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Performance guarantees for greedy maximization of non-submodular controllability metrics

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***Abstract*— A key problem in emerging complex cyber-physical networks is the design of information and control topologies, including sensor and actuator selection and communication network design. These problems can be posed as combinatorial set function optimization problems to maximize a dynamic performance metric for the network. Some systems and control metrics feature a property called *submodularity*, which allows simple greedy algorithms to obtain provably near-optimal topology designs. However, many important metrics lack submodularity and therefore lack provable guarantees for using a greedy optimization approach. Here we show that performance guarantees can be obtained for greedy maximization of certain *non-submodular* functions of the controllability and observability Gramians. Our results are based on two key quantities: the *submodularity ratio*, which quantifies how far a set function is from being submodular, and the *curvature*, which quantifies how far a set function is from being supermodular.**

I. Introduction

Many emerging complex dynamical networks, from critical infrastructure to industrial cyber-physical systems and biological networks, are increasingly able to be instrumented with new sensing, actuation, and communication capabilities. These networks comprise growing webs of interconnected feedback loops and must operate efficiently and resiliently in dynamic and uncertain environments. This motivates addressing fundamental network topology design problems to select the most effective sensors, actuators, and communication links, along with jointly designing the associated estimation, control, and communication policies.

There are a variety of quantitative notions of network controllability and observability to guide topology design in cyber-physical networks. Examples include Kalman rank conditions [1]–[5], controllability and observability Gramians [6]–[12], and optimal and robust feedback control and estimation performance metrics [13]–[20]. Topology design problems have also been considered for specific classes of networks, including leader selection and communication network design [21], [22]. Various optimization methods have been proposed for topology design, including greedy algorithms [8], [9], [17], [18], [21], convex relaxation heuristics with sparsity inducing regularization [13]–[16], [23], and mixed-integer semidefinite programming methods [19], [20]. These methods are all heuristic approximations to extremely difficult combinatorial optimization problems.

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A key combinatorial property in network topology design problems is *submodularity*; simple greedy algorithms have theoretical performance guarantees for submodular set function maximization problems. Submodularity has recently been discovered in several network topology design problems in systems and control, including certain Gramian metrics and leader selection problems [8], [9], [21], paralleling similar development for information optimization problems in machine learning. However, many other important topology design problems lack submodularity [17], [22]. Nevertheless, greedy algorithms were shown to be highly effective empirically for many non-submodular optimal control problems, despite the apparent lack of theoretical guarantees.

Here, we show that theoretical performance guarantees for greedy algorithms can be obtained for certain *non-submodular* set function optimization problems in systems and control. Our results are based upon recent fundamental work [24] that generalizes classical optimality bounds for submodular set functions. This work utilizes two key quantities: the *submodularity ratio*, which quantifies how far a set function is from being submodular, and the *curvature*, which quantifies how far a set function is from being modular. We focus on two *non-submodular* Gramian-based metrics for controllability and observability: the minimum eigenvalue and negative trace of the inverse. Specifically, we derive general bounds on the submodularity ratio and the curvature of these two functions based on eigenvalue inequalities for sums of symmetric matrices. The existence of these bounds support the use of the greedy algorithm beyond a heuristic for a much wider class of network topology design problems.

Our preliminary results appeared in an unpublished manuscript in [25]. Afterwards, two recent works also utilized approximate submodularity and supermodularity notions for network control design problems [26], [27]. Our work has been developed independently and prior to the above and our approach complements them as follows. First, [26] derive bounds by comparison of the non-submodular functions with a "close" submodular one. Second, [27] considers an objective function different than ours, arising in co-design of control and estimation for a network system.

The rest of the paper is organized as follows. Section II provides preliminaries on set function optimization and Gramian-based controllability metrics. Section III develops our results on bounds on the submodularity ratio and curvature for certain non-submodular functions of the controllability Gramian, leading to performance guarantees from the greedy algorithm. Section IV discusses the predictive power of the theory with case studies. We conclude in Section V.

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II. Preliminaries

A. Set functions and submodularity

Network topology design problems can be formulated as cardinality constrained set function optimization problems

$$\underset{S\subseteq V,\ |S|\leq k}{\text{maximize}} \quad f(S), \tag{1}$$

where $V = \{1, ..., M\}$ is a finite set, $f : 2^V \to \mathbf{R}$ is a set function that maps each subset of V to a real number, and k denotes a fixed number of elements to be selected from V. These problems are combinatorial and finite, and thus can be solved in principle by exhaustive search. However, this approach quickly becomes intractable even for moderately sized problems. The motivating context of large cyber-physical networks requires a different approach.

Greedy algorithms are a simple alternative to exhaustive search. The greedy algorithm for set function maximization is shown in Algorithm 1. When a set function maximization problem has a certain property called *submodularity*, the greedy algorithm achieves results that are provably within a constant factor of the optimal value.

Definition 1: A set function $f : 2^V \to \mathbf{R}$ is called *submodular* if for all subsets $A \subseteq B \subseteq V$ and all elements $s \notin B$, it holds that

$$f(A \cup \{s\}) - f(A) \geq f(B \cup \{s\}) - f(B). \tag{2}$$

A set function is *supermodular* if the reversed inequality in (2) holds and is *modular* if (2) holds with equality. A set function is *monotone nondecreasing* if $\forall A \subset V, s \in V$, $f(A\cup\{s\}) \geq f(A)$. A set function is *normalized* if $f(\emptyset) = 0$.

Intuitively, submodularity is a diminishing returns property, that is, adding an element to a smaller set gives a larger benefit than adding it to a larger set. This intuition is utilized and quantified to derive constant-factor approximation guarantees for the greedy algorithm applied to submodular maximization problems subject to cardinality constraints.

Theorem 1 (Nemhauser 1978 [28]): Let f^* be the optimal value of the set function optimization problem (1), and let $f(S_{greedy})$ be the value associated with the subset S_{greedy} obtained from applying the greedy algorithm on (1). If f is submodular nondecreasing, then

$$f(S_{greedy}) \geq \left(1 - \frac{1}{e}\right) f^* \tag{3}$$

The above theorem has rendered the greedy approach an algorithm of choice for several challenging combinatorial optimization problems[1].

[1]This bound can be refined by explicitly considering the number of elements k to be chosen or including further properties of f.

Algorithm 1 The greedy algorithm.

$S \leftarrow \emptyset$
while $|S| \leq k$ **do**
  $e^\star = \underset{e\in V\setminus S}{\text{argmax}} \quad f(S \cup \{e\}) - f(S)$
  $S \leftarrow S \cup \{e^\star\}$
$S^\star \leftarrow S$

Several problems in systems and control that feature sub- or supermodularity have been recently explored [8], [9], [21]. However, a large class of important set function optimization in network topology design fail to be sub- or supermodular [17], [22], [29]. It has been observed that by quantifying how close a function to being sub- or supermodular is, one can derive constant factor optimization for the greedy approach. This “closeness” is with respect to two notions defined below.

Let $\rho_A(B) := f(A \cup B) - f(B)$ denote the marginal benefit of the set $A \subset V$ with respect to the set $B \subset V$. For notational compactness, we use ω interchangeably with $\{\omega\}$ when considering a singleton subset of V.

Definition 2: The *submodularity ratio* of a nonnegative set function f is the largest $\gamma \in \mathbb{R}_+$ such that

$$\sum_{\omega\in\Omega\setminus S} \rho_\omega(S) \geq \gamma\rho_\Omega(S), \quad \forall\Omega, S \subseteq V. \tag{4}$$

Definition 3: The *curvature* of a nonnegative set function f is the smallest $\alpha \in \mathbb{R}_+$ such that

$$\rho_j(S \setminus j \cup \Omega) \geq (1 - \alpha)\rho_j(S \setminus j), \forall\Omega, S \subseteq V, \forall j \in S \setminus \Omega. \tag{5}$$

For a nondecreasing function $\gamma \in [0, 1]$, and $\gamma = 1$ if and only if f is submodular. The curvature α of a nondecreasing function is contained in $[0, 1]$, and $\alpha = 0$ if and only if f is supermodular [24]. The following recent result [24] generalizes Theorem 1 and provides performance guarantees for greedy maximization of *non-submodular* functions based on the submodularity ratio and curvature.

Theorem 2 ([24]): Let f be a nonnegative nondecreasing normalized set function with submodularity ratio $\gamma \in [0, 1]$ and curvature $\alpha \in [0, 1]$. Then, Algorithm 1 on problem (1) enjoys the following approximation guarantee:

$$f(S_{greedy}) \geq \frac{1}{\alpha}\left(1 - e^{-\alpha\gamma}\right) f^*.$$

It is intractable to compute the submodularity ratio and curvature for a given set function due to the combinatorial number of constraints (of order of $2^{2|V|}$) in (4) and (5), respectively (similar to the challenge in exhaustive search for solving Problem (1)). However, a positive lowerbound on the submodularity ratio and an upperbound on the curvature for a given f, justify the use of the greedy algorithm for Problem (1) via Theorem 2. Our goal is to derive such bounds for f's corresponding to non-submodular controllability metrics.

B. Gramian-based performance metrics

Consider the linear system describing network dynamics

$$\dot{x}(t) = Ax(t) + B_S u(t), \quad t = 0, ..., T, \tag{6}$$

where $x(t) \in \mathbf{R}^n$ is the network state at time t, $u(t) \in \mathbf{R}^{|S|}$ is the input at time t. Let $V = \{b_1, ..., b_M\}$ be a finite set of n-dimensional column vectors associated with possible locations for actuators that could be placed in the system, i.e., for $S \subset V$, the input matrix is $b_S = [b_{s_1}, ..., b_{s_{|S|}}] \in \mathbf{R}^{n\times|S|}$. We focus on the network topology design problem of selecting a set of actuators to optimize certain metrics of the controllability Gramian. (Analogous results follow for sensor selection based on the observability Gramian.)

The infinite-horizon controllability Gramian associated with a subset $S \subset V$ of actuators is the symmetric positive semidefinite matrix W_S, satisfying

$$W_S = \int_0^\infty e^{A\tau} b_S b_S^T e^{A^T\tau} d\tau \ \in \mathbf{R}^{n\times n}. \qquad (7)$$

To ensure the Gramian is well-defined we assume A is stable. Observe that $W_{S\cup\Omega} = W_S + W_{\Omega\setminus S}$, $\forall S, \Omega \subset V$. This additive dependence on the actuators is key in deriving properties of several performance metrics based on the Gramian.

The quantity $x^T W_S^{-1} x$ is the amount of input energy required to transfer the network state from the origin to the state x. As such, we can define the following scalar metrics of the matrix W_S, each of which defines a different set function that provides a basis for actuator selection.

- $f(S) = \mathbf{tr}(W_S)$ (modular): This metric is inversely related to the average input energy and can be interpreted as the average controllability in all directions in the state space. It also quantifies the system $\mathcal{H}_2$ norm.
- $f(S) = \log\det W_S$ (submodular): This is a volumetric measure of the set of states that can be reached with one unit of input energy. Note that even if trace of the Gramian is large the volume can be small, due to reachability only in certain state space directions.
- $f(S) = \mathbf{rank}(W_S)$ (submodular): This metric captures the dimension of controllable subspace.
- $f(S) = \lambda_{min}(W_S)$ (*not* submodular): This metric captures the energy for directions that are hard to control.
- $f(S) = -\mathbf{tr}(W_S^{-1})$ (*not* submodular): This metric captures the average energy required to reach any arbitrary direction of the state space.

The choice of a specific metric from above is dependent on the application at hand (see [8] for discussions). Along with each choice, one is faced with the problem of selecting actuators to optimize the metric. This selection is a combinatorial problem and hence, quickly becomes intractable as the network size increases. Past work used submodularity to support empirical evidence on effectiveness of the greedy algorithm for the first three metrics [8], [29], [30]. It was shown that the last two metrics $\lambda_{min}(W_S)$ and $-\mathbf{tr}(W_S^{-1})$, are *not* submodular [8], [29]. These two metrics are important since they refer to the worst-case and the average energy respectively, required to steer the system. However, the empirical performance of the greedy optimization were not supported theoretically for these cases.

III. Performance Guarantees for Non-Submodular Gramian Metrics

To support the use of greedy algorithm beyond a heuristic approach for maximizing $-\mathbf{tr}(W_S^{-1})$ and $\lambda_{min}(W_S)$, we will derive positive lowerbounds on the submodularity ratio and upperbounds on the curvature of these functions. Let $\mathcal{S}^n, \mathcal{S}^n_+, \mathcal{S}^n_{++}$ denote the set of n-dimensional symmetric, symmetric positive semidefinite, and symmetric positive definite matrices, respectively. For $M \in \mathcal{S}^n$, let $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$ denote the eigenvalues of the matrix M. Let I_n denote the identity matrix of dimension n.

Let us recall Weyl's inequalities for eigenvalues of sum of two symmetric matrices [31].

Lemma 1: Let $A, B \in \mathcal{S}^n$.

$$\lambda_i(A) + \lambda_n(B) \leq \lambda_i(A+B) \leq \lambda_i(A) + \lambda_1(B). \qquad (8)$$

A. Minimum eigenvalue of the Gramian

Proposition 1: The function $f(S) = \lambda_n(W_S)$ is nonnegative nondecreasing and normalized. The submodularity ratio γ, and the curvature α, of this function are bounded by

$$\gamma \geq \frac{\min_{\omega\in V}\lambda_n(W_\omega)}{\max_{\omega\in V}\lambda_1(W_\omega)}, \quad \alpha \leq 1 - \frac{\min_{\omega\in V}\lambda_n(W_\omega)}{\max_{\omega\in V}\lambda_1(W_\omega)}.$$

Proof: The nonnegativity of $\lambda_n(W_S)$ follows from the Gramian being positive semidefinite. The fact that it is nondecreasing follows from the eigenvalue inequality in (8) and from nonnegativity of $\lambda_n(W_S)$. In particular, note that for $\forall S \subset V$, $\forall \omega \in V$, $W_{S\cup\omega} = W_S + W_\omega$. Hence, $\lambda_n(W_{S\cup\omega}) \geq \lambda_n(W_S) + \lambda_n(W_\omega) \geq \lambda_n(W_S)$. It is easy to see that $\lambda_n(W_\emptyset) = 0$ and hence this function is normalized.

To bound the submodularity ratio, we first derive a lower-bound for the left-hand-side in (4). Note that $\forall S, \Omega \subset V$

$$\begin{aligned}\sum_{\omega\in\Omega\setminus S}\rho_\omega(S) &= \sum_{\omega\in\Omega\setminus S} f(S\cup\{\omega\}) - f(S)\\ &= \sum_{\omega\in\Omega\setminus S}\lambda_n(W_{S\cup\omega}) - \lambda_n(W_S)\\ &\geq \sum_{\omega\in\Omega\setminus S}\lambda_n(W_S) + \lambda_n(W_\omega) - \lambda_n(W_S)\\ &= \sum_{\omega\in\Omega\setminus S}\lambda_n(W_\omega) \geq |\Omega\setminus S|\min_{\omega\in V}\lambda_n(W_\omega),\end{aligned}$$

where in the first inequality we used Lemma 1. Next, for the right-hand-side we have $\forall S, \Omega \subset V$

$$\begin{aligned}\rho_\Omega(S) =& f(S\cup\Omega) - f(S) = \lambda_n(W_{S\cup\Omega}) - \lambda_n(W_S)\\ \leq& \lambda_n(W_S) + \lambda_1(W_{\Omega\setminus S}) - \lambda_n(W_S)\\ =& \lambda_1(W_{\Omega\setminus S}) \leq |\Omega\setminus S|\max_{\omega\in V}\lambda_1(W_\omega),\end{aligned}$$

where in the first inequality we also used Lemma 1. Putting the above two inequalities together yields

$$\gamma \geq \frac{\min_{\omega\in V}\lambda_n(W_\omega)}{\max_{\omega\in V}\lambda_1(W_\omega)}.$$

We similarly bound the curvature. Note that for the left-hand-side in (5), we have $\forall S, \Omega \subset V, j \in S\setminus\Omega$

$$\begin{aligned}\rho_j(S\setminus j\ \cup\Omega) =& \lambda_n(W_{S\cup\Omega}) - \lambda_n(W_{S\setminus j\ \cup\Omega})\\ \geq& \lambda_n(W_{S\setminus j\ \cup\Omega}) + \lambda_n(W_j) - \lambda_n(W_{S\setminus j\ \cup\Omega})\\ =& \lambda_n(W_j) \geq \min_{j\in V}\lambda_n(W_i).\end{aligned}$$

Next, for the right-hand-side we have $\forall S, \Omega \subset V, j \in S\setminus\Omega$

$$\begin{aligned}&\rho_j(S\setminus j) = \lambda_n(W_S) - \lambda_n(W_{S\setminus j})\\ &\quad\leq \lambda_n(W_{S\setminus j}) + \lambda_1(W_j) - \lambda_n(W_{S\setminus j}) \leq \max_{j\in V}\lambda_1(W_j).\end{aligned}$$

Putting the above two inequalities together, we have

$$\frac{\rho_j(S\setminus j\ \cup\Omega)}{\rho_j(S\setminus j)} \geq \frac{\min_{\omega\in V}\lambda_n(W_\omega)}{\max_{\omega\in V}\lambda_1(W_\omega)}, \quad \forall S, \Omega \subset V, j \in S\setminus\Omega.$$

Hence, we obtain the claimed lowerbound for the curvature

$$\alpha \leq 1 - \frac{\min_{\omega\in V}\lambda_n(W_\omega)}{\max_{\omega\in V}\lambda_1(W_\omega)}.$$

■

Remark 1: The above bound is useful in deriving performance guarantees via Theorem 2 only if $\min_{\omega\in V}\lambda_{min}(W_\omega) > 0$. This condition is equivalent to requiring that each actuator results in controllability of the network - an unreasonable requirement for large-scale sparse networks. A potential approach to get around this issue is to assume a set of existing actuators $B_0 \in \mathbb{R}^{n\times m}$ render the system controllable and the goal is to choose additional actuators to improve the controllability. Unfortunately, even with this assumption we face the same difficulty. In particular, note that in this case, the Gramian would be $\bar{W}_S = W_{B_0\cup S}$. Hence, $\bar{W}_{S\cup\omega} = \bar{W}_S + W_\omega$ and $\lambda_n(\bar{W}_{S\cup\omega}) - \lambda_n(\bar{W}_S) \geq \lambda_n(W_\omega)$. Since W_ω does not contain B_0 in general, its minimum eigenvalue would be zero and the same problem arises?. The bound in the recent work of [26] on the closeness of the minimum eigenvalue of the Gramian to a submodular function, seems to also suffer from the same drawback. Despite this theoretical limitation, our empirical estimates of the submodularity ratio and curvature, computed in the numerical section, for all problem instances considered were bounded (far) away from zero and one, respectively. As we will shortly see, in the metric described by inverse of the trace of the Gramian, we can avoid vacuous bounds by including B_0 corresponding to a set of base actuators ensuring controllability.

B. Trace of inverse of Gramian

The function $-\mathbf{tr}({W_S}^{-1})$ is not well-defined if W_S is not invertible. To avoid this issue, we assume that an existing set of actuators corresponding to B_0 provides controllability (considered also implicitly in [26], [32]). Hence, our input set is given by $B_S = [B_0, b_{s_1}, ..., b_{s_{|S|}}] \in \mathbf{R}^{n\times(m+|S|)}$. We use $\bar{W}_S$ for the Gramian corresponding to the augmented set.

Proposition 2: The set function $f(S) = -\mathbf{tr}(\bar{W}_S^{-1})$ is monotone nondecreasing. Its submodularity ratio γ, and curvature α, are bounded by

$$1 > \gamma \geq \frac{\min_{\omega\in V}\mathbf{tr}(W_\omega)\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2}{\max_{\omega\in V}\mathbf{tr}(W_\omega)\big(\lambda_1(\bar{W}_V)\big)^2} > 0, \quad (9)$$

$$0 < \alpha \leq 1 - \frac{\min_{\omega\in V}\mathbf{tr}(W_\omega)\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2}{\max_{\omega\in V}\mathbf{tr}(W_\omega)\big(\lambda_1(\bar{W}_V)\big)^2} < 1. \quad (10)$$

Proof: First, we show that $f(S)$ is nondecreasing. For all $\omega \in V, S \subset V$, we have

$$\begin{aligned}
&f(S\cup\{\omega\}) - f(S) = -\mathbf{tr}\big((\bar{W}_{S\cup\omega})^{-1}\big) + \mathbf{tr}\big((\bar{W}_S)^{-1}\big)\\
&= \sum_{i=1}^{n} -\lambda_i\big((\bar{W}_{S\cup\omega})^{-1}\big) + \lambda_i\big((\bar{W}_S)^{-1}\big)\\
&= \sum_{i=1}^{n} \frac{-1}{\lambda_i(\bar{W}_{S\cup\omega})} + \frac{1}{\lambda_i(\bar{W}_S)} = \sum_{i=1}^{n}\frac{\lambda_i(\bar{W}_{S\cup\omega}) - \lambda_i(\bar{W}_S)}{\lambda_i(\bar{W}_{S\cup\omega})\lambda_i(\bar{W}_S)}\\
&\geq \frac{\sum_{i=1}^{n}\lambda_i(\bar{W}_{S\cup\omega}) - \lambda_i(\bar{W}_S)}{\lambda_1(\bar{W}_V)\lambda_1(\bar{W}_V)} = \frac{\mathbf{tr}(\bar{W}_{S\cup\omega}) - \mathbf{tr}(\bar{W}_S)}{\big(\lambda_1(\bar{W}_V)\big)^2} \geq 0.
\end{aligned} \quad (11)$$

To derive a lowerbound for the submodularity ratio (4), we first derive a lowerbound for the left-hand-side in (4)

$$\begin{aligned}
&\sum_{\omega\in\Omega\setminus S} f(S\cup\{\omega\}) - f(S)\\
&= \sum_{\omega\in\Omega\setminus S} -\mathbf{tr}\big((\bar{W}_{S\cup\omega})^{-1}\big) + \mathbf{tr}\big((\bar{W}_S)^{-1}\big)\\
&\geq \sum_{\omega\in\Omega\setminus S}\frac{\mathbf{tr}(\bar{W}_{S\cup\omega}) - \mathbf{tr}(\bar{W}_S)}{\big(\lambda_1(\bar{W}_V)\big)^2} \geq |\Omega\setminus S|\frac{\min_{\omega\in V}\mathbf{tr}(W_\omega)}{\big(\lambda_1(\bar{W}_V)\big)^2}.
\end{aligned} \quad (12)$$

To get the second inequality above we summed (11) over $\omega \in \Omega \setminus S$. The last inequality trivially follows. Notice that the numerator above is greater than zero since the Gramian has at least one positive eigenvalue. Next, we upper bound the right-hand-side in (4).

$$\begin{aligned}
&f(S\cup\{\Omega\}) - f(S) = -\mathbf{tr}\big((\bar{W}_{S\cup\Omega})^{-1}\big) + \mathbf{tr}\big((\bar{W}_S)^{-1}\big)\\
&= \sum_{i=1}^{n}\frac{-1}{\lambda_i(\bar{W}_{S\cup\Omega})} + \frac{1}{\lambda_i(\bar{W}_S)} = \sum_{i=1}^{n}\frac{\lambda_i(\bar{W}_{S\cup\Omega}) - \lambda_i(\bar{W}_S)}{\lambda_i(\bar{W}_{S\cup\Omega})\lambda_i(\bar{W}_S)}\\
&\leq \frac{\sum_{i=1}^{n}\big(\lambda_i(\bar{W}_{S\cup\Omega}) - \lambda_i(\bar{W}_S)\big)}{\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)}\\
&= \frac{\mathbf{tr}(\bar{W}_{S\cup\Omega}) - \mathbf{tr}(\bar{W}_S)}{\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2} = \sum_{\omega\in\Omega\setminus S}\frac{\mathbf{tr}(W_\omega)}{\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2}\\
&\leq |\Omega\setminus S|\frac{\max_{\omega\in V}\mathbf{tr}(W_\omega)}{\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2}.
\end{aligned} \quad (13)$$

Notice that the denominator above is greater than zero since the assumption of having a set of existing actuators providing controllability, implies $\bar{W}_\emptyset = W_{B_0}$ is positive definite. Hence, $\lambda_n(\bar{W}_\omega) = \lambda_n(W_{B_0\cup\omega}) > 0$ for all $\omega \in V$ in the second to last inequality above. Putting inequalities (12) and (13) we obtain the positive lowerbound on γ as in (9).

Our technique for deriving a bound on curvature is very similar to that of the submodularity ratio. In particular, we first derive a lowerbound for the left-hand-side in (5)

$$\begin{aligned}
&\rho_j(S\setminus j\ \cup\Omega) = f(S\cup\Omega) - f(S\setminus j\ \cup\Omega)\\
&= -\mathbf{tr}\big((\bar{W}_{S\cup\Omega})^{-1}\big) + \mathbf{tr}\big((\bar{W}_{S\setminus j\ \cup\Omega})^{-1}\big)\\
&= \sum_{i=1}^{n}\frac{-1}{\lambda_i(\bar{W}_{S\cup\Omega})} + \frac{1}{\lambda_i(\bar{W}_{S\setminus j\ \cup\Omega})}\\
&= \sum_{i=1}^{n}\frac{\big(\lambda_i(\bar{W}_{S\cup\Omega}) - \lambda_i(\bar{W}_{S\setminus j\ \cup\Omega})\big)}{\lambda_i(\bar{W}_{S\cup\Omega})\lambda_i(\bar{W}_{S\setminus j\ \cup\Omega})}\\
&\geq \frac{\sum_{i=1}^{n}\big(\lambda_i(\bar{W}_{S\cup\Omega}) - \lambda_i(\bar{W}_{S\setminus j\ \cup\Omega})\big)}{\lambda_1(\bar{W}_V)\lambda_1(\bar{W}_V)}\\
&= \frac{\mathbf{tr}(\bar{W}_{S\cup\Omega}) - \mathbf{tr}(\bar{W}_{S\setminus j\ \cup\Omega})}{\big(\lambda_1(\bar{W}_V)\big)^2} = \frac{\mathbf{tr}(W_j)}{\big(\lambda_1(\bar{W}_V)\big)^2} \geq \frac{\min_{\omega\in V}\mathbf{tr}(W_\omega)}{\big(\lambda_1(\bar{W}_V)\big)^2}.
\end{aligned}$$

Next, we upper bound the right-hand-side in (5) as follows.

$$\begin{aligned}
&\rho_j(S\setminus j) = f(S) - f(S\setminus j)\\
&= -\mathbf{tr}\big((\bar{W}_S)^{-1}\big) + \mathbf{tr}\big((\bar{W}_{S\setminus j})^{-1}\big)\\
&= \sum_{i=1}^{n}\frac{-1}{\lambda_i(\bar{W}_S)} + \frac{1}{\lambda_i(\bar{W}_{S\setminus j})} = \sum_{i=1}^{n}\frac{\lambda_i(\bar{W}_S) - \lambda_i(\bar{W}_{S\setminus j})}{\lambda_i(\bar{W}_S)\lambda_i(\bar{W}_{S\setminus j})}\\
&\leq \frac{\sum_{i=1}^{n}\lambda_i(\bar{W}_S) - \lambda_i(\bar{W}_{S\setminus j})}{\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2} = \frac{\mathbf{tr}(\bar{W}_S) - \mathbf{tr}(\bar{W}_{S\setminus j})}{\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2}\\
&= \frac{\mathbf{tr}(W_j)}{\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2} \leq \frac{\max_{\omega\in V}\mathbf{tr}(W_\omega)}{\big(\min_{\omega\in V}\lambda_n(\bar{W}_\omega)\big)^2}.
\end{aligned}$$

Putting the above lowerbound and upperbound together, from the curvature definition in (3) we obtain the upperbound on the curvature given in (10). ■

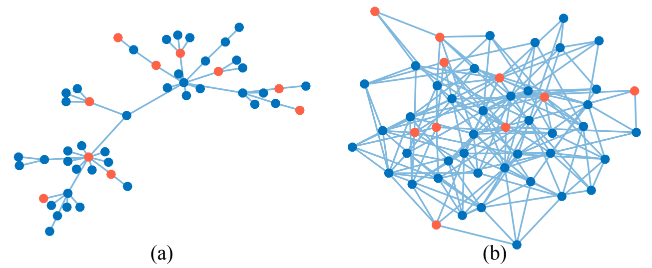

Fig. 1. (a) Barabási-Albert network on $n = 50$ nodes, with $k = 10$ nodes selected using the greedy algorithm with the Gramian trace inverse metric to receive control inputs (shown in red); (b) Erdős-Rényi network on $n = 50$ nodes, with $k = 10$ nodes selected using the greedy algorithm with the Gramian trace inverse metric to receive control inputs (shown in red).

Since $f(\emptyset) = -\mathbf{tr}((\bar{W}_\emptyset)^{-1}) = -\mathbf{tr}((W_{B_0})^{-1}) \neq 0$, f is not normalized. This offset appears in the suboptimality gap of the greedy algorithm through Theorem 2 as follows.

Corollary 1: Consider the function $f(S) = -\mathbf{tr}((\bar{W}_S)^{-1})$ with submodularity ratio γ and curvature α.

$$f(S_{greedy}) - f(\emptyset) \geq \frac{1}{\alpha}\left(1 - e^{-\alpha\gamma}\right)\left(f^* - f(\emptyset)\right).$$

Proof: Consider the function $\bar{f}(S) = f(S) - f(\emptyset) = -\mathbf{tr}(\bar{W}_S^{-1}) + \mathbf{tr}(W_{B_0}^{-1})$. It is normalized, i.e. $\bar{f}(\emptyset) = 0$. From Proposition 2, $f(S)$ is monotone nondecreasing and this implies $\bar{f}$ is nonnegative monotone nondecreasing. Since the submodularity ratio and the curvature remain invariant if a constant term is added to the function f, these parameters for $\bar{f}$ are equivalent to those of f. Hence, applying Theorem 2 to $\bar{f}$ gives the claim of the Corollary. ■

Remark 2: One might observe that in the considered instances of deriving the upper bound on the curvature, α^u, we obtained $\alpha^u = 1 - \gamma^l$, where γ^l was our lowerbound on the submodularity ratio. This connection is due to the (conservative) approach in deriving these bounds. Such connection does not exist for the true values of the submodularity ratio and the curvature in general. In particular, for a submodular function $\gamma = 1$. This clearly would not imply that f's curvature is $\alpha \leq 1 - 1 = 0$; otherwise, f would also be supermodular and hence, modular.

The above bounds are valid for any problem instance – any stable network dynamics matrix A and set of possible actuator locations B_S. Hence, these bounds are often conservative as will be seen in the next section. Nevertheless, their existence is promising as it supports empirical observations about effectiveness of the greedy algorithm for optimizing non-submodular set functions related to the Gramian.

IV. Case Studies

We present several illustrative numerical examples in random networks. In all examples, we first generate unweighted random graphs whose structure defines non-zero entries in the network dynamics matrix as discussed below. We then randomly generate edge weights associated with non-zero entries by drawing independently from a standard normal distribution. Finally, we shift the matrix so that it is stable, with the smallest eigenvalue(s) having real part -0.05. Figure 1(a) shows an instance of a Barabási-Albert network, whose edge structure is generated with a preferential attachment mechanism that produces power law degree distributions [33]. This network connectivity is motivated by link formations in social networks. Figure 1(b) shows an instance of an Erdős-Rényi network, with the edge probability chosen uniformly for all nodes to be 0.08 (just above the critical value of $\ln(50)/50$ to ensure connectivity of the network [34]). In both cases, there are $n = 50$ states and $k = 10$ possible inputs he selection of $k = 10$ inputs. We assume that an input signal could be injected into any state node, i.e., the set V corresponds to the standard basis in $\mathbf{R}^n$. The selected nodes using the greedy algorithm to minimize the trace of the controllability Gramian inverse are shown in Figure 1.

In the above problems, computing exact bounds for the submodularity ratio and curvature are prohibitive due to the network sizes. We empirically estimated the corresponding submodularity ratio and curvature by randomly generating the subsets in Definitions 2 and 3. In particular, for each set of sampled subsets, we determined the respective largest and smallest values of γ and α so that the inequalities in these definitions are satisfied. We never encountered sets that violated the submodularity inequality, indicating that although the set functions are not submodular in general, they may often be close to submodular empirically in typical instances. Similarly, the curvature ratios varied between zero and one, but on average were very close to the ideal value of zero. Representative results based on 5000 subset samples for each network type with $n = 50$ using the trace inverse metric are shown in Table I. Of course the theoretical bounds provide the only hard performance guarantees, but these empirical values may be stronger indicators of empirical performance of the greedy algorithm. In all examples, to find a Gramian whose inverse is well-defined, we included a small identity matrix in the Lyapunov equation (i.e., we solved $AW_S + W_S A^T + B_S B_S^T + \epsilon I$). This is consistent with the assumption needed for deriving the bounds, namely, having a set of existing actuators that provide controllability.

To provide evidence supporting the empirical effectiveness of the greedy algorithm despite lack of submodularity of minimum eigenvalue and trace inverse Gramian, we compared greedy results with globally optimal results for problems small enough to allow brute force search. We randomly generated 500 instances each for several types of networks, including random stable (via Matlab's rss function), Erdős-Rényi , and Barabási-Albert, with $n = 16$ and $k = 4$. We find that on average the greedy algorithm achieves over 90% of the globally optimal value across all networks for both the minimum eigenvalue and trace inverse metrics, and in many cases recovers a globally optimal actuator selection. This significantly outperforms even the worst-case guarantee for submodular functions (of $\sim 63\%$), and supports the boosts suggested by the empirical estimates of the submodularity ratio and curvature in Table 1. Note that for a submodular function f, a small curvature improves the performance guarantee of the greedy algorithm via Theorem 2, e.g. $\alpha = 0.01$ would ensure 99.5% optimality.). An

TABLE I

EMPIRICAL ESTIMATES OF SUBMODULARITY RATIO AND CURVATURE FOR VARIOUS NETWORKS, BASED ON 5000 RANDOM SUBSET PAIRS FROM DEFINITIONS 2 AND 3.

NETWORK	γ_{EMP}	α_{EMP} (RANGE, AVERAGE)
ERDŐS-RÉNYI	1	$[0, 0.72],\ 0.010$
BARABÁSI-ALBERT	1	$[0, 0.66],\ 0.009$
L-SHAPED MESH	1	$[0, 0.99],\ 0.007$

interesting future work is to understand probability of these metrics being submodular on certain classes of random graphs. A difficulty in implementing the algorithm as well as evaluating and interpreting the bounds and empirical estimates of submodularity ratio and curvature is that even for these moderately sized networks, the Gramian usually has several very small eigenvalues corresponding to state space directions that require large input energy to achieve state transfer. This observation is theoretically supported by the fundamental limitations discussed [6]. The pseudo-inverse or minimum non-zero eigenvalue can be used as alternatives, but these values are highly sensitive to an arbitrary threshold defining which eigenvalues are considered numerically zero. Appropriately deciding a controllability metric for large networks requires consideration of the application context.

V. CONCLUSIONS

We derived bounds on the submodularity ratio and curvature for two important non-submodular set functions related to the controllability Gramian. These bounds justify the use of the greedy approach beyond a heuristic, for large-scale network design problems corresponding to the Gramian. In simulations, we observed that the bounds derived might be very conservative. We are currently investigating reducing this conservatism for specific classes of networks. A major assumption in our work is that a base set of actuators for controllability exist. Currently, we are working on deriving alternative formulations of the problem that bypass this restrictive assumption, similar in spirit to [32] and can also provide a meaningful metric in the cases where several eigenvalues of the Gramian are near zero as proven in [6].

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