Structured Decentralized Control of Positive Systems With Applications to Combination Drug Therapy and Leader Selection in Directed Networks

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***Abstract*—We study a class of structured optimal control problems in which the main diagonal of the dynamic matrix is a linear function of the design variable. While such problems are in general challenging and nonconvex, for positive systems we prove convexity of the $\mathcal{H}_2$ and $\mathcal{H}_\infty$ optimal control formulations that allow for arbitrary convex constraints and regularization of the control input. Moreover, we establish differentiability of the $\mathcal{H}_\infty$ norm when the graph associated with the dynamical generator is weakly connected and develop a customized algorithm for computing the optimal solution even in the absence of differentiability. We apply our results to the problems of leader selection in directed consensus networks and combination drug therapy for human immunodeficiency virus (HIV) treatment. In the context of leader selection, we address the combinatorial challenge by deriving upper and lower bounds on optimal performance. For combination drug therapy, we develop a customized subgradient method for efficient treatment of diseases whose mutation patterns are not connected.**

***Index Terms*—Convex functions, decentralized control, H infinity control, network theory (graphs), optimization methods.**

I. Introduction

Modern applications require structured controllers that cannot be designed using traditional approaches. Except in special cases, e.g., in funnel causal and quadratically invariant systems [1], [2] and in system level synthesis [3], in which spatial and temporal sparsity constraints are imposed on the closed-loop response, posing optimal control problems in coordinates that preserve *controller structure* compromises convexity of the performance metric. In this paper, we study the structured decentralized control of positive systems. While structured decentralized control is challenging in general, we show that, for positive systems, the convexity of the $\mathcal{H}_2$ and $\mathcal{H}_\infty$ optimal control formulations is not lost by imposing structural constraints. We also derive a graph theoretic condition that guarantees continuous differentiability of the $\mathcal{H}_\infty$ performance metric and develop techniques to address combination drug therapy design and leader selection in directed consensus networks.

Positive systems arise in the modeling of systems with inherently nonnegative variables (e.g., probabilities, concentrations, and densities). Such systems have nonnegative states and outputs for nonnegative initial conditions and inputs [4]. In this paper, we examine models of HIV mutation [5]–[10] and consensus networks [11]–[16], where positivity comes from nonnegativity of populations and the structure of the underlying dynamics, respectively. Decentralized control, in which only the diagonal of the dynamical generator may be modified, is a suitable paradigm for modeling the effect of drugs on HIV [5] and the influence of leaders on the dynamics of leader-follower consensus networks [12]. In these applications, the structure of decentralized control is important for capturing the efficacy of the drugs on different HIV mutants and influence of noise on the quality of consensus, respectively. This model can also be used to study chemical reaction networks and transportation networks.

The mathematical properties of positive systems can be exploited for efficient or structured controller design. In [17], Tanaka and Langbort show that the kalman-yakubovich-popov lemma greatly simplifies for positive systems, thereby enabling decentralized $\mathcal{H}_\infty$ synthesis via semidefinite programming (SDP). In [18], it is shown that a static output-feedback problem can be solved via linear programming (LP) for a class of positive systems. Briat [19] and Ebihara *et al.* [20] develop necessary and sufficient conditions for robust stability of positive systems with respect to induced $\mathcal{L}_1$–$\mathcal{L}_\infty$ norm-bounded perturbations. In [21] and [22], it is shown that the structured singular value is equal to its convex upper bound for positive systems so assessing robust stability with respect to induced $\mathcal{L}_2$ norm-bounded perturbations becomes tractable.

Manuscript received November 28, 2017; revised March 4, 2018; accepted March 18, 2018. Date of publication March 28, 2018; date of current version March 14, 2019. This work was supported in part by the National Science Foundation under Awards ECCS-1739210 and CNS-1544887 and in part by the Air Force Office of Scientific Research under Award FA9550-16-1-0009. Recommended by Associate Editor Stephen L. Smith. *(Corresponding author: Mihailo R. Jovanovic.)*

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Digital Object Identifier 10.1109/TCNS.2018.2820499

It has been recently shown that the design of unconstrained decentralized controllers for positive systems can be cast as a convex problem [18], [23]. However, since structural constraints cannot be handled by the LP or linear matrix inequality approaches presented in [18] and [23], references [7]–[10] design $\mathcal{L}_1$ and $\mathcal{H}_\infty$ controllers that satisfy such constraints, but achieve suboptimal performance. Furthermore, convexity of the weighted $\mathcal{L}_1$ norm for structured decentralized control of positive systems was established in [24] and [25] and optimized switching strategies were considered in [26]–[28].

The paper is organized as follows. In Section II, we formulate the regularized optimal control problem for a class positive systems. In Section III, we establish convexity of both $\mathcal{H}_2$ and $\mathcal{H}_\infty$ control problems and derive a graph theoretic condition that guarantees continuous differentiability of the $\mathcal{H}_\infty$ objective function. In Section IV, we study leader selection in directed networks. In Section V, we design combination drug therapy for HIV treatment. Finally, in Section VI, we conclude the paper and summarize future research directions.

II. Problem Formulation and Background

We first provide background on graph theory and positive systems, describe the system under study, and formulate structured decentralized $\mathcal{H}_2$ and $\mathcal{H}_\infty$ optimal control problems.

A. Background Material

Notation: The set of real numbers is denoted by $\mathbb{R}$ and the sets of nonnegative and positive reals are $\mathbb{R}_+$ and $\mathbb{R}_{++}$. The set of $n \times n$ Metzler matrices (matrices with nonnegative off-diagonal elements) is denoted by $\mathbb{M}^{n\times n}$. We write $A > 0$ ($A \geq 0$) if A has positive (nonnegative) entries and $A \succ 0$ ($A \succcurlyeq 0$) if A is symmetric and positive (semi)definite. We define the sparsity pattern of a vector u, $\mathrm{sp}\,(u)$ as the set of indices for which u_i is nonzero, $\|u\|_1 := \sum_i |u_i|$ is the ℓ_1 norm, and $K^\dagger\colon \mathbb{R}^{n\times n} \to \mathbb{R}^m$ is the adjoint of a linear operator $K\colon \mathbb{R}^m \to \mathbb{R}^{n\times n}$ if it satisfies, $\langle X, K(u)\rangle = \langle K^\dagger(X), u\rangle$ for all $u \in \mathbb{R}^m$ and $X \in \mathbb{R}^{n\times n}$.

Definition 1 (Graph associated with a matrix): $\mathcal{G}(A) = (\mathcal{V}, \mathcal{E})$ is the graph associated with a matrix $A \in \mathbb{R}^{n\times n}$, with the set of nodes (vertices) $\mathcal{V} := \{1, \ldots, n\}$ and the set of edges $\mathcal{E} := \{(i,j) |\, A_{ij} \neq 0\}$, where (i,j) denotes an edge pointing from node j to node i.

Definition 2 (Strongly connected graph): A graph $(\mathcal{V}, \mathcal{E})$ is strongly connected if there is a directed path between any two distinct nodes in $\mathcal{V}$.

Definition 3 (Weakly connected graph): A graph $(\mathcal{V}, \mathcal{E})$ is weakly connected if replacing its edges with undirected edges results in a strongly connected graph.

Definition 4 (Balanced graph): A graph $(\mathcal{V}, \mathcal{E})$ is balanced if, for every node $i \in \mathcal{V}$, the sum of edge weights on the edges pointing *to* node i is equal to the sum of edge weights on the edges pointing *from* node i.

Definition 5: A dynamical system is positive if, for any nonnegative initial condition and any nonnegative input, the output is nonnegative for all time. A linear time-invariant system

$$\dot{x} = Ax + Bd$$
$$z = Cx$$

is positive if and only if $A \in \mathbb{M}^{n\times n}$, $B \geq 0$, and $C \geq 0$.

We now state three lemmas that are useful for the analysis of positive linear time invariant systems.

Lemma 1 (From [29]): Let $A \in \mathbb{M}^{n\times n}$ and let $Q \in \mathbb{R}^{n\times n}$ be a positive definite matrix with nonnegative entries. Then

1) $\mathrm{e}^A \geq 0$;
2) for Hurwitz A, the solution X to the algebraic Lyapunov equation
$$AX + XA^T + Q = 0$$
is elementwise nonnegative.

Lemma 2: The left and right principal singular vectors w and v of $A \in \mathbb{R}_+^{n\times n}$ are nonnegative. If $A \in \mathbb{R}_{++}^{n\times n}$, w and v are positive and unique.

Proof: The result follows from the application of the Perron theorem [30, Th. 8.2.11] to AA^T and $A^T A$. ■

Lemma 3 (From [24]): Let $b, c \in \mathbb{R}^n$ be nonnegative. Then, for any $t \geq 0$

$$c^T \mathrm{e}^{(A+K(u))t} b$$

is a convex function of u.

B. Decentralized Optimal Control

We consider a class of control problems

$$\begin{aligned} \dot{x} &= (A + K(u))\, x + Bd \\ z &= Cx \end{aligned} \tag{1}$$

where $x(t) \in \mathbb{R}^n$ is the state vector, $z(t) \in \mathbb{R}^m$ is the performance output, $d(t) \in \mathbb{R}^p$ is the disturbance input, and $u \in \mathbb{R}^m$ is the control input. Since control enters into the dynamics in a multiplicative fashion, optimal design of u for system (1) is, in general, a challenging nonconvex problem. In what follows, we introduce an assumption which implies that system (1) is positive for any u. As we demonstrate in Section III, under this assumption both the $\mathcal{H}_2$ and $\mathcal{H}_\infty$ structured decentralized optimal control problems are convex.

This class of problems can be used to model a variety of control challenges that arise in, e.g., chemical reaction networks and transportation networks. In this paper, we consider leader selection in directed consensus networks as well as combination drug therapy design for HIV treatment.

Assumption 1: The matrix A in (1) is Metzler, the matrices B and C are nonnegative, and the diagonal matrix $K(u) := \mathrm{diag}\,(Du)$ with $D \in \mathbb{R}^{n\times m}$ is a linear function of u.

Our objective is to design a stabilizing *diagonal* matrix $K(u)$ that minimizes amplification from d to z. To quantify the average effect of the impulsive disturbance input d, we consider the L_2 norm of the resulting impulse response, i.e.,

$$J_2(u) := \int_0^\infty \mathrm{trace}\left(C\,\mathrm{e}^{(A+K(u))t} B\, B^T \mathrm{e}^{(A+K(u))^T t}\, C^T\right) \mathrm{d}t. \tag{2a}$$

This performance metric is equivalent to the square of the $\mathcal{H}_2$ norm of system (1) which also has a well-known stochastic interpretation [31]. To quantify the worst-case input–output amplification of (1), we consider the $\mathcal{H}_\infty$ norm, defined as

$$J_\infty(u) \;:=\; \sup_{\omega\in\mathbb{R}} \; \bar{\sigma}\left(C\,(j\omega I - A - K(u))^{-1}B\right) \tag{2b}$$

where $\bar{\sigma}(\cdot)$ denotes the largest singular value of a given matrix when $A + K(u)$ is Hurwitz and ∞ otherwise. To limit the size of the control input u and promote desired structural properties, we consider the regularized optimal control problem

$$\begin{array}{ll} \underset{u}{\text{minimize}} & J(u) + g(u) \\ \text{subject to} & A + K(u) \text{ Hurwitz.} \end{array} \tag{3}$$

The regularization function g in (3) can be any convex function, e.g., a quadratic penalty $u^T Ru$ with $R \succ 0$ to limit the magnitude of u, an ℓ_1 penalty to promote sparsity of u, or the indicator function associated with a convex set $\mathcal{C}$ to ensure that $u \in \mathcal{C}$. We refer the reader to [32], [33] for an overview of recent uses of regularization in control-theoretic problems.

We now review some recent results. Under Assumption 1 the matrix $A + K(u)$ is a Metzler and its largest eigenvalue is real and a convex function of u [34]. Recently, it has been shown that the weighted $\mathcal{L}_1$ norm of the response of system (1) from a nonnegative initial condition $x_0 \geq 0$

$$\int_0^T c^T x(t)\mathrm{d}t$$

is a convex function of u for every $c \in \mathbb{R}^n_+$ [24], [25]. Furthermore, the approach in [17] can be used to cast the problem of *unstructured* decentralized $\mathcal{H}_\infty$ control of positive systems as an SDP and [23] can be used to cast it as an LP. However, both the SDP and LP formulations require a change of variables that does not preserve the structure of $K(u)$. Consequently, it is often difficult to design controllers that are feasible for a given noninvertible operator K or to impose structural constraints or penalties on u.

III. Convexity of Optimal Control Problems

We next establish the convexity of the $\mathcal{H}_2$ and $\mathcal{H}_\infty$ norms for systems that satisfy Assumption 1, derive a graph theoretic condition that guarantees continuous differentiability of J_∞, and develop a customized algorithm for solving optimization problem (3) even in the absence of differentiability.

A. Convexity of J_2 and J_∞

We first establish convexity of the $\mathcal{H}_2$ optimal control problem and provide the expression for the gradient of J_2.

Proposition 4: Let Assumption 1 hold and let $A_{\rm cl}(u) := A + K(u)$ be a Hurwitz matrix. Then, J_2 is a convex function of u and its gradient is given by

$$\nabla J_2(u) = 2K^\dagger(X_c X_o) \tag{4}$$

where X_c and X_o are the controllability and observability gramians of the closed-loop system (1)

$$A_{\rm cl}(u)X_c + X_c A_{\rm cl}^T(u) + BB^T = 0 \tag{5a}$$

$$A_{\rm cl}^T(u)X_o + X_o A_{\rm cl}(u) + C^T C = 0. \tag{5b}$$

Proof: We first establish convexity of $J_2(u)$ and then derive its gradient. The square of the $\mathcal{H}_2$ norm is given by

$$J_2(u) = \begin{cases} \left\langle C^T C, X_c\right\rangle, & A_{\rm cl}(u) \text{ Hurwitz} \\ \infty, & \text{otherwise} \end{cases}$$

where the controllability gramian X_c of the closed-loop system is determined by the solution to Lyapunov equation (5a). For Hurwitz $A_{\rm cl}(u)$, X_c can be expressed as,

$$X_c = \int_0^\infty \mathrm{e}^{A_{\rm cl}(u)t} BB^T \mathrm{e}^{A_{\rm cl}^T(u)t}\mathrm{d}t.$$

Substituting into $\langle C^T C, X_c\rangle$ and rearranging terms yields

$$\begin{aligned} J_2(u) &= \int_0^\infty \|C\mathrm{e}^{A_{\rm cl}(u)t}B\|_F^2\,\mathrm{d}t \\ &= \int_0^\infty \sum_{i,j}\left(c_i^T\mathrm{e}^{A_{\rm cl}(u)t}b_j\right)^2\mathrm{d}t \end{aligned}$$

where c_i^T is the ith row of C and b_j is the jth column of B. From Lemma 3, it follows that $c^T\mathrm{e}^{A_{\rm cl}(u)t}b$ is a convex function of u for nonnegative vectors c and b. Since the range of this function is $\mathbb{R}_+$ and $(\cdot)^2$ is nondecreasing over $\mathbb{R}_+$, the composition rules for convex functions [35] imply that $(c_i^T\mathrm{e}^{A_{\rm cl}(u)t}b_j)^2$ is convex in u. Convexity of $J_2(u)$ follows from the linearity of the sum and integral operators.

To derive ∇J_2, we form the associated Lagrangian

$$\begin{aligned} \mathcal{L}(u, X_c, X_o) = &\left\langle C^T C, X_c\right\rangle \\ &+ \left\langle X_o, A_{\rm cl}(u)X_c + X_c A_{\rm cl}^T(u) + BB^T\right\rangle \end{aligned}$$

where X_o is the Lagrange multiplier associated with equality constraint (5a). Taking variations of $\mathcal{L}$ with respect to X_o and X_c yields Lyapunov equations (5a) and (5b) for controllability and observability gramians, respectively. Using $A_{\rm cl}(u) = A + K(u)$ and the adjoint of K, we rewrite the Lagrangian as

$$\begin{aligned} \mathcal{L}(u, X_c, X_o) = &\, 2\left\langle K^\dagger(X_c X_o), u\right\rangle + \left\langle C^T C, X_c\right\rangle \\ &+ \left\langle X_o, AX_c + X_c A^T + BB^T\right\rangle. \end{aligned}$$

Taking the variation of $\mathcal{L}$ with respect to u yields (4). ■

Remark 1: The quadratic cost

$$\int_0^T x^T(t)\,C^T C\,x(t)\,\mathrm{d}t$$

is also convex over a finite or infinite time horizon for a piecewise constant u. This follows from [24, Lemma 4] and suggests that an approach inspired by the model predictive control (MPC) framework can be used to compute a time-varying optimal control input for a finite horizon problem.

Remark 2: The expression for ∇J_2 in Proposition 4 remains valid for any linear system and any linear operator $K\colon \mathbb{R}^m \to \mathbb{R}^{n\times n}$. However, convexity of J_2 holds under Assumption 1 and is not guaranteed in general.

We now establish the convexity of the $\mathcal{H}_\infty$ control problem and provide expression for the subdifferential set of J_∞.

Proposition 5: Let Assumption 1 hold and let $A_{\rm cl}(u) := A + K(u)$ be a Hurwitz matrix. Then, J_∞ is a convex function of u and its subdifferential set is given by

$$\partial J_\infty(u) = \left\{ \sum_i \alpha_i K^\dagger \left(A_{\rm cl}^{-1}(u) B v_i w_i^T C A_{\rm cl}^{-1}(u) \right) \mid w_i^T (C A_{\rm cl}^{-1}(u) B) v_i = J_\infty(u), \alpha \in \mathcal{P} \right\} \tag{6}$$

where $K^\dagger$ is the adjoint of the operator K and $\mathcal{P}$ is the simplex, $\mathcal{P} := \{\alpha_i | \; \alpha_i \geq 0, \sum_i \alpha_i = 1\}$.

Proof: We first establish convexity of $J_\infty(u)$ and then derive the expression for its subdifferential set. For positive systems, the $\mathcal{H}_\infty$ norm achieves its largest value at $\omega = 0$ [17] and from (2b) we thus have $J_\infty(u) = \bar{\sigma}(-C A_{\rm cl}^{-1}(u) B)$. To show convexity of $J_\infty(u)$, we show that $-C A_{\rm cl}^{-1}(u) B$ is a convex and nonnegative function of u, that $\bar{\sigma}(X)$ is a convex and nondecreasing function of a nonnegative argument X and leverage the composition rules for convex functions [35].

Since $A_{\rm cl}(u)$ is Hurwitz, its inverse can be expressed as

$$-A_{\rm cl}^{-1}(u) = \int_0^\infty \mathrm{e}^{A_{\rm cl}(u) t} \mathrm{d}t. \tag{7}$$

Convexity of $c_i \mathrm{e}^{A_{\rm cl}(u)t} b_j$ by Lemma 3 and linearity of integration implies that each element of the matrix

$$-C A_{\rm cl}^{-1}(u) B = C \int_0^\infty \mathrm{e}^{A_{\rm cl}(u) t} \mathrm{d}t \, B$$

is convex in u and, by part (a) of Lemma 1, nonnegative.

The largest singular value $\bar{\sigma}(X)$ is a convex function of the entries of X [35]

$$\bar{\sigma}(X) = \sup_{\|w\|=1, \|v\|=1} w^T X v \tag{8}$$

and Lemma 2 implies that the principal singular vectors v_i and w_i that achieve the supremum in (8) are nonnegative for $X \geq 0$. Thus

$$w_i^T \left(X + \beta \mathrm{e}_j \mathrm{e}_k^T \right) v_i \geq w_i^T X v_i$$

for any $\beta \geq 0$, thereby implying that $\bar{\sigma}(X)$ is nondecreasing over $X \geq 0$. Since each element of $-C A_{\rm cl}^{-1}(u) B \geq 0$ is convex in u, these properties of $\bar{\sigma}(\cdot)$ and the composition rules for convex functions [35] imply convexity of $J_\infty(u) = \bar{\sigma}(-C A_{\rm cl}^{-1}(u) B)$.

To derive $\partial J_\infty(u)$, we note that the subdifferential set of the supremum over a set of differentiable functions

$$f(x) = \sup_{i \in \mathcal{I}} f_i(x)$$

is the convex hull of the gradients of the functions that achieve the supremum [36, Th. 1.13],

$$\partial f(x) = \left\{ \sum_{j | f_j(x) = f(x)} \alpha_j \nabla f_j(x) | \alpha \in \mathcal{P} \right\}.$$

Thus, the subgradient of $\bar{\sigma}(X)$ with respect to X is given by

$$\partial \bar{\sigma}(X) = \left\{ \sum_j \alpha_j w_j v_j^T \mid w_j^T X v_j = \bar{\sigma}(X), \alpha \in \mathcal{P} \right\}.$$

Finally, the matrix derivative of X^{-1} in conjunction with the chain rule yield (6). ∎

Remark 3: For a positive system all induced norms are convex functions of $-CA^{-1}(u)B$, which is the transfer matrix evaluated at zero frequency. Lemma 3 thus implies that all induced norms of system (1) are convex functions of u. We show convexity of the $\mathcal{H}_\infty$ norm as it is of particular interest in our study and the proof facilitates the derivation of the gradient.

Remark 4: The adjoint of the linear operator K, introduced in Assumption 1, with respect to the standard inner product is $K^\dagger(X) = D^T \operatorname{diag}(X)$. For positive systems, Lemma 1 implies that the gramians X_c and X_o are nonnegative matrices. Thus, the diagonal of the matrix $X_c X_o$ is positive and it follows that J_2 is a monotone function of the diagonal matrix $K(u)$. Similarly, $-A_{\rm cl}^{-1}(u) B v_i$ and $-w_i^T C A_{\rm cl}^{-1}(u)$ are nonnegative and thus J_∞ is also a monotone function of $K(u)$.

B. Differentiability of the $\mathcal{H}_\infty$ Norm

In general, the $\mathcal{H}_\infty$ norm is a nondifferentiable function of the control input u. Even though, under Assumption 1, the decentralized $\mathcal{H}_\infty$ optimal control problem (3) for positive systems is convex, it is still difficult to solve because of the lack of differentiability of J_∞. Nondifferentiable objective functions often necessitate the use of subgradient methods, which can converge slowly to the optimal solution.

In what follows, we prove that J_∞ is a continuously differentiable function of u for weakly connected $\mathcal{G}(A)$. Then, by noting that J_∞ is nondifferentiable only when $\mathcal{G}(A)$ contains disconnected components, we develop a method for solving (3) that outperforms the standard subgradient algorithm.

1) Differentiability Under Weak Connectivity: In this section, we assume that the matrices B and C are square and that their main diagonals are positive. To show the result, we first require two technical lemmas.

Lemma 6: Let $M \geq 0$ be a matrix whose main diagonal is strictly positive and whose associated graph $\mathcal{G}(M)$ is weakly connected. Then, the graphs associated with $\mathcal{G}(MM^T)$ and $\mathcal{G}(M^T M)$ have self loops and are strongly connected.

Proof: Positivity of the main diagonal of M implies that if M_{ij} is nonzero, then $(M^T M)_{ij}$ and $(MM^T)_{ij}$ are nonzero; by symmetry, $(M^T M)_{ji}$ and $(MM^T)_{ji}$ are also nonzero. Thus, $\mathcal{G}(M^T M)$ and $\mathcal{G}(MM^T)$ contain all the edges (i, j) in $\mathcal{G}(M)$ as well as their reversed counterparts (j, i). Since $\mathcal{G}(M)$ is weakly connected, $\mathcal{G}(M^T M)$ and $\mathcal{G}(MM^T)$ are strongly connected. The presence of self loops follows directly from the positivity of the main diagonal of M. ∎

Lemma 7: Let $M \geq 0$ be a matrix whose main diagonal is strictly positive and whose associated graph $\mathcal{G}(M)$ is weakly connected. Then, the principal singular value and the principal singular vectors of M are unique.

Proof: Note that $\mathcal{G}(M^k)$ has an edge from i to j if M contains a directed path of length k from i to j [37, Lemma 1.32]. Since $\mathcal{G}(MM^T)$ and $\mathcal{G}(M^T M)$ are strongly connected with self loops, Lemma 6 implies the existence of $\bar{k}$ such that $(M^T M)^k > 0$ and $(MM^T)^k > 0$ for all $k \geq \bar{k}$, and the Perron Theorem [30, Th. 8.2.11] implies that $(M^T M)^k$ and $(MM^T)^k$ have unique maximum eigenvalues for all $k \geq \bar{k}$.

The eigenvalues of $(M^T M)^k$ and $(MM^T)^k$ are related to the singular values of M by

$$\lambda_i\left(\left(M^T M\right)^k\right) = \lambda_i\left(\left(MM^T\right)^k\right) = (\sigma_i(M))^{2k}$$

and the eigenvectors of $(M^T M)^k$ and $(MM^T)^k$ are determined by the right and the left singular vectors of M, respectively. Since the principal eigenvalue and eigenvectors of these matrices are unique, the principal singular value and the associated singular vectors of M are also unique. ■

Theorem 8: Let Assumption 1 hold, let $A_{\rm cl}(u) := A + K(u)$ be a Hurwitz matrix, and let matrices B and C have strictly positive main diagonals. If the graph $\mathcal{G}(A)$ associated with A is weakly connected, $J_\infty(u)$ is continuously differentiable.

Proof: Lemma 1 implies that $\mathrm{e}^{A_{\rm cl}(u)} \geq 0$. From [37, Lemma 1.32], $\mathcal{G}(M^k)$ has an edge from i to j if there is a directed path of length k from i to j in $\mathcal{G}(M)$. Weak connectivity of $\mathcal{G}(A)$ implies weak connectivity of $\mathcal{G}(A_{\rm cl}(u))$, $\mathcal{G}(A_{\rm cl}^k(u))$, $\mathrm{e}^{A_{\rm cl}(u)t}$ and, by (7), of $\mathcal{G}(-A_{\rm cl}^{-1}(u))$.

Since $A_{\rm cl}(u)$ is Hurwitz and Metzler, its main diagonal must be strictly negative; otherwise, $\frac{\mathrm{d}}{\mathrm{d}t}x_i \geq 0$ for some x_i, contradicting stability and thus the Hurwitz assumption. Equation (7) and Lemma 1 imply $A_{\rm cl}^{-1}(u) \leq 0$ and, since $A_{\rm cl}(u)$ is Metzler, $A_{\rm cl}^{-1}(u)A_{\rm cl}(u) = I$ can only hold if the main diagonal of $-A_{\rm cl}^{-1}(u)$ is strictly positive.

Moreover, since the diagonals of B and C are strictly positive, $\mathcal{G}(-CA_{\rm cl}^{-1}(u)B)$ is weakly connected and the diagonal of $-CA_{\rm cl}^{-1}(u)B$ is also strictly positive. Thus, Lemma 7 implies that the principal singular value and singular vectors of $-CA_{\rm cl}^{-1}(u)B$ are unique, that (6) is unique for each stabilizing u, and that $J_\infty(u)$ is continuously differentiable. ■

2) Nondifferentiability for Disconnected $\mathcal{G}(A)$: Theorem 8 implies that under a mild assumption on B and C, J_∞ is only nondifferentiable when the graph associated with A has disjoint components. Proximal methods and its accelerated variants [38] generalize gradient descent to nonsmooth problems when the proximal operator of the nondifferentiable term in the objective function is readily available. However, since there is no explicit expression for the proximal operator of J_∞, in general we have to use subgradient methods to solve (3).

To a large extent, subgradient methods are inefficient because they do not guarantee descent of the objective function. However, under the following mild assumption, the subgradient of J_∞, ∂J_∞, can be conveniently expressed and a descent direction can be obtained by solving a linear program.

Assumption 2: Without loss of generality, let $A_{\rm cl}(u)$ be permuted such that $A_{\rm cl}(u) = \mathrm{blkdiag}(A_{\rm cl}^1(u), \ldots, A_{\rm cl}^m(u))$ is block diagonal and let $\mathcal{G}(A_{\rm cl}^i(u))$ be weakly connected for every i. Moreover, the matrices $B = \mathrm{blkdiag}(B^1, \ldots, B^m)$ and $C = \mathrm{blkdiag}(C^1, \ldots, C^m)$ are block diagonal and partitioned conformably with the matrix $A_{\rm cl}(u)$.

Theorem 9: Let Assumptions 1 and 2 hold and let $A_{\rm cl}(u) := A + K(u)$ be a Hurwitz matrix. Then,

$$J_\infty(u) = \max_i J_\infty^i(u) \tag{9a}$$

where $J_\infty^i(u) := \bar{\sigma}(C^i(A_{\rm cl}^i(u))^{-1}B^i)$. Moreover, every element of the subgradient of $J_\infty(u)$ can be expressed as the convex combination of a finite number of vectors $f^j := \nabla J_\infty^j(u)$ corresponding to the gradients of the functions $J_\infty^j(u)$ that achieve the maximum in (9a), i.e., $J_\infty(u) = J_\infty^j(u)$

$$\partial J_\infty(u) = \{F\alpha | \alpha \in \mathcal{P}\} \tag{9b}$$

where the columns of F are given by f^j and $\mathcal{P}$ is the simplex.

Proof: Since $A_{\rm cl}(u)$ is a block diagonal matrix, so is $A_{\rm cl}^{-1}(u)$ and Assumption 2 implies that $-CA_{\rm cl}^{-1}(u)B = \mathrm{blkdiag}(-C^i(A_{\rm cl}^i(u))^{-1}B^i)$ is also block diagonal. Thus,

$$J_\infty(u) = \bar{\sigma}(-CA_{\rm cl}^{-1}(u)B) = \max_i \bar{\sigma}\left(-C^i(A_{\rm cl}^i(u))^{-1}B^i\right)$$

which proves (9a). Theorem 8 implies that each $J_\infty^i(u)$ is continuously differentiable which establishes (9b). ■

When g is differentiable, we leverage the above convenient expression for ∂J_∞ to select an element of the subdifferential set which, with an abuse of terminology, we call the *optimal* subgradient. The optimal subgradient is guaranteed to be a descent direction for (3) and it is defined as the member of $\partial(J_\infty(u) + g(u))$ that solves

$$\begin{aligned} &\underset{v,\alpha}{\text{minimize}} && \max_j \left(v^T\left(f^j + \nabla g(u)\right)\right) && \text{(10a)}\\ &\text{subject to} && v = -(F\alpha + \nabla g(u)), \alpha \in \mathcal{P} && \text{(10b)}\\ & && v^T\left(f^j + \nabla g(u)\right) < 0, \text{for all } j && \text{(10c)}\end{aligned}$$

where F and f^j are defined as in Theorem 9. By (9a), $J_\infty(u)$ is the maximum of differentiable functions $J_\infty^i(u)$ and problem (10) forms a search direction using the gradients of the functions J_∞^j that achieve that maximum. While constraint (10b) ensures that $v \in \partial J_\infty(u) + \nabla g(u)$, (10c) ensures that v is a descent direction for each J_∞^j and thereby guarantees that v is a descent direction for J_∞. Finally, objective function (10a) is the maximum of the directional derivatives of J_∞^j in the direction v, i.e., the directional derivative of the objective function in (3) in the search direction.

Problem (10) can be solved efficiently because it is a linear program. Moreover, the optimality condition for (3), $\partial J_\infty(u) + \nabla g(u) \ni 0$, can be checked by solving a linear program to verify the existence of an $\alpha \in \mathcal{P}$ such that $F\alpha + \nabla g(u) = 0$.

3) Customized Algorithm: Ensuring a descent direction enables principled rules for step-size selection and makes problem (3) with nondifferentiable g tractable via the augmented-Lagrangian-based approaches. Reformulation of (3)

$$\begin{aligned} &\underset{u,v}{\text{minimize}} && J_\infty(u) + g(v)\\ &\text{subject to} && u - v = 0 \end{aligned} \tag{11}$$

leads to the associated augmented Lagrangian

$$\mathcal{L}_\mu(u, v; \lambda) := J_\infty(u) + g(v) + \lambda^T(u - v) + \tfrac{1}{2\mu}\|u - v\|^2$$

where v is an auxiliary variable and μ is a positive parameter. Formulation (11) is convenient for the alternating direction method of multipliers (ADMM) [39], which minimizes $\mathcal{L}_\mu$ separately over u and v and updates λ until convergence. ADMM is highly sensitive to the choice of μ and it may require many iterations to converge. In contrast, the more mature and robust method of multipliers (MM) [40] has effective rules for adaptively updating μ, which leads to faster convergence. It is difficult to directly apply MM to (11) because it requires joint minimization of $\mathcal{L}_\mu$ over (u, v) and both g and J_∞ are nondifferentiable. However, when the proximal operator of g is readily available, e.g., when g is the ℓ_1 norm or an indicator function of a convex set with simple projection [41], explicit minimization over v is achieved by $v_\mu^\star(u,\lambda) = \mathbf{prox}_{\mu g}(u + \mu\lambda)$. Substitution of $v_\mu^\star(u,\lambda)$ into $\mathcal{L}_\mu$ yields the proximal augmented Lagrangian [42]

$$\mathcal{L}_\mu\left(u, v_\mu^\star(u,\lambda);\lambda\right) = J_\infty(u) + M_{\mu g}(u + \mu\lambda) - \tfrac{\mu}{2}\|\lambda\|^2$$

where $M_{\mu g}$ is the Moreau envelope of g and is continuously differentiable, even when g is not [41]; see [42] for details. Since J_∞ is the only nondifferentiable component of the proximal augmented Lagrangian, the optimal subgradient (10) can be used to minimize it over u. This equivalently minimizes $\mathcal{L}_\mu(u, v; \lambda)$ over (u, v) and leads to a tractable MM algorithm

$$u^{k+1} = \underset{u}{\operatorname{argmin}}\, \mathcal{L}_\mu\left(u, v_{\mu^k}^\star(u,\lambda^k);\lambda^k\right)$$

$$\lambda^{k+1} = \lambda^k + \tfrac{1}{\mu^k}\left(u^{k+1} - \mathbf{prox}_{\mu^k g}\left(u^{k+1} + \mu^k\lambda^k\right)\right).$$

This algorithm minimizes the proximal augmented Lagrangian over u, updates λ via gradient ascent, and it represents an appealing alternative to ADMM for problems of the form (3). In particular, an adaptive selection of the parameter μ leads to improved practical performance relative to ADMM [42].

IV. Leader Selection in Directed Networks

We now consider the special case of system (1), in which the matrix A is given by a graph Laplacian, and study the leader selection problem for directed consensus networks. The question of how to optimally assign a predetermined number of nodes to act as leaders in a network of dynamical systems with a given topology has recently emerged as a useful proxy for identifying important nodes in a network [11]–[16]. Even though significant theoretical and algorithmic advances for undirected networks have been made, the leader selection problem in directed networks remains open.

A. Problem Formulation

We describe consensus dynamics and state the problem.

1) Consensus Dynamics: The weighted directed network $\mathcal{G}(L)$ with n nodes and the graph Laplacian L obeys consensus dynamics, in which each node i updates its state x_i using relative information exchange with its neighbors

$$\dot{x}_i = -\sum_{j\in\mathcal{N}_i} L_{ij}(x_i - x_j) + d_i.$$

Here, $\mathcal{N}_i := \{j | (i,j) \in \mathcal{E}\}$, $L_{ij} \geq 0$ is a weight that quantifies the importance of the edge from node j to node i, d_i is a disturbance, and the aggregate dynamics are [43]

$$\dot{x} = -Lx + d$$

where L is the graph Laplacian of the directed network [44].

The graph Laplacian always has an eigenvalue at zero that corresponds to a right eigenvector of all ones, $L\mathbb{1} = 0$. If this eigenvalue is simple, all node values x_i converge to a constant $\bar{x}$ in the absence of an external input d. When $\mathcal{G}(L)$ is balanced, $\bar{x} = (1/n)\mathbb{1}^T x(0)$ is the average of the initial node values. In general, $\bar{x} = w^T x(0)$, where w is the left eigenvector of L corresponding to zero eigenvalue, $w^T L = 0$. If $\mathcal{G}(L)$ is not strongly connected, L may have additional eigenvalues at zero and the node values converge to distinct groups whose number is equal to or smaller than the multiplicity of the zero eigenvalue.

2) Leader Selection: In consensus networks, the dynamics are governed by relative information exchange and the node values converge to the network average. In the leader selection paradigm [12], certain "leader" nodes are additionally equipped with *absolute* information that introduces negative feedback on the states of these nodes. If suitable leader nodes are present, the dynamical generator becomes a Hurwitz matrix and the states of all nodes asymptotically converge to zero.

The node dynamics in a network with leaders is

$$\dot{x}_i = -\sum_{j\in\mathcal{N}_i} L_{ij}(x_i - x_j) - u_i x_i + d_i$$

where $u_i \geq 0$ is the weight that node i places on its absolute information. The node i is a leader if $u_i > 0$, otherwise it is a follower. The aggregate dynamics can be written as

$$\dot{x} = -\left(L + \operatorname{diag}(u)\right)x + d$$

and placed in the form (1) by taking $A = -L$, $B = C = I$, and $K(u) = -\operatorname{diag}(u)$. We evaluate the performance of a leader vector $u \in \mathbb{R}^n$ using the $\mathcal{H}_2$ or $\mathcal{H}_\infty$ performance metrics J_2 or J_∞, respectively. We note that this system is marginally stable in the absence of leaders and much work on consensus networks focuses on driving the *deviations* from the average node values to zero [45]. Instead, we here focus on driving the node values themselves to zero.

We formulate the combinatorial problem of selecting N leaders to optimize either $\mathcal{H}_2$ or $\mathcal{H}_\infty$ norm as follows.

Problem 1: Given a network with a graph Laplacian L and a fixed leader weight κ, find the optimal set of N leaders that solves

$$\begin{array}{ll} \underset{u}{\text{minimize}} & J(u) \\ \text{subject to} & \mathbb{1}^T u = N\kappa,\, u_i \in \{0, \kappa\} \end{array}$$

where J is a performance metrics described in Section II-B, with $A = -L$, $B = C = I$, and $K(u) = \operatorname{diag}(u)$.

Fitch *et al.* [13] and [14] derive explicit expressions for leaders in undirected networks. However, these expressions are efficient only for very few or very many leaders. Instead, we follow [12] and develop an algorithm that relaxes the integer constraint to obtain a lower bound on Problem 1 and use greedy heuristics to obtain an upper bound.

Considering leader selection in directed networks adds the challenge of ensuring stability. At the same time, we can leverage existing results on leader selection in undirected networks to derive efficient upper bounds on Problem 1.

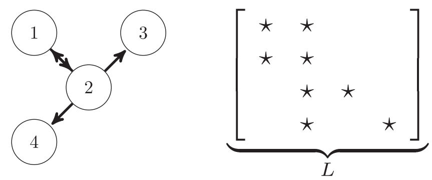


Fig. 1. Directed network and the sparsity pattern of the corresponding graph Laplacian. This network is stabilized if and only if either node 1 or node 2 are made leaders.

B. Stability for Directed Networks

For a vector of leader weights u to be feasible for Problem 1, it must stabilize system (1), i.e., $-(L + \mathrm{diag}(u))$ must be a Hurwitz matrix. When $\mathcal{G}(L)$ is undirected and connected, any leader will stabilize (1). However, this is not the case for directed networks. For example, making node 1 or 2 a leader stabilizes the network in Fig. 1, but making node 3 or 4 a leader does not. Theorem 10 provides a necessary and sufficient condition for stability.

Theorem 10: Let L be a weighted directed graph Laplacian and let $u \geq 0$. The matrix $-(L + \mathrm{diag}(u))$ is Hurwitz if and only if $w \circ u \neq 0$ for all nonzero w with $w^T L = 0$, where $\circ$ is the elementwise product.

Proof: ($\Leftarrow$) If $w \circ u = 0$, $w^T \mathrm{diag}(u) = 0$. If, in addition, $w^T L = 0$, we have

$$-w^T (L + \mathrm{diag}(u)) = 0 \tag{12}$$

and, therefore, zero is an eigenvalue of $-(L + \mathrm{diag}(u))$.

($\Rightarrow$) Since the graph Laplacian L is row stochastic and $\mathrm{diag}(u)$ is diagonal and nonnegative, the Gershgorin circle theorem [30] implies that the eigenvalues of $-(L + \mathrm{diag}(u))$ are at most 0. To show that $-(L + \mathrm{diag}(u))$ is Hurwitz, we show that it has no eigenvalue at zero. Assume there exists a nonzero w such that (12) holds. This implies that either $w^T L = w^T \mathrm{diag}(u) = 0$ or that $w^T L = -w^T \mathrm{diag}(u)$. The first case is not possible because, by assumption, $w^T \mathrm{diag}(u) = (w \circ u)^T \neq 0$ for any w such that $w^T L = 0$. If the second case is true, then $w^T L v = -w^T \mathrm{diag}(u) v$ must also hold for all v. However, if we take $v = \mathbb{1}$, then $w^T L \mathbb{1} = 0$ but $-w^T \mathrm{diag}(u)\mathbb{1}$ is nonzero. ■

Remark 5: Only the set of leader nodes is relevant to the question of stability. If u does not stabilize (1), no positive weighting of the vector of leader nodes, $\alpha \circ u$ with $\alpha \in \mathbb{R}^N_{++}$, will stabilize (1). Similarly if u stabilizes (1), every $\alpha \circ u$ will.

Corollary 11: If $\mathcal{G}(L)$ is strongly connected, any choice of leader node will stabilize (1).

Proof: Since the graph Laplacian associated with a strongly connected graph is irreducible, the Perron–Frobenius theorem [30] implies that the left eigenvector associated with $-L$ is positive. Thus, $w \circ u \neq 0$ for any nonzero u and system (1) is stable by Theorem 10. ■

Remark 6: The condition in Theorem 10 requires that there is a path from the set of leader nodes to every node in the network. This can be enforced by extracting disjoint "leader subsets" $\mathcal{S}_j$ which are not influenced by the rest of the network, i.e., $(v^j)^T L = 0$ where $v^j_i = 1$ if $i \in \mathcal{S}_j$ and $v^j_i = 0$ otherwise, and which are each strongly connected components of the original network. Stability is guaranteed if there is at least one leader node in each such subset $\mathcal{S}_j$, e.g., for the network in Fig. 1, there is one leader subset $\mathcal{S}_1 = \{1, 2\}$. By Corollary 11, $\mathcal{S}_1$ contains all nodes when the network is strongly connected.

C. Bounds for Problem 1

To approach combinatorial Problem 1, we derive bounds on its optimal objective value. These bounds can also be used to implement a branch-and-bound approach [46].

1) Lower Bound: By relaxing the combinatorial constraint in Problem 1, we formulate the optimization problem

$$\begin{array}{ll} \underset{u}{\text{minimize}} & J(u) \\ \text{subject to} & u \in \kappa\mathcal{P}_N \end{array} \tag{13}$$

where $\kappa\mathcal{P}_N := \{u | \sum_i u_i = N\kappa, u_i \leq \kappa\}$ is the "capped" simplex. The results of Section III, establish the convexity of problem (13). Using a recent result on efficient projection onto $\mathcal{P}_N$ [47], this problem can be solved efficiently via proximal gradient methods [38] to provide a lower bound on Problem 1.

When $\mathcal{G}(L)$ is not strongly connected, additional constraints can be added to enforce the condition in Theorem 10 and thus guarantee stability. Let the sets $\mathcal{S}_j$ denote "leader subsets" from which a leader must be chosen, as discussed in Remark 6. Then, the convex problem

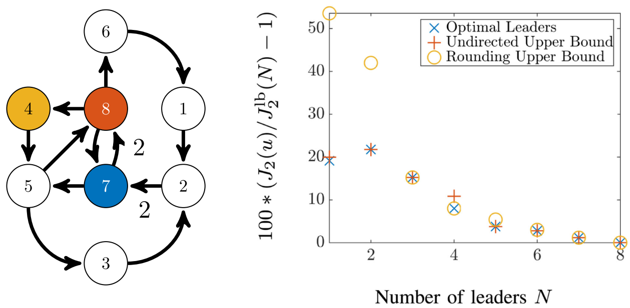
$$\begin{array}{ll} \text{minimize} & J(u) \\ \text{subject to} & u \in \kappa\mathcal{P}_N, \displaystyle\sum_{i \in \mathcal{S}_j} u_i \geq \kappa, \text{for all } j \end{array} \tag{14}$$

relaxes the combinatorial constraint and guarantees stability. We denote the resulting lower bounds on the optimal values of the $\mathcal{H}_2$ and $\mathcal{H}_\infty$ versions of Problem 1 with N leaders by $J_2^{\mathrm{lb}}(N)$ and $J_\infty^{\mathrm{lb}}(N)$, respectively.

2) Upper Bounds for Problem 1: If k denotes the number of subsets $\mathcal{S}_j$, a stabilizing candidate solution to Problem 1 can be obtained by "rounding" the solution to (14) by taking N leaders to contain the largest element from each subset $\mathcal{S}_j$ and $N - k$ largest remaining elements. The greedy swapping algorithm proposed in [12] can further tighten this upper bound.

Recent work on leader selection in undirected networks can also provide upper bounds for Problem 1 when $\mathcal{G}(L)$ is balanced. The symmetric component of the Laplacian of a balanced graph, $L_s := \frac{1}{2}(L + L^T)$, is the Laplacian of an undirected network. The exact optimal leader set for an undirected network can be efficiently computed when N is either small or large [13], [14]. Since the performance of the symmetric component of a system provides an upper bound on the performance of the original system, these sets of leaders will have better performance with L than with L_s for both the $\mathcal{H}_2$ [48, Corollary 3] and $\mathcal{H}_\infty$ norms [49, Proposition 4].

Even when L does not represent a balanced network, J_2 and J_∞ are, respectively, upper bounded by the trace and the maximum eigenvalue of $\frac{1}{2}(L_s + K)^{-1}$. For small numbers of leaders, they can be efficiently computed using rank-one inversion updates. A similar approach was used in [13] and [14] to derive optimal leaders for undirected networks. Moreover, this approach yields a stabilizing set of leaders [48, Lemma 1].



(a) (b)

Fig. 2. $\mathcal{H}_2$ performance of optimal leader set (blue $\times$) and upper bounds resulting from "rounding" (yellow $\circ$) and the optimal leaders for the undirected network (red $+$). Performance is shown as a percent increase in J_2 relative to $J_2^{\text{lb}}(N)$. (a) Balanced Network with 8 nodes, 12 edges. (b) Performance of optimal leaders and two leader selection.

D. Additional Comments

We now provide additional discussion on interesting aspects of Problem 1. We first consider the gradients of J_2 and J_∞.

Remark 7: When $K(u) = -\text{diag}(u)$, we have $\nabla J_2 = -2\text{diag}(X_c X_o)$. The matrix $X_c X_o$ often appears in model reduction and $(\nabla J_2(u))_i$ corresponds to the inner product between the ith columns of X_c and X_o.

Remark 8: When $K(u) = -\text{diag}(u)$, $(\partial J_\infty(u))_i$ is given by the product of $-\text{e}_i^T A_{\text{cl}}^{-1}(u) v$ and $w^T A_{\text{cl}}^{-1}(u)\text{e}_i$. The former quantifies how much the forcing, which causes the largest overall response of system (1), affects node i, and the latter captures how much the forcing at node i affects the direction of the largest output response.

The optimal leader sets for balanced graphs are interesting because they are invariant under reversal of all edge directions.

Proposition 12: Let $\mathcal{G}(L)$ be balanced, let $\hat{L} := L^T$ so that $\mathcal{G}(\hat{L})$ contains the reversed edges of the graph $\mathcal{G}(L)$, and let $\hat{J}_2$ and $\hat{J}_\infty$ denote the performance metrics (2) with $A = -\hat{L}$, $K(u) = -\text{diag}(u)$, and $B = C = I$ as in Problem 1. Then, $J_2(u) = \hat{J}_2(u)$ and $J_\infty(u) = \hat{J}_\infty(u)$.

Proof: The controllability gramian of (1) defined with $A_{\text{cl}} = -(L + \text{diag}(u))$ solves Lyapunov equation (5a), $-(L + \text{diag}(u))X_c - X_c(L + \text{diag}(u))^T + I = 0$, and is also the observability gramian $\hat{X}_o$ of (1) defined with $A_{\text{cl}} = -(\hat{L} + \text{diag}(u)) = -(L^T + \text{diag}(u))$ that solves (5b). By definition of the $\mathcal{H}_2$ norm, $\hat{J}_2(u) = \text{trace}(\hat{X}_o) = \text{trace}(X_c) = J_2(u)$. Since $\bar{\sigma}(M) = \bar{\sigma}(M^T)$, $\hat{J}_\infty(u) = \bar{\sigma}(-(\hat{L} + \text{diag}(u))^{-1}) = \bar{\sigma}(-(L + \text{diag}(u))^{-1}) = J_\infty(u)$. ∎

This invariance is intriguing because the space of balanced graphs is spanned by cycles. Zelazo *et al.* [50] explored how undirected cycles affect undirected consensus networks. Proposition 12 suggests that directed cycles also play a fundamental role in directed consensus networks.

E. Computational Experiments

Here, we illustrate our approach to Problem 1 with N leaders and the weight $\kappa = 1$. The "rounding" approach that we employ is described in Section IV-C2.

1) Synthetic Example: For the directed network in Fig. 2(a), let the edges from node 2 to node 7 and from node 7 to node 8 have an edge weight of 2 and let all other edges have unit edge weights. We compare the optimal set of leaders, determined by exhaustive search, to the set of leaders obtained by "rounding" the solution to relaxed problem (14); and by the optimal selection for the undirected version of the graph via [13], [14], as discussed in Section IV-C2. In Fig. 2(a), blue node 7 represents the optimal single leader, yellow node 4 represents the single leader selected by "rounding," and red node 8 represents the optimal single leader for the undirected network. In Fig. 2(b), we show the $\mathcal{H}_2$ performance for 1 to 8 leader nodes resulting from different methods. Since in general, we do not know the optimal performance *a priori*, we plot performance degradation (in percents) relative to the lower bound on Problem 1 obtained by solving problem (14).

Fig. 2(b) shows that neither "rounding" (yellow $\circ$) nor the optimal selection for undirected networks (red $+$) achieve unilaterally better $\mathcal{H}_2$ performance (performance of the optimal leader sets are shown in blue $\times$). While the procedure for the undirected networks selects better sets of 1, 2, and 5 leaders relative to "rounding," identifying them is expensive except for large or small number of leaders [13], [14] and "rounding" identifies a better set of 4 leaders. This suggests that, when possible, *both* sets of leaders should be computed and the one that achieves better performance should be selected.

2) Neural Network of the Worm C. Elegans: We now consider the network of neurons in the brain of the worm C. Elegans with 297 nodes and 2359 weighted directed edges. The data was compiled by [51] from [52]. Inspired by the use of leader selection as a proxy for identifying important nodes in a network [11]–[15], we employ this framework to identify important neurons in the brain of C. Elegans.

Three nodes in the network have zero in-degree, i.e., they are not influenced by the rest of the network. Thus, as discussed in Remark 6, there are three "leader subsets," each comprised of one of these nodes. Theorem 10 implies that system (1) can only be stable if each of these nodes are leaders.

In Fig. 3(c) and (d), we show J_2 and J_∞ resulting from "rounding" the solution to problem (14) to select the additional 1 to 294 leaders. Performance is plotted as an increase (in percents) relative to the lower bound $J^{\text{lb}}(N)$ obtained from (14). This provides an upper bound on suboptimality of the identified set of leaders. While this value does not provide information about how $J(u)$ changes with the number of leaders, Remark 4 implies that it monotonically decreases with N.

For both J_2 and J_∞ performance metrics, Fig. 3(c) and (d) illustrates that the upper bound is loosest for 25 leaders (1.56% and 0.48%, respectively). As seen in Fig. 2(b) from the previous example, whose small size enabled exhaustive search to solve Problem 1 exactly, the upper bound on suboptimality is not tight and the exact optimal solution to Problem 1 can differ by as much 21.75% from the lower bound. This suggests that "rounding" selects very good sets of leaders for this example.

In Fig. 3(a) and (b), we show the network with ten identified J_2 and J_∞ optimal leaders. The size of the nodes is related to their out-degree and the thickness of the edges is related to the weight. The red $\diamond$ marks nodes that *must* be leaders and the blue $\circ$ marks the seven additional leaders selected by "rounding."

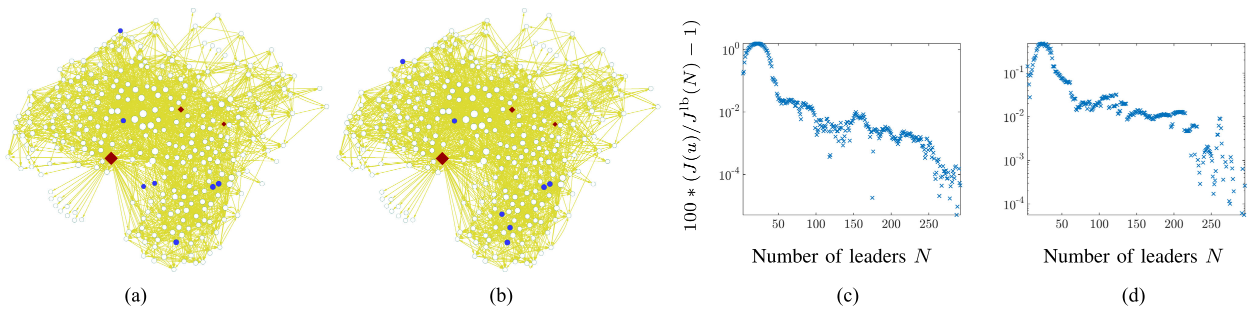


Fig. 3. C. Elegans neural network with $N = 10$ (a) J_2 and (b) J_∞ leaders along with the (c) J_2 and (d) J_∞ performance of varying numbers of leaders N relative to $J^{\rm lb}(N)$. In all cases, leaders are selected via "rounding."

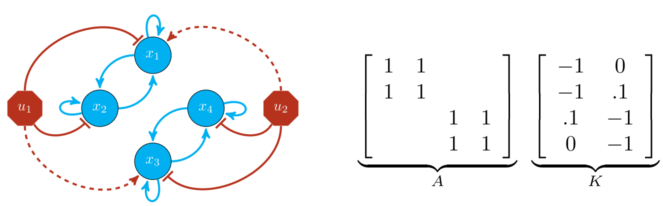


Fig. 4. Directed network and corresponding A matrix for a virus with four mutants and two drugs. For this system, J_∞ is nondifferentiable.

V. Combination Drug Therapy

System (1) also arises in the modeling of combination drug therapy [5], [7]–[10], and it provides a model for the evolution of populations of mutants of the HIV virus x in the presence of a combination of drugs u. The HIV virus is known to be present in the body in the form of different mutant strands; in (1), the ith component of the state vector x represents the population of the ith HIV mutant. The diagonal entries of the matrix A represent the net replication rate of each mutant, and the off diagonal entries of A, which are all nonnegative, represent the rate of mutation from one mutant to another. The control input u_k is the dose of drug k and each column D_k of the matrix D in $K(u) = \operatorname{diag}(Du)$ specifies at what rate drug k kills each HIV mutant.

A. Nondifferentiability of J_∞

The mutation patterns of viruses need not be connected. In Fig. 4, we show a sample mutation network with two disconnected components. For this network, the $\mathcal{H}_\infty$ norm is nondifferentiable when $u_1 = u_2$. Nondifferentiability and the lack of an efficiently computable proximal operator necessitates the use of subgradient methods for solving

$$\underset{u}{\text{minimize}} \quad J_\infty(u) + u^T u.$$

As shown in Fig. 5 with $h(u) := J_\infty(u) + u^T u$, subgradient methods are not descent methods so small constant or a divergent series of diminishing step-sizes must be employed.

We compare the performance of the subgradient method with a constant step-size of 10^{-2} (blue) and a diminishing step-size $\frac{7\times 10^{-2}}{k}$ (red) with our optimal subgradient method in which the step-size is chosen via backtracking to ensure descent of the objective function (yellow). We show the objective function value with respect to iteration number in Fig. 5(a) and the iterates u^k in the (u_1, u_2)-plane in Fig. 5(b).

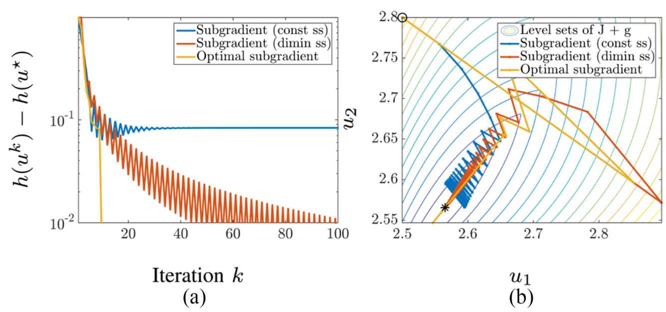


Fig. 5. Comparison of different algorithms starting from initial condition $[2.5\ 2.8]^T$. The algorithms are the subgradient method with a constant step-size (blue), the subgradient method with a diminishing step-size (red) and our optimal subgradient method where the step-size is chosen via backtracking to ensure descent of the objective function (yellow). (a) Descent of objective function. (b) Iterates in the (u_1, u_2)-plane.

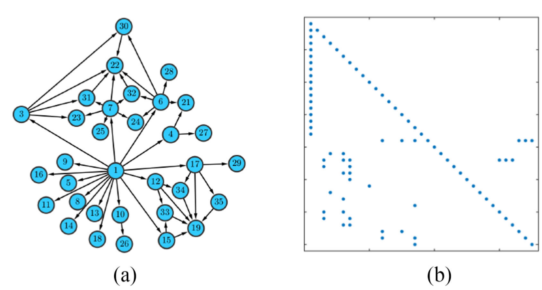


Fig. 6. Mutation pattern of the HIV mutants from [53]. (a) HIV mutation network. (b) Sparsity pattern of A.

We run the subgradient methods for 1000 iterations as there is no principled stopping criterion. Our optimal subgradient method converged with an accuracy of 10^{-4} (i.e., there was a $v \in \partial J_\infty(u)$ such that $\|v + \nabla g(u)\| \le 10^{-4}$), in 23 iterations.

B. Clinically Relevant Example

Following [7], [8] and using data from [53], we study a system with 35 mutants and 5 drugs. The sparsity pattern of the matrix A, shown in Fig. 6, corresponds to the mutation pattern and replication rates of 33 mutants and $K(u)$ specifies the effect of drug therapy. Two mutants are not shown in Fig. 6(a) as they have no mutation pathways to or from other mutants.

Several clinically relevant properties, such as maximum dose or budget constraints, may be directly enforced in our formulation. Other combinatorial conditions can be promoted via convex penalties, such as drug j requiring drug i via $u_i \ge u_j$ or

TABLE I
OPTIMAL BUDGETED DOSES AND $\mathcal{H}_2/\mathcal{H}_\infty$ PERFORMANCE

Antibody	$\mathbf{u}_2^\star$	$u_\infty^\star$
3BC176	0.5952	0.9875
PG16	0	0
45-46G54W	0.2484	0.0125
PGT128	0.1564	0
10-1074	0	0

$J_2(u_2^\star)$	0.6017
$J_2(u_\infty^\star)$	1.1947
$J_\infty(u_2^\star)$	0.1857
$J_\infty(u_\infty^\star)$	0.1084

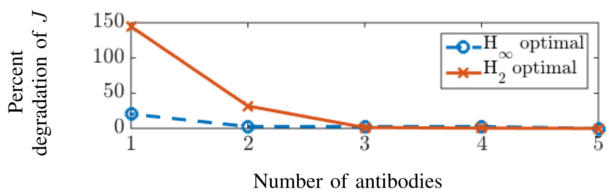


Fig. 7. Performance degradation (in percents) relative to the optimal $\mathcal{H}_2$ and $\mathcal{H}_\infty$ strategies that use all five drugs.

Algorithm 1: Sparsity-promoting Algorithm for N Drugs.

Set $\gamma > 0$, $R \succ 0$, $w = \mathbb{1}$, $\varepsilon > 0$
while $\mathrm{card}(u_\gamma) > N$ **do**
  $u_\gamma = \mathrm{argmin}_u \; J(u) + u^T R u + \gamma \sum_i w_i |u_i|$
  increase γ, set $w_i = 1/(u_i + \varepsilon)$
end
  $u_N^\star = \mathrm{argmin}_u \quad J(u) + u^T R u$
    subjectto $\quad \mathrm{sp}(u) \subseteq \mathrm{sp}(u_\gamma)$

mutual exclusivity of drugs i and j via $u_i + u_j \leq 1$. We design optimal drug doses using two convex regularizers g.

1) Budget Constraint: We impose a unit budget constraint on the drug doses and solve the J_2 and J_∞ problems using proximal gradient methods [38], [40]. These can be cast in the form (3), where g is the indicator function associated with the probability simplex $\mathcal{P}$. Table I contains the optimal doses and illustrates the tradeoff between $\mathcal{H}_2$ and $\mathcal{H}_\infty$ performance.

2) Sparsity-Promoting Framework: Although the above budget constraint is naturally sparsity-promoting, in Algorithm 1, we augment a quadratically regularized optimal control problem with a reweighted ℓ_1 norm [54] to select a homotopy path of successively sparser sets of drugs. We then perform a "polishing" step to design the optimal doses of the selected set of drugs. We use 50 logarithmically spaced increments of the regularization parameter γ between 0.01 and 10 to identify the drugs and then replace the weighted ℓ_1 penalty with a constraint to prescribe the selected drugs. In Fig. 7, we show performance degradation (in percents) relative to the optimal dose that uses all five drugs with $B = C = I$ and $R = I$.

VI. CONCLUDING REMARKS

We introduce a unifying framework for the $\mathcal{H}_2$ and $\mathcal{H}_\infty$ synthesis of positive systems and use it to address the problems of leader selection in directed consensus networks and the design of combination drug therapy for HIV treatment. We identify classes of networks for which the $\mathcal{H}_\infty$ norm is a differentiable function of the control input and develop efficient customized algorithms that perform well even in the absence of differentiability. Our ongoing work focuses on the design of time-varying strategies within an MPC framework.

ACKNOWLEDGMENT

We would like to thank A. Rantzer and K. Fitch for useful discussion on positive systems and leader selection, respectively, and to V. Jonsson for providing us with the HIV model and for her insights on combination drug therapy.

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