the outer loop is bounded by \( \log \lambda_{\text{max}} \). For each iteration of the inner loop, the objective function \( r_\lambda(S) \) is evaluated \( kn \) times. Computing \( r_\lambda(S) \) is equivalent to computing the volume of a linear polytope, which can be approximated in \( O(n^5) \) time [31], for a total runtime of \( O(kn^6 \log \lambda_{\text{max}}) \).

From [32], for any monotone submodular function \( f(S) \) and the optimization problem
\[ \min \{ |S| : f(S) \leq \alpha \}, \]
the set \( \hat{S} \) returned by the algorithm satisfies
\[ \frac{|\hat{S}|}{|S^*|} \leq 1 + \log \left\{ \frac{f(V) - f(\emptyset)}{f(V) - f(\hat{S}_{T-1})} \right\}, \]
Algorithm 2 Algorithm for selecting a set of states $S$ to minimize average cost per cycle.

1: procedure $\text{MIN\_ACPC}(G = (V, E), U, P, R, k)$

2: \hspace{1em} Input: Graph $G = (V, E)$, set of actions $U_i$ at each node $i$, probability distribution $P$, number of states $k$.

3: \hspace{1em} Output: Set of nodes $S$

4: $\lambda_{\text{max}} \leftarrow \max \text{ ACPC for any } v \in \{1, \ldots, n\}$

5: $\lambda_{\text{min}} \leftarrow 0$

6: while $|\lambda_{\text{max}} - \lambda_{\text{min}}| > \delta$ do

7: \hspace{1em} $S \leftarrow \emptyset$

8: \hspace{2em} $\lambda \leftarrow \frac{\lambda_{\text{max}} + \lambda_{\text{min}}}{2}$

9: \hspace{2em} while $r_\lambda(S) > 0$ do

10: \hspace{3em} $v^* \leftarrow \arg \min \{r_\lambda(S \cup \{v\}) : v \in \{1, \ldots, n\}\}$

11: \hspace{3em} $S \leftarrow S \cup \{v^*\}$

12: \hspace{2em} end while

13: \hspace{1em} if $|S| \leq k$ then

14: \hspace{2em} $\lambda_{\text{max}} \leftarrow \lambda$

15: \hspace{1em} else

16: \hspace{2em} $\lambda_{\text{min}} \leftarrow \lambda$

17: \hspace{1em} end if

18: \hspace{1em} end while

19: \hspace{1em} return $S$

20: end procedure

where $\hat{S}_{T-1}$ is the set obtained at the second-to-last iteration of the algorithm. Applied to this setting, we have

$$\frac{|\hat{S}|}{|S^*|} \leq 1 + \log \left\{ \frac{r_\lambda(V) - r_\lambda(\emptyset)}{r_\lambda(V) - r_\lambda(\hat{S}_{T-1})} \right\}$$

$$= 1 + \log \left\{ \frac{r_\lambda(\emptyset)}{r_\lambda(\hat{S}_{T-1})} \right\}$$

$$\leq 1 + \log \left\{ \frac{r_\lambda(\emptyset)}{\min_v \{r_\lambda(\hat{S} \setminus \{v\})\}} \right\}.$$
We note that the complexity of Algorithm 2 is mainly determined by the complexity of computing the volume of the polytope $P(\lambda, S)$. This complexity can be reduced to $O(n^3)$ by computing the volume of the minimum enclosing ellipsoid of $P(\lambda, S)$ instead.

The ACPC problem can be extended to the case where the random walk is not irreducible, making the graph $G$ disconnected, and hence the set $S$ must be divided among a set of connected components $G_1, \ldots, G_m$. This case can be considered by modifying Algorithm 2 to have $r_\lambda(S|G_i) = 0$ for all $i = 1, \ldots, m$ as the termination condition, thus ensuring that the ACPC is at most $\lambda$ for all of the connected components.

C. Joint Optimization of Reachability and ACPC

In this section, we consider the problem of selecting a set $S$ to satisfy safety and liveness constraints with maximum probability and minimum cost. This problem can be viewed as combining the maximum reachability and minimum ACPC problems formulated in the previous sections. As a preliminary, we define an end component of an MDP.

**Definition 7:** For an MDP $\mathcal{M} = (V, A, P)$, an end component (EC) is a subset of nodes $V' \subseteq V$, together with sets of actions $\{A'_i : i \in V'\}$ and a transition mapping $P' : V' \times A' \times V' \to [0, 1]$. The set $V'$ satisfies $v \in V'$, $u \in A'_v$, and $P(v, u, v') > 0$ implies $v' \in V$.

Intuitively, an end component $(V', A', P')$ is a set of states and actions such that if only the actions in $A'$ are played, the MDP will remain in $V'$ for all time. A maximal end component (MEC) is an end component such that for any $V'$ and $A''$, $V' \subseteq V''$ and $A' \subseteq A''$ implies that $V''$ and $A''$ are not an EC. The following result shows the relationship between MECs and safety and liveness constraints.

**Lemma 4 ([30]):** The probability that an MDP satisfies a safety and liveness specification defined by $R$ and $S$ is equal to the probability that the MDP reaches an MEC $(V', U', P')$ with $V' \cap S \neq \emptyset$ and $V' \cap R = \emptyset$.

We define an MEC with $V' \cap R = \emptyset$ to be an accepting maximal end component (AMEC). By Lemma 4, the problem of maximizing the probability of satisfying the safety and liveness constraints is equal to the probability of reaching an MEC. This problem can be mapped to a maximum reachability problem by introducing an augmented MDP $\tilde{\mathcal{M}} = (\tilde{V}, \tilde{A}, \tilde{P})$, defined as follows. Let $\mathcal{M}_1 = (V'_1, A'_1, P'_1), \ldots, \mathcal{M}_N = (V'_N, A'_N, P'_N)$ denote the set of MECs satisfying $V'_i \cap S \neq \emptyset$. The node set of the augmented graph is equal to $V \setminus (\bigcup_{i=1}^N V'_i) \cup \{m_1, \ldots, m_N\}$.
The actions for nodes in $V$ are unchanged, while the nodes $m_1, \ldots, m_N$ have empty action sets. The transition probabilities are given by

$$
\tilde{P}(i, u, j) = \begin{cases} 
P(i, u, j), & i, j \notin \bigcup_{i=1}^{M} V'_i, u \in A_i \\
\sum_{j \in V'_i} P(i, u, j), & i \notin \bigcup_{s=1}^{M} V'_s, j = m_l, u \in A_i \\
1, & i = j = m_l \\
0, & i = m_l, i \neq j
\end{cases}
$$

In this MDP, the probability of reaching the set $\{m_1, \ldots, m_N\}$ is equal to the probability of satisfying the safety and liveness constraints, and hence maximizing the probability of satisfying the constraints is equivalent to a reachability problem.

We now formulate two problems of joint reachability and ACPC. The first problem is to minimize the ACPC, subject to the constraint that the probability of satisfying the constraints is maximized. The second problem is to maximize the probability of satisfying safety and liveness properties, subject to a constraint on the average cost per cycle. In order to address the first problem, we characterize the sets $S$ that maximize the reachability probability.

**Lemma 5:** Suppose that for each AMEC $(V', U', P')$, $S \cap V' \neq \emptyset$. Then $S$ maximizes the probability of satisfying the safety and liveness constraints of the MDP.

**Proof:** By Lemma 4, the safety and liveness constraints are satisfied if the walk reaches an MEC satisfying $S \cap V' \neq \emptyset$. Hence, for any policy $\mu$, the probability of satisfying the constraints is maximized when the $S \cap V' \neq \emptyset$ for all MECs.

Note that the converse of the lemma may not be true. There may exist policies that maximize the probability of satisfaction and yet do not reach some AMECs with positive probability.

**Lemma 5** implies that in order to formulate the problem of minimizing the ACPC such that the probability of achieving the specifications is maximized, it suffices to ensure that there is at least one node in each AMEC that belongs to $S$. We will show that this is equivalent to a matroid constraint on $S$. Define a partition matroid by $\mathcal{M}_1 = (V, \mathcal{I})$ where

$$
\mathcal{I} = \{ S : |S \cap V'| \leq 1 \ \forall \ \text{AMEC} \ V' \}.
$$

Let $r$ denote the number of AMECs, and let $\mathcal{M}_{k-r}$ denote the uniform matroid with cardinality $(k-r)$. Finally, let $\mathcal{M} = \mathcal{M}_1 \vee \mathcal{M}_{k-r}$. The following theorem gives the equivalent formulation.
Theorem 4: Let \( q(S) \) denote the ACPC for set \( S \). Then the problem of selecting a set of up to \( k \) nodes in order to minimize the ACPC while maximizing reachability probability is equivalent to

\[
\begin{align*}
\text{minimize} & \quad q(S) \\
\text{s.t.} & \quad S \in \mathcal{M}
\end{align*}
\]  

(13)

Proof: Since \( q(S) \) is strictly decreasing in \( S \), the minimum value of the ACPC is achieved when \( |S| = k \). In order to maximize the probability of satisfying the safety and liveness constraints, \( S \) must also contain at least one node in each AMEC, implying that \( S \) contains a basis of \( \mathcal{M}_1 \). Hence the optimal set \( S^* \) consists of the union of one node from each AMEC (a basis of \( \mathcal{M}_1 \)) and \((k-r)\) other nodes (a basis of \( \mathcal{M}_{k-r} \)), and hence is a basis of \( \mathcal{M} \). Conversely, we have that the optimal solution to (13) satisfies the constraint \(|S| \leq k\) and contains at least one node in each AMEC, and thus is also a feasible solution to the joint reachability and ACPC problem.

Hence, we can formulate the problem of selecting \( S \) to minimize the ACPC as

\[
\begin{align*}
\text{minimize} & \quad \max \lambda \\
S \in \mathcal{M} & \\
\text{s.t.} & \quad \lambda + h(i) \leq 1 + \sum_{j=1}^{n} P(i, u, j) h(j) \\
& \quad + \lambda \sum_{j \notin S} P(i, u, j)
\end{align*}
\]

(14)

If there are multiple AMECs, then each AMEC \((V'_i, U'_i, P'_i)\) will have a distinct value of average per cycle cost \( \lambda_i \), which will be determined by \( S \cap V'_i \). The problem of minimizing the worst-case ACPC is then given by

\[
\begin{align*}
\text{minimize} & \quad \max_m \lambda_m(S \cap V'_m) \\
S \in \mathcal{M} & \\
\text{s.t.} & \quad \lambda_m + h(i) \leq 1 + \sum_{j=1}^{n} P(i, u, j) h(j) \\
& \quad + \lambda \sum_{j \notin S} P(i, u, j) \quad \forall i \in V'_m, \ u \in A'_i
\end{align*}
\]

(15)

This problem is equivalent to

\[
\begin{align*}
\text{minimize} & \quad \zeta \\
S & \\
\text{s.t.} & \quad \zeta + h(i) \leq 1 + \sum_{j=1}^{n} P(i, u, j) h(j) \\
& \quad + \zeta \sum_{j \notin S} P(i, u, j) \quad \forall i, u \in A'_i \\
& \quad |S| \leq k
\end{align*}
\]

(16)
By Proposition 2, Eq. (16) can be rewritten as

$$\begin{align*}
\text{minimize} & \quad \zeta \\
\text{s.t.} & \quad \sum_{m=1}^{M} r_{\zeta}^m (S \cap V'_m) = 0 \\
& \quad |S| \leq k
\end{align*}$$

(17)

where $r_{\zeta}^i(S)$ is the volume of the polytope $P(\zeta, S \cap V'_m)$ defined as in Section IV-B. A bijection-based approach, analogous to Algorithm 2, suffices to approximately solve (17). This approach is given as Algorithm 3.

The following proposition describes the optimality bounds of Algorithm 3.

**Proposition 3**: Algorithm 3 returns a value of $\zeta$, denoted $\hat{\zeta}$, that satisfies $\hat{\zeta} < \zeta^*$, where $\zeta^*$ is the minimum ACPC that can be achieved by any set $S$ satisfying

$$|S| \leq k \left( 1 + \log \frac{\sum_{m=1}^{M} r_{\zeta}^m (\emptyset)}{\min_v \sum_{m=1}^{M} r_{\zeta}^m (S \setminus \{v\})} \right).$$

(18)

**Proof**: The proof is analogous to the proof of Theorem 3. The submodularity of $r_{\zeta}^i(S)$ implies that the set $|\hat{S}|$ is within the bound (18) of the minimum-size set $|S^*|$ with $\sum_{m=1}^{M} r_{\zeta}^m (S) = 0$.

We now turn to the second joint optimization problem, namely, maximizing the reachability probability subject to a constraint $\zeta$ on the average cost per cycle. We develop a two-stage approach. In the first stage, we select a set of input nodes for each AMEC $V_1, \ldots, V_r$ in order to guarantee that the ACPC is less than $\zeta$. In the second stage, we select the set of AMECs to include in order to satisfy the ACPC constraint while minimizing the number of inputs needed.

For the first stage, for each AMEC we approximate the problem

$$\begin{align*}
\text{minimize} & \quad |S_i| \\
\text{s.t.} & \quad r_{\zeta}^i (S_i) = 0
\end{align*}$$

(19)

where $r_{\zeta}^i(S_i) = \text{vol}(P(\zeta, S_i))$ is defined as in Section IV-B and restricted to $(V'_i, A'_i, P'_i)$, and thus obtain a set of nodes $S_i$ such that the ACPC is bounded above by $\lambda$ on the AMEC $V_i$ when the set of desired states is $S_i$. We let $c_i = |S_i|$ denote the number of nodes required for each AMEC. The problem of selecting a subset of nodes to maximize reachability while satisfying this constraint on $\zeta$ can then be formulated as

$$\begin{align*}
\text{minimize} & \quad \max_{S: \sum_{i \in S} c_i \leq k} \left( \sum_{i=1}^{N} x_i - \lambda \sum_{i \in S} x_i \right) \\
\text{s.t.} & \quad x \in \Pi
\end{align*}$$

(20)
Algorithm 3 Algorithm for selecting a set of states $S$ to minimize average cost per cycle.

1: procedure MIN_ACPC_MAX_REACH($G = (V, E)$, $U$, $P$, $R$, $k$)
2: Input: Graph $G = (V, E)$, set of actions $U_i$ at each node $i$, probability distribution $P$, number of states $k$.
3: Output: Set of nodes $S$
4: \( \zeta_{\text{max}} \leftarrow \text{max ACPC for any } v \in \{1, \ldots, n\} \)
5: \( \zeta_{\text{min}} \leftarrow 0 \)
6: while \( |\zeta_{\text{max}} - \zeta_{\text{min}}| > \delta \) do
7: for $i = 1, \ldots, M$ do
8: \( S \leftarrow \emptyset \)
9: \( \zeta \leftarrow \frac{\zeta_{\text{max}} + \zeta_{\text{min}}}{2} \)
10: while \( r_{\lambda}(S) > 0 \) do
11: \( v^* \leftarrow \text{arg min } \{ r_{\zeta}(S \cup \{v\}) : v \in \{1, \ldots, n\} \} \)
12: \( S \leftarrow S \cup \{v^*\} \)
13: end while
14: end for
15: if \( |S| \leq k \) then
16: \( \lambda_{\text{max}} \leftarrow \lambda \)
17: else
18: \( \lambda_{\text{min}} \leftarrow \lambda \)
19: end if
20: end while
21: return $S$
22: end procedure

by analogy to (7). The inner optimization problem of (20) is a knapsack problem, and hence is NP-hard and must be approximated at each iteration. In order to reduce the complexity of the problem, we introduce the following alternative formulation. We let $P_\lambda$ denote the polytope
satisfying the inequalities

\[ 1^T v = \beta \]

\[ v_i (1 - \lambda_1 \mathbf{1} \{i \in S\}) \geq \sum_{j=1}^{n} v_j P(i, u, j) \]

By Proposition 2, the condition that the reachability probability is at most \( \zeta \) is equivalent to \( \text{vol}(P(\zeta, S_i)) = 0 \). Letting \( r_\lambda(S) \) denote the volume of \( \mathcal{P}_\lambda \) when the set of desired states is \( S \), the problem is formulated as

\[
\begin{align*}
\text{minimize} & \quad \sum_{i \in T} c_i \\
\text{s.t.} & \quad r_\lambda(T) = 0
\end{align*}
\]

Problem (21) is a submodular knapsack problem with coverage constraints. An algorithm for solving it is as follows. The set \( T \) is initialized to \( \emptyset \). At each iteration, find the element \( i \) that minimizes

\[ \frac{c_i}{r_\lambda(T) - r_\lambda(T \cup \{i\})}, \]

terminating when the condition \( r_\lambda(T) = 0 \) is satisfied.

Hence, the overall approach is to select a collection of subsets \( S_i : i = 1, \ldots, M \), representing the minimum-size subsets to satisfy the ACPC constraint on each AMEC \( V_i \). We then select a set of AMECs to include in order to satisfy a desired constraint on reachability while minimizing the total number of inputs. The set \( S \) is then given by

\[ S = \bigcup_{i \in T} S_i. \]

The optimality gap of this approach is described as follows.

**Proposition 4:** The set \( T \) chosen by the greedy algorithm satisfies

\[ \frac{|T|}{|T^*|} \leq 1 + \log \left\{ \frac{1}{r_\lambda(T)} \right\}, \]

where \( T^* \) is the optimal solution to (21).

**Proof:** We have that \( r_\lambda \) is monotone decreasing and supermodular. Hence, by Theorem 1 of [32], the optimality bound holds.

Combining the optimality bounds yields

\[ \frac{|S|}{|S^*|} \leq \left( 1 + \log \left\{ \frac{1}{r_\lambda(T)} \right\} \right) \left( 1 + \log \left\{ \frac{1}{r_\lambda(T)} \right\} \right). \]
D. Optimal Hitting Time

In this section, we consider the problem of minimizing the hitting time under a joint selection of the probability distribution and set. We have that the hitting time of node $i$ under policy $\mu$, denoted $H(i, \mu, S)$, satisfies

$$H(i, \mu, S) = 1 + \sum_{u \in A_i} \sum_{j=1}^{n} P(i, u, j) Pr(\mu_i = u)H(j, S)$$

for $i \notin S$ and $H(i, S) = 0$ for $i \in S$. Hence the optimal hitting time for a given set $S$ is given by

$$H(i, S) = 1 + \min_u \left\{ \sum_{j=1}^{n} P(i, u, j)H(j, S) \right\}.$$ 

Thus the optimal hitting time problem is equivalent to the linear program

$$\begin{align*}
\text{maximize} & \quad 1^T v \\
\text{s.t.} & \quad v_i \leq 1 + \sum_{j=1}^{n} P(i, u, j)v_j \forall i, u \in A_i \\
& \quad v_i = 0, \quad i \in S
\end{align*} \quad (22)$$

The following lemma leads to an equivalent formulation to (22).

**Lemma 6:** For a given graph $G$, there exists $\lambda > 0$ such that the conditions

$$\begin{align*}
v_i & \leq 1 + \sum_{j=1}^{n} P(i, u, j)v_j \forall i, u \in U_i \\
v_i & = 0 \forall i \in S
\end{align*} \quad (23)$$

are equivalent to

$$v_i + \lambda \mathbf{1}\{i \in S\}v_i \leq 1 + \sum_{j=1}^{n} P(i, u, j)v_j. \quad (25)$$

**Proof:** If (25) holds, then for $\lambda$ sufficiently large we must have $v_i = 0$ for all $i \in S$. The condition then reduces to

$$v_i \leq 1 + \sum_{j=1}^{n} P(i, u, j)v_j$$

for all $i \notin S$ and $u \in U_i$, which is equivalent to (23).

From Lemma 6, it follows that in order to ensure that the optimal hitting time for each node is no more than $\zeta$, it suffices to ensure that for each $v$ satisfying $1^T v \geq \zeta$, there exists at least one $i$ and $u$ such that

$$1 + \sum_{j=1}^{n} P(i, u, j)v_j < (1 + \lambda \mathbf{1}\{i \in S\})v_i.$$
We define the function $\chi_v(S)$ as

$$\chi_v(S) = \begin{cases} 1, & (23) \text{ and (24) hold} \\ 0, & \text{else} \end{cases}$$

The following lemma relates the function $\chi_v(S)$ to the optimality conditions of Lemma 6.

**Lemma 7:** The optimal hitting time corresponding to set $S$ is bounded above by $\zeta$ if and only if

$$\chi_\zeta(S) \triangleq \int_{\{v: 1^Tv \geq \zeta\}} \chi_v(S) \ dv = 0.$$

**Proof:** Suppose that $\chi_\zeta(S) = 0$. Then for each $v$ satisfying $1^Tv \geq \zeta$, we have that $\chi_v(S) = 0$ and hence

$$\sum_{j=1}^n P(i, u, j)v_j < (1 + \lambda 1_{i \in S})v_i$$

holds for some $i$ and $u \in U_i$, and hence there is no $v$ satisfying the conditions of (22) with $1^Tv = \zeta$ for the given value of $S$.

The following result then leads to a submodular optimization approach to computing the set $S$ that minimizes the hitting time.

**Proposition 5:** The function

$$\chi(S) = \int_{\{v: 1^Tv \geq \zeta\}} \chi_v(S) \ dv$$

is supermodular as a function of $S$.

**Proof:** We first show that $\chi_v(S)$ is supermodular. We have that $\chi_v(S) = 1$ if and only if there exists $i \in S$ with $v_i \neq 0$, or equivalently, $\text{supp}(v) \cap S \neq \emptyset$. If $\chi_v(S) = \chi_v(S \cup \{u\}) = 0$, then the condition $\text{supp}(v) \cap S \neq \emptyset$ already holds, and hence $\chi_v(T) = \chi_v(T \cup \{u\})$. Since $\chi(S)$ is an integral of supermodular functions, it is supermodular as well.

Furthermore, $\chi(S)$ can be approximated in polynomial time via a sampling-based algorithm [2]. Hence the problem of selecting a set of states $S$ in order to minimize the optimal hitting time can be stated as

$$\begin{align*}
\text{minimize} \quad & \zeta \\
\text{s.t.} \quad & \min \{|S|: \chi_\zeta(S) = 0\} \leq k
\end{align*}$$

(26)

Problem (26) can be approximately solved using an algorithm analogous to Algorithm 2, with $r_\lambda(S)$ replaced by $\chi_\zeta(S)$ in Lines 9 and 10, and $\lambda$ replaced by $\zeta$ throughout. The following proposition gives optimality bounds for the revised algorithm.
Proposition 6: The modified Algorithm\cite{2} guarantees that the hitting time satisfies $\zeta^*(S) \geq \zeta^*(\hat{S})$, where $\hat{S}$ is the optimal solution when $\hat{k} = k \left( 1 + \log \frac{\chi(\emptyset)}{\min_v \chi(S \setminus \{v\})} \right)$.

Proof: Since the function $\zeta^*(S)$ is supermodular, the number of states $S$ selected by the greedy algorithm to satisfy $\zeta^*(S) = 0$ satisfies (27). Hence, for the set $\hat{S}$, since $|S| \leq \hat{k}$, we have that $\zeta^*(S) \geq \zeta^*(\hat{S})$.

V. Submodularity with Fixed Probability Distribution

This section demonstrates submodularity of random walk times for walks with a probability distribution that does not depend on the set of nodes $S$. We first state a general result on submodularity of stopping times, and then prove submodularity of hitting, commute, cover, and coupling times as special cases.

A. General Result

Consider a set of stopping times $Z_1, \ldots, Z_N$ for a random process $X_k$. Let $W = \{1, \ldots, N\}$, and define two functions $f, g : 2^W \rightarrow \mathbb{R}$ by

$$f(S) = \mathbb{E}\{\max\{Z_i : i \in S\}\}$$

$$g(S) = \mathbb{E}\{\min\{Z_i : i \in S\}\}$$

We have the following general result.

Proposition 7: Let $W = \{1, \ldots, N\}$. The functions $f(S)$ and $g(S)$ are nondecreasing submodular and nonincreasing supermodular, respectively.

Proof: For any $S$ and $T$ with $S \subseteq T$, we have that

$$f(T) = \mathbb{E}\{\max\{\max\{Z_i : i \in S\}, \max\{Z_i : i \in T \setminus S\}\}\}$$

$$\geq \mathbb{E}\{\max\{Z_i : i \in S\}\} = f(S),$$

implying that $f(S)$ is nondecreasing. The proof of monotonicity for $g(S)$ is similar.

To show submodularity of $f(S)$, consider any sample path $\omega$ of the random process $X_k$. For any sample path, $Z_i$ is a deterministic nonnegative integer. Consider any sets $S, T \subseteq \{1, \ldots, N\},$
and suppose without loss of generality that \( \max \{ Z_i(\omega) : i \in S \} \geq \max \{ Z_i(\omega) : i \in T \} \). Hence for any sets \( S, T \subseteq \{1, \ldots, N\} \), we have

\[
\max_{i \in S} Z_i(\omega) + \max_{i \in T} Z_i(\omega) = \max_{i \in S \cup T} Z_i(\omega) + \max_{i \in S \cap T} Z_i(\omega).
\]

Now, let \( Q = (i_1, \ldots, i_N) \), where each \( i_j \in \{1, \ldots, N\} \), be a random variable defined by \( Z_{i_1} \leq Z_{i_2} \leq \cdots \leq Z_{i_N} \) for each sample path, so that \( Q \) is the order in which the stopping times \( Z_i \) are satisfied. For any ordering \((i_1, \ldots, i_N)\), we have

\[
E \left\{ \max_{i \in S} \{ Z_i \} | Q = (i_1, \ldots, i_n) \right\} = \max_{j : i_j \in S} E(Z_{i_j} | Q = (i_1, \ldots, i_n)) = \max_{j : i_j \in S} \alpha_{i_j Q},
\]

which is submodular by the same analysis as above. Taking expectation over all the realizations of \( Q \), we have

\[
f(S) = \sum_{(i_1, \ldots, i_N)} E \left\{ \max_{i \in S} \{ Z_i \} | Q = (i_1, \ldots, i_N) \right\} \cdot Pr(Q = (i_1, \ldots, i_N))
\]

\[
= \sum_{(i_1, \ldots, i_N)} \left[ \max_{j : i_j \in S} \alpha_{i_j Q} \right] \cdot Pr(Q = (i_1, \ldots, i_N))
\]

which is a finite nonnegative weighted sum of submodular functions and hence is submodular.

The proof of supermodularity of \( g(S) \) is similar.

Proposition [7] is a general result that holds for any random process, including random processes that are non-stationary. In the following sections, we apply these results and derive tighter conditions for hitting, commute, and cover times.

B. Submodularity of Hitting and Commute Times

In this section, we consider the problem of selecting a subset of nodes \( S \) in order to minimize the hitting time to \( S \), \( H(\pi, S) \). The following result is a corollary of Proposition [7].

**Lemma 8:** \( H(\pi, S) \) is supermodular as a function of \( S \).

**Proof:** Let \( Z_i \) denote the stopping time corresponding to the event \( \{ X_k = i \} \), where \( X_k \) is a random walk on the graph. Then \( H(\pi, S) \) is supermodular by Proposition [7].
The results of Lemma 8 imply that a greedy algorithm is sufficient to achieve an upper bound of $(1 - 1/e)$ on the hitting time. An analogous lemma for the commute time is as follows.

**Lemma 9:** For any distribution $u$, the function $K(S, u)$ is supermodular as a function of $S$.

**Proof:** Let $Z_i$ denote the stopping time corresponding to the event $\{X_{k} = u, X_l = i\}$ for some $l < k$. Then $K(S, u) = E(\min_{i \in S} Z_i)$, and hence $K(S, u)$ is supermodular as a function of $S$. ■

Lemma 9 can be extended to distributions $\pi$ over the initial state $u$ as $K(S, \pi) = \sum_u K(S, u)\pi(u)$. The function $K(S, \pi)$ is then a nonnegative weighted sum of supermodular functions, and hence is supermodular.

### C. Submodularity of Cover Time

The submodularity of the cover time is shown as follows.

**Proposition 8:** The cover time $C(S)$ is nondecreasing and submodular as a function of $S$.

**Proof:** The result can be proved by using Proposition 7 with the set of events $\{Z_i : i \in S\}$ where the event $Z_i$ is given as $Z_i = \{X_{k} = i\}$.

An alternative proof is as follows. Let $S \subseteq T \subseteq V$, and let $v \in V \setminus T$. The goal is to show that

$$C(S \cup \{v\}) - C(S) \geq C(T \cup \{v\}) - C(T).$$

Let $\tau_v(S)$ denote the event that the walk reaches $v$ before reaching all nodes in the set $S$, noting that $\tau_v(T) \subseteq \tau_v(S)$. Let $Z_S$, $Z_T$, and $Z_v$ denote the times when $S$, $T$, and $v$ are reached by the
walk, respectively. We prove that the cover time is submodular for each sample path of the walk by considering different cases.

In the first case, the walk reaches node $v$ before reaching all nodes in $S$. Then $C(S) = C(S \cup \{v\})$ and $C(T) = C(T \cup \{v\})$, implying that submodularity holds trivially. In the second case, the walk reaches node $v$ after reaching all nodes in $S$, but before reaching all nodes in $T$. In this case, $C(S \cup \{v\}) - C(S) = Z_v - Z_S$, while $C(T \cup \{v\}) - C(T) = 0$. In the last case, the walk reaches $v$ after reaching all nodes in $T$. In this case,

$$C(S \cup \{v\}) - C(S) = Z_v - Z_S \geq Z_v - Z_T = C(T \cup \{v\}) - C(T),$$

implying submodularity. Taking the expectation over all sample paths yields the desired result.

The submodularity of cover time implies that the problem of maximizing the cover time can be approximated up to a provable optimality bound. Similarly, we can select a set of nodes to minimize the cover time by

$$\min \{C(S) - \lambda|S| : S \subseteq V\}.$$ 

The cover time, however, is itself computationally difficult to approximate. Instead, upper bounds on the cover time can be used. We have the following preliminary result.

**Proposition 9 ([1]):** For any set of nodes $A$, define $t_{\min}^A = \min_{a,b \in A, a \neq b} E_a(\tau_b)$. Then the cover time $C(S)$ is bounded by

$$C(S) \geq \max_{A \subseteq S} \left\{ t_{\min}^A \left( 1 + \frac{1}{2} + \cdots + \frac{1}{|A| - 1} \right) \right\} \triangleq f'(S).$$

Define $c(k) = 1 + \frac{1}{2} + \cdots + \frac{1}{|A| - 1}$. The approximation $f'(S)$ can be minimized as follows. We first have the following preliminary lemma.

**Lemma 10:** The function $f'(S)$ is equal to

$$f'(S) = \max_{k=1, \ldots, |S|} \alpha_k c(k),$$

where $\alpha_k$ is the $k$-th largest value of $E_a(\tau_b)$ among $b \in S$.

**Proof:** Any set $A$ with $|A| = k$ will have the same value of $c(A)$. Hence it suffices to find, for each $k$, the value of $A$ that maximizes $t_{\min}^A$ with $|A| = k$. That maximizer is given by the $k$ elements of $S$ with the largest values of $\min_{a \in V} E_a(\tau_b)$, and the corresponding value is $\alpha_k$. ■

By Lemma 10 in order to select the minimizer of $f'(S) - \lambda|S|$, the following procedure is sufficient. For each $k$, select the $k$ smallest elements of $S$, and compute $\beta_k c(k) - \lambda k$, where $\beta_k$ is the $k$-th smallest value of $\min_{a \in V} E_a(\tau_b)$ over all $b \in S$. 




In addition, we can formulate the following problem of minimizing the probability that the cover time is above a given threshold. The value of \( Pr(C(S) > K) \) can be approximated by taking a set of sample paths \( \omega_1, \ldots, \omega_N \) of the walk and ensuring that \( C(S; \omega_i) > K \) in each sample path. This problem can be formulated as

\[
Pr(C(S) > K) \approx \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}\{C(S; \omega_i) > K\}.
\]

The function \( \mathbb{1}\{C(S; \omega_i) > K\} \) is increasing and submodular, since it is equal to 1 if there is a node in \( S \) that is not reached during the first \( K \) steps of the walk and 0 otherwise. Hence the problem of minimizing the probability that the cover time exceeds a given threshold can be formulated as

\[
\min \left\{ Pr(C(S) > K - \lambda|S| : S \subseteq V \right\}
\]

and solved in polynomial time.

VI. Numerical Results

We evaluated our approach through numerical study using Matlab. We simulated both the fixed and optimal distribution cases. In the case of fixed distribution, our goal was to determine how the minimum cover time varied as a function of the number of input nodes and the network size. We generated an Erdos-Renyi random graph \( G(N, p) \), in which there is an edge \( (i, j) \) from node \( i \) to node \( j \) with probability \( p \), independent of all other edges, and the total number of nodes is \( N \). The value of \( N \) varied from \( N = 10 \) to \( N = 50 \).

Figure 1(a) shows the minimum cover time as a function of the cardinality of \( S \). Each data point was obtained by varying the parameter \( \lambda \) in \( f(S) - \lambda|S| \), resulting in a trade-off curve between the cover time \( C(S) \) and the cardinality \( |S| \). The minimum cover time is an increasing function of the number of inputs. We observed that the cover times were similar for the three network sizes.

Figure 1(b) compares the optimal selection algorithm with a greedy heuristic and random selection of inputs. We found that the greedy algorithm closely approximates the optimum at a lower computation cost, while both outperformed the random input selection.

In the optimal distribution case, we simulated the average cost per cycle (ACPC) problem. We first considered a lattice graph. The set of actions corresponded to moving left, right, up, or down. For each action, the walker was assumed to move in the desired direction with probability...
$p_c$, and to move in a uniformly randomly chosen direction otherwise. If an “invalid” action was chosen, such as moving up from the top-most position in the lattice, then a feasible step was chosen uniformly at random.

Figure 1(c) shows a comparison between three algorithms. The first algorithm selects a random set of $k$ nodes as inputs. The second algorithm selects input nodes via a centrality-based heuristic, in which the most centrally located nodes are chosen as inputs. The third algorithm is the proposed submodular approach (Algorithm 2). We found that the submodular approach slightly outperformed the centrality-based method while significantly improving on random selection.

VII. CONCLUSION

This paper studied the time required for a random walk to reach one or more nodes in a target set. We demonstrated that the problem of selecting a set of nodes in order to minimize random walk times including commute, cover, and hitting times has an inherent submodular structure that enables development of efficient approximation algorithms, as well as optimal solutions for some special cases.

We considered two cases, namely, walks with fixed distribution, as well as walks in which the distribution is jointly optimized with the target set in order to minimize the walk times. In the first case, we developed a unifying framework for proving submodularity of the walk times, based on proving submodularity of selecting a subset of stopping times, and derived submodularity of commute, cover, and hitting time as special cases. As a consequence, we showed that a set of nodes that minimizes the cover time can be selected using only polynomial number of evaluations of the cover time, and further derived solution algorithms for bounds on the cover time.

In the case where the distribution and target set are jointly optimized, we investigate the problems of maximizing the probability of reaching the target set, minimizing the average cost per cycle of the walk, as well as joint optimization of these parameters. We proved that the former problem admits a relaxation that can be solved in polynomial time, while the latter problem can be approximated via submodular optimization methods. In particular, the average cost per cycle can be minimized by minimizing the volume of an associated linear polytope, which we proved to be a supermodular function of the input set.

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