Data-Driven Control of Complex Networks

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Our ability to manipulate the behavior of complex networks depends on the design of efficient control algorithms and, critically, on the availability of an accurate and tractable model of the network dynamics. While the design of control algorithms for network systems has seen notable advances in the past few years, knowledge of the network dynamics is a ubiquitous assumption that is difficult to satisfy in practice, especially when the network topology is large and, possibly, time-varying. In this paper we overcome this limitation, and develop a data-driven framework to control a complex dynamical network optimally and without requiring any knowledge of the network dynamics. Our optimal controls are constructed using a finite set of experimental data, where the unknown complex network is stimulated with arbitrary and possibly random inputs. In addition to optimality, we show that our data-driven formulas enjoy favorable computational and numerical properties even when compared to their model-based counterpart. Finally, although our controls are provably correct for networks with deterministic linear dynamics, we also characterize their performance against noisy experimental data and for a class of nonlinear dynamics that arise when manipulating neural activity in brain networks.

With the development of sensing, processing, and storing capabilities of modern sensors, massive volumes of information-rich data are now rapidly expanding in many physical and engineering domains, ranging from robotics (1), to biological (2, 3) and economic sciences (4). Data are often dynamically generated by complex interconnected processes, and encode key information about the structure and operation of these networked phenomena. Examples include temporal recordings of functional activity in the human brain (5), phasor measurements of currents and voltages in the power distribution grid (6), and streams of traffic data in urban transportation networks (7). When first-principle models are not conceivably, costly, or difficult to obtain, this unprecedented availability of data offers a great opportunity for scientists and practitioners to better understand, predict, and, ultimately, control the behavior of real-world complex networks.

Existing works on the controllability of complex networks have focused exclusively on a model-based setting (8–14), although, in practice, constructing accurate models of large-scale networks is a challenging, often unfeasible, task (15–17). In fact, errors in the network model (i.e., missing or extra links, incorrect link weights) are unavoidable, especially if the network is identified from data (see, e.g., (18, 19) and Fig. 1(a)). This uncertainty is particularly important for network controllability, since, as exemplified in Fig. 1(b)–(c), the computation of model-based network controls tends to be unreliable and highly sensitive to model uncertainties, even for moderate size networks (20, 21). It is therefore natural to ask whether network controls can be learned directly from data, complex networks | dynamical systems | big data | data-driven control

Significance Statement
Manipulating the behavior of complex networks is necessary in critical situations ranging from the disruption of power generation in the grid, to the containment of spreading pathogens and the design of innovative treatments for neurological diseases. To design targeted interventions, an accurate and tractable model of the network structure and dynamics is needed. Yet, such a model is typically too difficult to estimate or derive from first principles, thus limiting, or even preventing, the use of existing control strategies to manipulate any real complex network. In this work we develop an alternative control framework, which relies on experimental data and does not require any model. We show that our data-driven controls are optimal, computationally reliable, and robust, especially for large networks.

G.B., D.S.B., and F.P. contributed to the conceptual and theoretical aspects of the study, wrote the manuscript and the SI Appendix. G.B. carried out the numerical studies and prepared the figures.

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and, if so, how well these data-driven control policies perform.

Data-driven control of dynamical systems has attracted increasing interest over the last few years, triggered by recent advances and successes in machine learning and artificial intelligence (22, 23). The classic (indirect) approach to learn controls from data is to use a sequential system identification and control design approach. That is, one first identifies a model of the system from the available data, and then computes the desired controls using the estimated model (24). However, identification algorithms are sometimes inaccurate and time-consuming, and several direct data-driven methods have been proposed to by-pass the identification step. These include, among others, (model-free) reinforcement learning (25, 26), iterative learning control (27), adaptive and self-tuning control (28), and behavior-based methods (29, 30).

The above techniques differ in the data generation procedure, class of system dynamics considered, and control objectives. In classic reinforcement learning settings, data are generated online and updated under the guidance of a policy evaluator or reward simulator, which in many applications is represented by an offline-trained (deep) neural network (31). Iterative learning control is used to refine and optimize repetitive control tasks: data are recorded online during the execution of a task repeated multiple times, and employed to improve tracking accuracy from trial to trial. In adaptive control, the structure of the controller is fixed and a few control parameters are optimized using data collected on the fly. A widely known example is the auto-tuning of PID controllers (32). Behavior-based techniques exploit a trajectory-based (or behavioral) representation of the system, and data that typically consist of a single, noiseless, and sufficiently long input-output system trajectory (30). Each of the above data-driven approaches has its own limitations and merits, which strongly depend on the intended application area. However, a common feature of all these approaches is that they are tailored to or have been employed for closed-loop control tasks, such as stabilization or tracking, and not for finite-time point-to-point control tasks.

In this paper, we address the problem of learning from data point-to-point optimal controls for complex dynamical networks. Precisely, following recent literature on the controllability of complex networks (33, 34), we focus on control policies that optimally steer the state of (a subset of) network nodes from a given initial value to a desired final one within a finite time horizon. To derive analytic, interpretable results that capture the role of the network structure, we consider networks governed by linear time-invariant dynamics. Importantly, experimental data are not required to be optimal, and can even be generated through random control experiments. In this setting, we establish closed-form expressions of optimal data-driven control policies to reach a desired target state and, in the case of noiseless data, characterize the minimum number of experiments needed to exactly reconstruct optimal control inputs. Further, we introduce suboptimal yet computationally simple data-driven expressions, and discuss the numerical and computational advantages of using our data-driven approach when compared to the classic model-based one. Finally, we illustrate by means of a numerical study how our framework can be applied to control, and characterize the controllability properties of, functional brain networks. While the focus of this paper is on designing optimal control inputs, the expressions derived in this work also provide an alternative, computationally reliable, and efficient way of analyzing the controllability properties of large network systems. This constitutes a significant contribution to the extensive literature on the model-based analysis of network controllability, where the limitations imposed by commonly used Gramian-based techniques limit the investigation to small and well-structured networks (20, 21).

**Results**

**Network dynamics and optimal point-to-point control.** We consider networks governed by linear time-invariant dynamics

\[
\begin{align*}
x(t + 1) &= Ax(t) + Bu(t), \\
y(t) &= Cx(t),
\end{align*}
\]  

where \(x(t) \in \mathbb{R}^n\), \(u(t) \in \mathbb{R}^m\), and \(y(t) \in \mathbb{R}^p\) denote, respectively, the state, input, and output of the network at time \(t\). The matrix \(A \in \mathbb{R}^{n \times n}\) describes the (directed and weighted) adjacency matrix of the network, and the matrices \(B \in \mathbb{R}^{n \times m}\) and \(C \in \mathbb{R}^{p \times n}\), respectively, are typically chosen to single out prescribed sets of input and output nodes of the network.

In this work, we are interested in designing open-loop control policies that steer the network output \(y(t)\) from an initial value \(y(0) = y_0\) to a desired one \(y(T) = y_f\) in \(T\) steps. If \(y_T\) is output controllable (33, 35) (a standing assumption in this paper), then the latter problem admits a solution and, in fact, there are many ways to accomplish such a control task. Here, we assume that the network is initially relaxed \((x(0) = 0)\), and we seek the control input \(u_{0:T-1}^* = [u^* (T - 1)^T \cdots u^* (0)^T]^T\) that drives the output of the network to \(y_f\) in \(T\) steps and, at the same time, minimizes a prescribed quadratic combination of the control effort and locality of the controlled trajectories.

Mathematically, we study and solve the following constrained minimization problem:

\[
\begin{align*}
\min_{u_{0:T-1}} & \quad y_{y_{f:T-1}}^T Q y_{y_{f:T-1}} + u_{y_{0:T-1}}^T R u_{y_{0:T-1}} \\
\text{s.t.} & \quad \text{Eq. (1)} \quad \text{and} \quad y_T = y_f,
\end{align*}
\]  

where \(Q \succeq 0\) and \(R > 0\) are tunable matrices\(^*\) that penalize output deviation and input usage, respectively, and subscript \(y_{1:T-1}\) denotes the vector containing the samples of a trajectory in the time window \([t_1, t_2]\), \(t_1 \leq t_2\) (if \(t_1 = t_2\), we simply write \(y_{1}\)). If \(Q = 0\) and \(R = I\), then \(u_{0:T-1}^*\) coincides with the minimum-energy control to reach \(y_f\) in \(T\) steps (35).

Eq. (2) admits a closed-form solution whose computation requires the exact knowledge of the network matrix \(A\) and suffers from numerical instabilities (Materials and Methods). In the following section, we address this limitation by deriving model-free and reliable expressions of \(u_{0:T-1}^*\) that solely rely on experimental input/output data collected during the network operation.

**Learning optimal controls from non-optimal data.** We assume that the network matrix \(A\) is unknown and that \(N\) control experiments have been performed with the dynamical network in Eq. (1). The \(i\)-th experiment consists of generating and applying the input sequence \(u_{0:T-1}^{(i)}\) and measuring the resulting output trajectory \(y_{f,T}^{(i)}\) (Fig. 2(a)). Here, as in, e.g., (36), we consider episodic experiments where the network state is

\(^*\)We let \(A > (\succeq) 0\) denote a positive definite (semi-definite) matrix, and \(A^T\) the transpose of \(A\).
reset to zero before running a new trial, and refer to the SI Appendix for an extension to the non-episodic setting. We let $U_{0:T-1}$, $Y_{1:T-1}$, and $Y_T$ denote the matrices containing, respectively, the experimental inputs, the output measurements in the time interval $[1, T - 1]$, and the output measurements at time $T$. Namely,

$$U_{0:T-1} = \begin{bmatrix} u_{0:T-1}^{(1)} & \cdots & u_{0:T-1}^{(N)} \end{bmatrix},$$

$$Y_{1:T-1} = \begin{bmatrix} y_{1:T-1}^{(1)} & \cdots & y_{1:T-1}^{(N)} \end{bmatrix},$$

$$Y_T = \begin{bmatrix} y_T^{(1)} & \cdots & y_T^{(N)} \end{bmatrix}. \quad [3]$$

An important aspect of our analysis is that we do not require the input experiments to be optimal, in the sense of Eq. (2), nor do we investigate the problem of experiment design, i.e., generating data that are “informative” for our problem. In our setting, data are given, and these are generated from arbitrary, possibly random, or carefully chosen experiments.

By relying on the data matrices in Eq. (3), we derive the following data-driven solution to the minimization problem in Eq. (2) (see the SI Appendix):

$$\hat{u}_{0:T-1} = U_{0:T-1}(I - KY_T(LKY_T)^{-1}L)^{-1}Y_T^{-1}y_T, \quad [4]$$

where $L$ is any matrix satisfying $L^T L = Y_{1:T-1}^T Q Y_{1:T-1} + U_{0:T-1}^T R U_{0:T-1} - K Y_T$. $K Y_T$ denotes a matrix whose columns form a basis of the kernel of $Y_T$, and the superscript symbol $^{-1}$ stands for the Moore–Penrose pseudoinverse operation (37).

**Minimum number of data to learn optimal controls.** Finite data suffice to exactly reconstruct the optimal control input via the data-driven expression in Eq. (4) (see the SI Appendix). In Fig. 2(c), we illustrate this fact for the class of Erdős–Rényi networks of Fig. 2(b). Specifically, the data-driven input $\hat{u}_{0:T-1}$ equals the optimal one $u_{0:T-1}^*$ for any target $y_T$ if the data matrices in Eq. (3) contain $mT$ linearly independent experiments; that is, if $U_{0:T-1}$ is full rank (Fig. 2(c), left).

We stress that linear independence of the control experiments is a mild condition that is normally satisfied when the experiments are generated randomly. Further, if the number of independent trials is smaller than $mT$ but larger than or equal to $p$, the data-driven control $\hat{u}_{0:T-1}$ still correctly steers the network output to $y_T$ in $T$ steps (Fig. 2(c), right), but with a cost that is typically larger than the optimal one. In this case, $\hat{u}_{0:T-1}$ is a suboptimal solution to Eq. (2), which becomes optimal (for any $y_T$) if the collected data contain $p$ independent trials that are optimal as well.

**Data-driven minimum-energy control.** By letting $Q = 0$ and $R = I$ in Eq. (4), we recover a data-driven expression for the $T$-step minimum-energy control to reach $y_T$. We remark that the family of minimum-energy controls has been extensively employed to characterize the fundamental capabilities and limitations of controlling networks, e.g., see (9,11,14). After some algebraic manipulations, the data-driven minimum-energy control input can be compactly rewritten as (see the SI Appendix)

$$\hat{u}_{0:T-1} = (Y_T^T U_{0:T-1}^{-1})^{-1} y_T. \quad [5]$$

The latter expression relies on the final output measurements only (matrix $Y_T$) and, thus, it does not exploit the full output data (matrix $Y_{1:T-1}$). Eq. (5) can be further approximated as

$$\hat{u}_{0:T-1} \approx U_{0:T-1} Y_T^{-1} y_T. \quad [6]$$

This is a simple, suboptimal data-based control sequence that correctly steers the network to $y_T$ in $T$ steps, as long as $p$ independent data are available. Further, and more importantly, when the input data samples are drawn randomly and independently from a distribution with zero mean and finite variance, Eq. (6) converges to the minimum-energy control in the limit of infinite data (see the SI Appendix).

Fig. 3(a) compares the performance (in terms of control effort and error in the final state) of the two data-driven expressions in Eq. (5) and Eq. (6), and the model-based control as a function of the data size $N$. While the data-driven control in Eq. (5) becomes optimal for a finite number of data (specifically, for $N = mT$), the approximate expression in Eq. (6) tends to the optimal control only asymptotically in the number of data (Fig. 3(a), left plot). In both cases, the error in the final state goes to zero after collecting $N = p$ data.
Fig. 3. Performance of minimum-energy data-driven network controls. Panel (a) shows the value of the cost function (left) and the error in the final state (right) for the minimum-energy data-driven control inputs in Eq. (5), Eq. (6), and the model-based one as a function of the number of data $N$. We consider Erdős–Rényi networks as in Fig. 2(b) with $\varepsilon = 0.05$, and $n = 100$, $T = 10$, $m = 5$, $p = 20$. In Panel (b), we compare the error in the final state of the data-driven approach (Eq. (5), Eq. (6)), and the classic two-step approach (identification and model-based control design) as a function of the network size $n$. We use the subspace-based identification procedure described in Materials and Methods, Erdős–Rényi networks as in Fig. 2(b) with two different edge densities, and parameters $T = 40$, $n = n/10$, $p = p$, $N = mT + 10$. The curves in panels (a) and (b) represent the average over 500 realizations of data, networks, and input/output nodes, and the light-colored regions in panel (b) contain the values of all realizations. Panel (c), left, compares the time needed to compute the optimal controls via data-driven and model-based strategies as a function of the network size, for one realization of the Erdős–Rényi network model and data. Panel (c), right, shows the errors in the final state. We use the following parameters: $\varepsilon = 0.05$, $n = n/100$, $p = n/50$, $T = 50$, and $N = mT + 10$. In all simulations the entries of the input data matrix $U$ are normal i.i.d. variables, and the input and output nodes are randomly selected. Target controllability is always ensured for all choices of input nodes by adding self-loops and edges that guarantee strong connectivity when needed. For additional computational details, see Materials and Methods.

Numerical and computational benefits of data-driven controls. By relying on the same set of experimental data, in Fig. 3(b), we compare the numerical accuracy, as measured by the error in the final state, of the data-driven controls in Eq. (5) and Eq. (6) and the minimum-energy control computed via a standard two-step approach comprising a network identification step followed by model-based control design. We consider Erdős–Rényi networks as in Fig. 2(b) in which the state of all nodes can be accessed ($C = I$), and, to reconstruct the network matrices $A$ and $B$, the subspace-based identification technique described in Materials and Methods. Data-driven strategies significantly outperform the standard sequential approach for both dense (Fig. 3(b), top) and sparse topologies (Fig. 3(b), bottom). This is not surprising because, independently of the network identification procedure, the standard two-step approach requires a number of operations larger than those required by the data-driven approach, resulting in an increased sensitivity to round-off errors. Nevertheless, it is interesting to note that the data-driven approach is especially effective for large, dense networks for which the standard approach leads to errors of considerable magnitude (up to approximately $10^5$).

A further advantage in using data-driven controls over model-based ones arises when dealing with massive networks featuring a small fraction of input and output nodes. Specifically, in Fig. 3(c) we plot the time needed to numerically compute the data-driven and model-based controls as a function of the size of the network. We focus on Erdős–Rényi networks as in Fig. 2(b) of dimension $n \geq 1000$ with $n/100$ input and output nodes and a control horizon $T = 50$. The model-based control input requires the computation of the first $T−1$ powers of $A$ (Materials and Methods). The computation of the data-driven expressions in Eq. (5) and Eq. (6) involves, instead, linear-algebraic operations on two matrices $U_0 T−1$ and $Y_T$ that are typically smaller than $A$ (precisely, when $T < n/m$ and $N < n$). Thus, the computation of the control input via the data-driven approach is normally faster than the classic model-based computation (Fig. 3(c), right). In particular, the data-driven control in Eq. (6), although suboptimal, yields the most favorable performance due to its particularly simple expression. Importantly, this computational speed-up does not come at the expense of accuracy. Indeed, the error in the final state achieved by the data-driven controls is approximately the same as the one achieved by the model-based strategy (Fig. 3(c), right).

Data-driven controls with noisy data. The analysis so far has focused on noiseless data. A natural question is how the data-driven controls behave in the case of noisy data. Here, we consider data corrupted by additive i.i.d. noise with zero mean and known variance. Namely, the available data read as

\[
U_{0,T−1} = \bar{U}_{0,T−1} + \Delta U,
\]

\[
Y_{1,T−1} = \bar{Y}_{1,T−1} + \Delta Y,
\]

\[
Y_T = \bar{Y}_T + \Delta Y_T,
\]

where $\bar{U}_{0,T−1}$, $\bar{Y}_{1,T−1}$, $\bar{Y}_T$ denote the ground truth values and $\Delta U$, $\Delta Y$, and $\Delta Y_T$ are random matrices with i.i.d. entries with zero mean and variance $\sigma^2_U$, $\sigma^2_Y$, and $\sigma^2_{Y_T}$, respectively. In this setting, it can be shown that the data-driven control in Eq. (4) and the data-driven minimum-energy controls in Eq. (5) and Eq. (6) are typically not consistent; that is, they do not converge to the true control inputs as the data size tends to infinity (see SI Appendix for a concrete example). However, by

1The different types of noise are assumed to be zero-mean to simplify the exposition. With slight modifications, non-zero-mean noise could also be accommodated by our approach. Further, the second-order statistics of the different types of noise may be estimated from prior knowledge of the accuracy of measurement sensors.
suitably modifying these expressions, it is possible to recover asymptotically correct data-driven formulas (SI Appendix). The key idea is to add correction terms that compensate for the noise variance arising from the pseudoinverse operations. In particular, the asymptotically correct version of the data-driven controls in Eq. (5) and Eq. (6) read, respectively, as

\[
\begin{align*}
\hat{u}_{0:T-1} &= \hat{Y}_T U_{0:T-1}^T (U_{0:T-1} U_{0:T-1}^T - N \sigma_y^2 I)^{-1} y_T \quad \text{[8]} \\
\hat{u}_{0:T-1} &= U_{0:T-1} Y_T^2 (Y_T Y_T^2 - N \sigma_y^2 I)^{-1} y_T \quad \text{[9]}
\end{align*}
\]

where we used the fact that \( X^\dagger = X^T (XX^T)^{-1} \) for any matrix \( X \) (37), and \( N \sigma_y^2 I \) and \( N \sigma_y^2 I \) represent the noise-dependent correction terms. Note, in particular, that if the noise corrupts the output data \( Y_T \) only, then Eq. (8) coincides with the original data-driven control in Eq. (5), so that no correction is needed. Similarly, if the noise corrupts the input data \( U_T \) only, then Eq. (9) coincides with the original data-driven control in Eq. (6).

**Controlling functional brain networks via fMRI snapshots.**

To demonstrate the potential relevance and applicability of the data-driven framework presented thus far, we investigate the problem of generating prescribed patterns of activity in functional brain networks directly from task-based functional magnetic resonance imaging (task-fMRI) time series. Specifically, we examine a dataset of task-based fMRI experiments related to motor activity and extracted from the Human Connectome Project (HCP) (41) (see Fig. 4(a)). In these experiments, participants are presented with visual cues that ask them to execute specific motor tasks; namely, tap their left or right fingers, squeeze their left or right toes, and move their tongue. We consider a set of \( m = 6 \) input channels associated with different task-related stimuli; that is, the motor tasks’ stimuli and the visual cue preceding them. As in (38), we encode the input signals as binary time series taking the value of 1 when the corresponding task-related stimulus occurs and 0 otherwise. The output signals consist of minimally pre-processed blood-oxygen-level-dependent (BOLD) time series associated with the fMRI measurements at different regions of the brain (see also Materials and Methods). In our numerical study, we parcellated the brain into \( p = 148 \) brain regions (74 regions per hemisphere) according to the Destrieux 2009 atlas (39).

Further, as a baseline for comparison, we approximate the dynamics of the functional network with a low-dimensional \((n = 20)\) linear model computed via the approach described in (38), which has been shown to accurately capture the underlying network dynamics.

In Fig. 4(b), we plot the inputs (top) and outputs (center) of one subject for the first sequence of five motor tasks. The bottom plot of the same figure shows the outputs obtained by approximating the network dynamics with the above-mentioned linear model. In Fig. 4(c), we compare the performance of the minimum-energy data-driven control in Eq. (5) with the model-based one, assuming that the network obeys the dynamics of the approximate linear model. We consider a control horizon \( T = 150 \), form the data matrices in Eq. (3) by sliding a window of fixed size \( T \) over the available fMRI data, and consider a set of 20 orthogonal targets corresponding to eigenvectors of the estimated \( T \)-step controllability Gramian (see Materials and Methods for further details). The top plot of Fig. 4(c) reports the error (normalized by the output dimension) in the final state of the two strategies, while the bottom plot shows the corresponding control energy (that is, the norm of the control input). In the plots, the targets are ordered from the most \((y_{11})\) to the least \((y_{20})\) controllable. The data-driven and the model-based inputs exhibit an almost identical behavior with reference to the most controllable targets. As we shift towards the least controllable targets, the data-driven...
strategy yields larger errors but, at the same time, requires less energy to be implemented, thus being potentially more feasible in practice. Importantly, since the underlying brain dynamics are not known, errors in the final state are computed using the identified linear dynamical model. It is thus expected that data-driven inputs yield larger errors in the final state than model-based inputs, although these errors may not correspond to control inaccuracies when applying the data-driven inputs to the actual brain dynamics. Ultimately, our numerical study suggests that the data-driven framework could represent a viable alternative to the classic model-based approach (e.g., see (12, 42, 43)) to infer controllability properties of brain networks, and (by suitably modulating the reconstructed inputs) enforce desired functional configurations.

Discussion

In this paper we present a framework to control complex dynamical networks from data generated by non-optimal (and possibly random) experiments. We show that optimal point-to-point controls to reach a desired target state, including the widely used minimum-energy control input, can be determined exactly from data. We provide closed-form and approximate data-based expressions of these control inputs and characterize the minimum number of samples needed to compute them. Further, we show by means of numerical simulations that data-driven inputs are more accurate and computationally more efficient than model-based ones, and can be used to analyze and manipulate the controllability properties of real networks.

More generally, our framework and results suggest that many network control problems may be solved by simply relying on experimental data, thus promoting a new, exciting, and practical line of research in the field of complex networks. Because of the abundance of data in modern applications and the computationally appealing properties of data-driven controls, we expect that this new line of research will benefit a broad range of research communities, spanning from engineering to biology, which employ control-theoretic methods and tools to comprehend and manipulate complex networked phenomena.

Some limitations of this study should also be acknowledged and discussed. First, in our work we consider networks governed by linear dynamics. On the one hand, this is a restrictive assumption since many real-world networks are inherently nonlinear. On the other hand, linear models are used successfully to approximate the behavior of nonlinear dynamical networks around desired operating points, and capture more explicitly the impact of the network topology. Second, in many cases a closed-loop control strategy is preferable than a point-to-point one, especially if the control objective is to stabilize an equilibrium when external disturbances corrupt the dynamics. However, we stress that point-to-point controls, in addition to being able to steer the network to arbitrary configurations, are extensively used to characterize the fundamental control properties and limitations in networks of dynamical nodes. For instance, the expressions we provide for point-to-point control can also lead to novel methods to study the energetic limitations of controlling complex networks (9), select sensors and actuators for optimized estimation and control (44), and design optimized network structures (45). Finally, although we provide data-driven expressions that compensate for the effect of noise in the limit of infinite data, we do not provide non-asymptotic guarantees on the reconstruction error. Overcoming these limitations represents a compelling direction of future work, which can strengthen the relevance and applicability of our data-driven control framework, and ultimately lead to viable control methods for complex networks.

Materials and Methods

Model-based expressions of optimal controls

The model-based solution to Eq. (2) can be written in batch form as

$$u_{t-1}^* = (I - K_{t} (MK_{t} + M)^{-1}) M C T_{1} y_1,$$

where $C_T = [C B C A B \ldots C A T^{-1} B]$ is the T-step output controllability matrix of the dynamical network in Eq. (1), $K_T$ denotes a basis of the kernel of $C_T$, and $M$ is any matrix satisfying $M M = H_T^Q H_T + R$, with

$$H_T = \begin{bmatrix} 0 & \cdots & \cdots & 0 & CB \\ \vdots & \ddots & \ddots & \cdots & CB \\ \vdots & \cdots & \ddots & \cdots & \cdots \\ 0 & CB & \cdots & \cdots & CA T^{-2} B \end{bmatrix},$$

and 0 entries denoting $p \times m$ zero matrices. If $Q = 0$ and $R = I$ (minimum-energy control input), Eq. (10) simplifies to $u_{t-1}^* = C T_{1} y_1$. Alternatively, the minimum-energy input can be compactly written in terms of the T-step output controllability Gramian of the system in Eq. (1):

$$u^*(t) = B^T A^{T-t-1} C W_{T}^{-1} y_{T}, \quad t = 0, 1, 2, \ldots, T-1.$$

Eq. (11) is the classical (Gramian-based) expression of the minimum-energy control input (35). It is well-known that this expression is numerically unstable, even for moderate size systems, e.g., see (20).

Subspace-based system identification.

Given the data matrices $U_{0:T-1}$ and $Y_{T}$ as defined in Eq. (3) and assuming that $C = I$, a simple deterministic subspace-based procedure (46, Ch. 6) to estimate the matrices $A$ and $B$ from the available data consists of the following two steps:

1. Compute an estimate of the T-step controllability matrix of the network as the solution of the minimization problem

$$\hat{C}_T = \arg \min_{C_T} \| Y_T - C_T U_{0:T-1} \|_F^2,$$

where $\| \cdot \|_F$ denotes the Frobenius norm of a matrix. The solution to Eq. (12) has the form $\hat{C}_T = Y_T Y_{0:T-1}^{-1}$.

2. In view of the definition of the controllability matrix, obtain an estimate of the matrix $B$ by extracting the first m columns of $\hat{C}_T$. Namely, $\hat{B} = [\hat{C}_T]_{1:m},$ where $[X]_{i:j}$ indicates the sub-matrix of X obtained from keeping the entries from the i-th to j-th columns and all of its rows. An estimate of the matrix $A$ can be obtained as the solution to the least-squares problem

$$\hat{A} = \arg \min_A \| [\hat{C}_T]_{1:m+1:mT} - A [\hat{C}_T]_{1:(T-1)m} \|_F^2,$$

which yields the matrix $\hat{A} = [\hat{C}_T]_{1:m+1:mT} [\hat{C}_T]_{1:(T-1)m}^{-1}$.

If the data are noiseless, the system is controllable in $T - 1$ steps, and $U_{0:T-1}$ has full row rank, then this procedure provably returns correct estimates of $A$ and $B$ (46).

Task-fMRI dataset, pre-processing pipeline, and identification setup.

The motor task fMRI data used in our numerical study are extracted from the HCP S1200 release (41, 47). The details for data acquisition and experiment design can be found in (47). The BOLD measurements have been pre-processed according to the minimal pipeline described in (40), and, as in (38), filtered with a band-pass filter to attenuate the frequencies outside the 0.06–0.12 Hz band. Further, as common practice, the effect of the physiological signals (cardiac, respiratory, and head motion signals) is removed from the BOLD measurements by means of the regression procedure in (38).
We approximate the input-output dynamics with a linear model. The data matrices in Eq. (3) are generated via a sliding window of fixed length $T = 150$ with initial time in the interval $[140, 10]$. We assume that the inputs and states are zero for times less than or equal to 10, i.e., the instant at which the first task condition is issued. We approximate the input-output dynamics with a linear model with state dimension $n = 20$ computed using input-output data in the interval $[0, 200]$ and the identification procedure detailed in (38).

Computational details. All numerical simulations have been performed via standard linear-algebra LAPACK routines available as built-in functions in Matlab® R2019b, running on a 2.6 GHz Intel Core i5 processor with 8 GB of RAM. In particular, for the computation of pseudoinverses we use the singular value decomposition method (command pinv in Matlab®) with a threshold of $10^{-8}$.

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