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An operator theoretic approach to linear ensemble control

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ABSTRACT

In this paper, we revisit the original least squares formulation of the ensemble control problem. Based on new considerations, we are able to resolve the longstanding problem of formulating general, and easily verifiable conditions for an ensemble to be controllable in the least-squares sense. The key is to take a purely operator theoretic approach from the very beginning, i.e. to study the ensemble control problem by virtue of the associated Fredholm integral equation. By establishing a direct connection to a recently introduced moment-based approach, the theoretical question of least-squares ensemble controllability is eventually settled. In the second part, we take the very same integral operator theoretic approach to consider the equally longstanding problem of synthesizing inputs that realize a desired steering between two ensemble states. By means of a suitable discretization of the integral operator, we obtain a computational procedure to synthesize control signals that steer ensembles in both a robust and minimum energy fashion. This yields a unified framework for the ensemble control of linear systems.

1. Introduction

The strikingly intriguing problem of coordinating an ensemble of nearly identical systems by merely exerting a common control signal to all systems in the ensemble, known as the ensemble control problem, has generated considerable attention in recent years. This prototype problem, formulated here in rather pure systems-theoretic terms, in fact quite naturally arises in numerous application domains ranging from quantum physics [1–3] and cell biology and cancer treatment [4–6] to problems related to human engineered systems [5,7–9], such as the control of particle processes or robotic swarms. The reason for the premise of applying a broadcast input on all systems in the ensemble simply stems from the fact that once the number of systems in the ensemble to be considered reaches a certain size, e.g., on the order of Avogadro's constant, say 10^{23}, the idea of being able to address individual systems in an individual manner becomes less and less applicable.

After this general phenomenon has been first formulated in purely systems theoretic terms about a decade ago, it has been the subject of extensive studies with different systems theoretic approaches. Starting with the work in [10,11] for the study of linear and bilinear ensemble systems, it slowly became apparent that one of the central objectives in the newly established field of ensemble control would involve establishing systems-theoretic descriptions for ensemble controllability [10–22]. In parallel to the purely theoretical investigations of ensemble controllability conditions, the development of tractable computational methods for computing the actual steering signals [23–28] needed in practical problems was recognized to be an equally important and challenging problem.

The first approach to theoretical investigation of ensemble controllability of linear ensemble systems was in a functional analytic setting [10]. However, the characterization was formulated in terms of a singular value expansion, which was not able to yield a desirable characterization for ensemble controllability in terms of the system matrices. At the same time, the problem of constructing control signals to steer linear ensembles from one state (configuration) to another in a practically acceptable manner turned out to be particularly challenging with this approach as well, as the control synthesis problem is severely ill-conditioned [29]. This may intuitively explained by virtue of the whole ensemble system being highly underactuated. In following years, another line of attack for resolving parts of the issues was being developed. In this approach, it was found that a discretization of the input signal by means of a zero-order hold strategy would translate the ensemble control problem into a polynomial approximation problem. By leveraging this connection to approximation theory, input signals for steering ensemble systems between ensemble states of interest can be designed using pseudospectral methods, by which an optimal ensemble control problem is mapped to a discrete nonlinear program through approximating the state and control functions using interpolating polynomials [23,30–32], and a polynomial expansion approach [25]. Most recently, a moment-based approach was

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introduced in [16], shedding some new light on the systematic analysis of controllability and optimal input signal design for linear ensemble systems in the least squares sense.

In this paper, we build upon insights from [16] and establish for the most basic class of ensembles

$$\frac{\partial}{\partial t}x(t,\theta) = \theta Ax(t,\theta) + Bu(t), \qquad \theta \in [a,b], \tag{1}$$

the long sought after simple reading sufficient condition for least squares ensemble controllability. Within this class, our results are general enough to encompass all the considered cases of controllable ensembles that have been studied so far using other methods. Furthermore, based on the same circle of ideas, we provide a general computational framework that encompasses several different practical problem types arising in the computational ensemble control problem for linear systems. The scope of the computational framework applies to the larger class of ensembles of the form

$$\frac{\partial}{\partial t}x(t,\theta) = A(\theta)x(t,\theta) + B(\theta)u(t), \qquad \theta \in [a,b].$$

In this sense, the framework proposed in this paper may be described as both coherent and general.

Essentially, the key idea underlying the approach advocated in this paper stems from the realization to finally accept the fact that studying this problem from a truly dynamic and systems theoretic perspective might be futile. This is in parts owed to the fact that any dynamic descriptions of an ensemble, e.g. in terms of moments do not close, etc.

Thus, we will consequently focus our entire attention to the original starting point of the ensemble control problem, which is given by the equation

$$x(T,\theta) = e^{A(\theta)T}x_0(\theta) + \int_0^T e^{A(\theta)(T-t)}B(\theta)u(t)\,\mathrm{d}t.$$

Assuming the very relevant case that $x_0(\theta) = 0$ for all $\theta \in [a,b]$, we arrive at the simpler reading expression

$$x(T,\theta) = \int_0^T e^{A(\theta)(T-t)}B(\theta)u(t)\,\mathrm{d}t. \tag{2}$$

This is a Fredholm integral equation (see e.g., [33–36]), in which we seek for an input signal $t \mapsto u(t)$ so that the integral on the right-hand side over the time variable yields the desired terminal configuration, which is a function of the second variable θ that appears in the equation. The function $K(t,\theta) = e^{A(\theta)(T-t)}B(\theta)$ is the kernel of the integral.

We may regard this relation in a more operator theoretic fashion by introducing the operator

$$R_T : L^2([0,T],\mathbb{R}^m) \to L^2([a,b],\mathbb{R}^n),$$

which maps the signal $u(\cdot)$ to $R_T u \in L^2([a,b],\mathbb{R}^n)$, given by

$$(R_T u)(\theta) = \int_0^T e^{A(\theta)(T-t)}B(\theta)u(t)\,\mathrm{d}t.$$

While there are a number of theoretical results regarding Fredholm integral equations, none of those available are constructive in the sense that they provide analytical solutions, with the exception of very special kernels. Thus, the (numerical) solution of Fredholm integral equations continues to draw great interest in different scientific communities.

Based on this circumstance, and the fact that all the other approaches so far have not led to comprehensive, and encompassing solutions (theoretically and computationally), in this paper we make (2) our starting point for both theoretical and computational considerations. As it turns out, this approach will also serve as an inherent link between the theoretical and the computational results, thereby yielding a coherent and general framework for ensemble control. In summary, the main contributions of this paper are the establishment of a general coherent framework that provides a complete and unified solution for both the theoretical L^2-ensemble controllability problem and the practical problem of synthesizing actual control inputs that solve a given ensemble steering task.

2. Review of L^2-ensemble controllability and moment-controllability with respect to monomials

The starting point for our theoretical investigation in the first part of the paper is the following definition of L^2-ensemble controllability of a linear ensemble system [10].

Definition 1 (L^2-*Ensemble Controllability*)**.** A linear ensemble

$$\frac{\partial}{\partial t}x(t,\theta) = \theta Ax(t,\theta) + Bu(t), \qquad \theta \in [a,b],$$

is said to be L^2-*ensemble controllable* if for any two configurations $x_0(\cdot), x_f(\cdot) \in L^2([a,b],\mathbb{R}^n)$, all $T > 0$ and all $\epsilon > 0$ there exists a measurable input $u : [0,T] \to \mathbb{R}^m$ that steers the ensemble from the initial configuration $x_0(\cdot)$ at $t = 0$ to a terminal configuration $x(T,\cdot)$ with $\|x(T,\cdot) - x_f(\cdot)\|_{L^2([a,b],\mathbb{R}^n)} < \epsilon$.

Despite extensive decade-long efforts to obtain practically verifiable characterizations of L^2-ensemble controllability of linear ensembles, previously established characterizations are somewhat specialized and disparate, leaving the search for a more general and coherent framework for characterizing L^2-ensemble controllability open. A promising recent approach has been established through the consideration of the evolution of the moments of an ensemble given by

$$\xi_p(T,u) = \int_a^b \theta^p x(T,\theta)\,\mathrm{d}\theta,$$

with $p \in \mathbb{N}_0$, which has provided (necessary) conditions for L^2-ensemble controllability that are formulated in terms of structural considerations of the matrices A and B and furthermore allow for a graphical interpretation of the moment dynamics [16].

The idea of the moment-based approach to ensemble controllability first introduced in [16] was to consider the problem of controlling the moments of an ensemble as a proxy to controlling the ensemble's actual state. In more detail, a linear ensemble of the form

$$\frac{\partial}{\partial t}x(t,\theta) = \theta Ax(t,\theta) + Bu(t), \qquad \theta \in [a,b],$$

would be considered moment-controllable if for any sequence of real numbers, there exists an input signal u that steers the sequence of moments $\xi_p = \int_a^b \theta^p x(T,\theta)\,\mathrm{d}\theta$ arbitrarily close to the desired sequence of moments matching the sequence of moments of a desired terminal ensemble state; see also [37] for a related but slightly different idea of "ensemble controllability in momenta". By considering the dynamics of the moments via differentiating the pth order moment ξ_p, it was found that for the system in (1), one has

$$\begin{aligned}\frac{d}{dt}\xi_p(t) &= \frac{d}{dt}\int_a^b \theta^p x(t,\theta)\,d\theta = \int_a^b \theta^{p+1}Ax(t,\theta) + \theta^p Bu(t)\,d\theta\\ &= A\xi_{p+1}(t) + \left(\int_a^b \theta^p\,d\theta\right)Bu(t).\end{aligned}$$

The moment dynamics of the linear ensemble is thus

$$\frac{d}{dt}\begin{pmatrix}\xi_0\\ \xi_1\\ \xi_2\\ \vdots\end{pmatrix} = \begin{pmatrix}0 & A & 0 & 0 & \cdots\\ 0 & 0 & A & 0 & \cdots\\ 0 & 0 & 0 & A & \cdots\\ \vdots & \vdots & \vdots & \ddots & \ddots\end{pmatrix}\begin{pmatrix}\xi_0\\ \xi_1\\ \xi_2\\ \vdots\end{pmatrix} + \begin{pmatrix}\mu_0 B\\ \mu_1 B\\ \mu_2 B\\ \vdots\end{pmatrix}u, \tag{3}$$

with the initial state $\xi_p(0) = \int_a^b \theta^p x_0(\theta)\,d\theta$. With a temporary additional technical assumption that $[a,b] \subset [-1,1]$, which will be lifted in the remainder of the paper through a result showing invariance of L^2-ensemble controllability under linear scalings of the parameter interval, it can be shown that the ensemble moments $(\xi_p)_{p\in\mathbb{N}_0}$ evolve in the space of square-summable sequences.

Lemma 2. *Let $0 < M < 1$ and consider some function $g \in L^2([-M,M],\mathbb{R})$. Then the sequence $(\xi_r)_{r\in\mathbb{N}_0}$ defined by*

$$\xi_r = \int_{[-M,M]} \theta^r g(\theta)\,d\theta$$

is square-summable.

Proof. By Hölder's inequality (with $p = q = 2$), one has

$$\left|\int_{[-M,M]} \theta^r g(\theta)\,d\theta\right| \le \|\theta^r\|_2 \|g\|_2.$$

Thus

$$\xi_r^2 = \left(\int_a^b \theta^r g(\theta)\,d\theta\right)^2 \le \|\theta^r\|_2^2\|g\|_2^2 = \|g\|_2^2\left(\int_a^b \theta^{2r}\,d\theta\right) = 2\|g\|_2^2\left(\frac{M^{2r+1}}{2r+1}\right).$$

From the assumption $0 < M < 1$, it can be directly concluded (from, say, a ratio test for the convergence of a series) that $\sum_{r=0}^{\infty}\xi_r^2 < \infty$. In other words $(\xi_r)_{r\in\mathbb{N}_0} \in \ell^2$. □

Furthermore, the result that allows us to merely focus our theoretical studies to the case that $[-M,M] \subset [-1,1]$ without any loss of generality is as follows.

Proposition 3. *An ensemble of the form*

$$\frac{\partial}{\partial t}x(t,\theta) = \theta A x(t,\theta) + Bu(t),$$

that is L^2-ensemble controllable for $\theta \in [a,b]$ is also L^2-ensemble controllable for $\theta \in [aR, bR]$ for all $R > 0$.

This result illustrates that it is essential for the ensemble controllability analysis whether or not the origin is an interior point of the parameter interval $[a,b]$, which is also the motivation for the two main theorems of the paper, Theorems 8 and 9.

Proof. A more technical formulation of the statement of the proposition is as follows. Consider two structurally identical linear ensemble systems of the form

$$\frac{\partial}{\partial t}x(t,\theta) = \theta A x(t,\theta) + Bu(t), \qquad \theta \in [a,b], \tag{4}$$

$$\frac{\partial}{\partial t}\tilde{x}(t,\tilde{\theta}) = \theta A \tilde{x}(t,\tilde{\theta}) + B\tilde{u}(t), \qquad \tilde{\theta} \in [a/R, b/R], \tag{5}$$

that differ only in a scaling of the parameter interval with a scaling factor $R > 0$. Given a steering $\tilde{u}^\star : [0,T] \to \mathbb{R}^m$ of the scaled ensemble system (5) between $\tilde{x}_0(\cdot) \in L^2([a/R,b/R],\mathbb{R}^n)$ and $\tilde{x}_f(\cdot) \in L^2([a/R,b/R],\mathbb{R}^n)$, the modified input

$$u^\star : [0, T/R] \to \mathbb{R}^m$$
$$t \mapsto u^\star(t) = R\tilde{u}^\star(Rt)$$

results in the steering of (4) between $\theta \mapsto x_0(\theta) = \tilde{x}_0(\frac{\theta}{R})$ and $\theta \mapsto x_f(\theta) = \tilde{x}_f(\frac{\theta}{R})$ within the parameter interval $\theta \in [a,b]$. As a result, L^2-ensemble controllability of linear ensemble systems of the form $\frac{\partial}{\partial t}x(t,\theta) = \theta A x(t,\theta) + Bu(t)$, $\theta \in [a,b]$ is invariant under linear scalings of the parameter interval.

To prove this result, we proceed as follows. The input $\tilde{u}^\star : [0,T] \to \mathbb{R}^m$ steers the scaled ensemble system (5) between $\tilde{x}_0(\cdot) \in L^2([a/R,b/R],\mathbb{R}^n)$ and $\tilde{x}_f(\cdot) \in L^2([a/R,b/R],\mathbb{R}^n)$, i.e.,

$$\tilde{x}_f(\tilde{\theta}) \approx \tilde{x}(T,\tilde{\theta}) = e^{\tilde{\theta}AT}\tilde{x}_0(\tilde{\theta}) + \int_0^T e^{\tilde{\theta}A(T-t)}B\tilde{u}^\star(t)\,dt.$$

We need to show that by applying $u^\star : [0,\frac{T}{R}] \to \mathbb{R}^m$, $t \mapsto u^\star(t) = R\tilde{u}^\star(Rt)$ to (4) with initial state $\theta \mapsto x_0(\theta) = \tilde{x}_0(\frac{\theta}{R})$ will result in the final ensemble state

$$\theta \mapsto x_f(\theta) = \tilde{x}_f\left(\frac{\theta}{R}\right) \approx e^{\frac{\theta}{R}AT}\tilde{x}_0\left(\frac{\theta}{R}\right) + \int_0^T e^{\frac{\theta}{R}A(T-t)}B\tilde{u}^\star(t)\,dt.$$

We have

$$\begin{aligned} x\left(\frac{T}{R},\theta\right) &= e^{\theta A\frac{T}{R}}\underbrace{x_0(\theta)}_{:=\tilde{x}_0\left(\frac{\theta}{R}\right)} + \int_0^{\frac{T}{R}} e^{\theta A(\frac{T}{R}-t)}BR\tilde{u}^\star(Rt)\,dt \\ &= e^{\frac{\theta}{R}AT}\tilde{x}_0\left(\frac{\theta}{R}\right) + \int_0^T e^{\frac{\theta}{R}A(T-\tau)}B\tilde{u}^\star(\tau)\,d\tau, \end{aligned}$$

where we have used the substitution $\tau := Rt$ in the integration. □

Thus, within the context of studying L^2-ensemble controllability of the original ensemble, we can assume without loss of generality that the parameter interval $[a,b]$ is scaled so that $[a,b] \subset [-1,1]$ and consider the definition of the operators

$$\begin{aligned} &\mathcal{A} : \ell^2(\mathbb{R}^n) \to \ell^2(\mathbb{R}^n), \quad x = (x_1, x_2, \dots) \mapsto (Ax_2, Ax_3, \dots) \\ &\mathcal{B} : \mathbb{R}^m \to \ell^2(\mathbb{R}^n), \qquad\qquad u \mapsto (\mu_0 Bu, \mu_1 Bu, \dots). \end{aligned}$$

We can now rewrite (3) as an infinite-dimensional linear system

$$\dot{x}(t) = \mathcal{A}\xi(t) + \mathcal{B}u(t) \tag{6}$$

defined on the state space $\ell^2(\mathbb{R}^n)$.

By leveraging classical results from infinite-dimensional linear systems theory [38], the moment system is approximately controllable if and only if

$$\overline{\operatorname{span}}_{k\ge 0}(\mathcal{A}^k\mathcal{B})(\mathbb{R}^m) = \ell^2,$$

or, equivalently, if all row truncations of the "infinite Kalman matrix" $(\mathcal{B}, \mathcal{A}\mathcal{B}, \mathcal{A}^2\mathcal{B}, \dots)$ given by

$$K^{(M)} = \begin{pmatrix} \mu_0 B & \mu_1 AB & \mu_2 A^2 B & \dots \\ \mu_1 B & \mu_2 AB & \mu_3 A^2 B & \dots \\ \vdots & \vdots & \vdots & \\ \mu_M B & \mu_{M+1} AB & \mu_{M+2} A^2 B & \dots \end{pmatrix}, \tag{7}$$

contain columns which span $\mathbb{R}^{n(M+1)}$. We can summarize our foregoing discussions and findings as follows.

Definition 4 (*Moment-Controllability with Respect to Monomials*)**.** A linear ensemble

$$\frac{\partial}{\partial t}x(t,\theta) = \theta A x(t,\theta) + Bu(t), \qquad \theta \in [a,b] \subset [-1,1]$$

is said to be moment-controllable with respect to monomials if the dynamics of the monomial moments $\xi_p(t,u) = \int_a^b \theta^p x(t,\theta)\,d\theta$ given by

$$\frac{d}{dt}\begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 & A & 0 & 0 & \cdots \\ 0 & 0 & A & 0 & \cdots \\ 0 & 0 & 0 & A & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}\begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \vdots \end{pmatrix} + \begin{pmatrix} \mu_0 B \\ \mu_1 B \\ \mu_2 B \\ \vdots \end{pmatrix} u,$$

evolving in $\ell^2(\mathbb{R}^n)$ is approximately controllable, or, equivalently, if for all $M \in \mathbb{N}_0$ the column-infinite "matrices"

$$K^{(M)} = \begin{pmatrix} \mu_0 B & \mu_1 AB & \mu_2 A^2 B & \dots \\ \mu_1 B & \mu_2 AB & \mu_3 A^2 B & \dots \\ \vdots & \vdots & \vdots & \\ \mu_M B & \mu_{M+1} AB & \mu_{M+2} A^2 B & \dots \end{pmatrix},$$

contain columns that span the whole ambient space.

The latter test has already been leveraged in [16] to establish valuable new insights regarding (necessary) conditions on L^2-ensemble controllability of the original ensemble system given in terms of the matrices A and B. The equivalence between moment-controllability with respect to monomials and L^2-ensemble controllability was also already conjectured then, but not fully established.

3. Moment-controllability with respect to Legendre polynomials

The approach of considering ensemble moments with respect to monomials is very favorable in terms of the resulting simple structure found in the moment dynamics, as well as the resulting favorable test for controllability of the moment dynamics via the matrices A and B of the original ensemble $\frac{\partial}{\partial t}x(t,\theta) = \theta A x(t,\theta) + Bu(t)$, $\theta \in [a,b]$. The exact connection between controllability of the monomial moment dynamics and the most established notion of L^2-ensemble controllability is, however, not immediately clear. If we instead focus on moments with respect to Legendre polynomials (see e.g., [33–36]), denoted by P_p, i.e.,

$$\eta_p(T,u) = \int_a^b P_p(\theta) x(T,\theta)\,\mathrm{d}\theta,$$

the connection to L^2-ensemble controllability is immediately clear. This consideration of the modified moments involving the Legendre polynomials is essentially the key to arrive at L^2-ensemble controllability results due to the following basic Hilbert space argument. Given Legendre polynomials $P_p : [a,b] \to \mathbb{R}$ (recentered on $[a,b]$ and normalized), it is straightforward to define the (vector-valued) Legendre polynomials via

$$\left\{ \begin{pmatrix} P_p \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ P_p \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \dots, \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ P_p \end{pmatrix} \right\}_{p \in \mathbb{N}_0}.$$

These form an orthonormal basis for $L^2([a,b],\mathbb{R}^n)$. Expanding the ensemble state $x(t,\cdot)$ in this vector-valued Legendre orthonormal basis, we have

$$x(t,\cdot) = \sum_{p=0}^{\infty} \left(\left\langle x(t,\cdot), \begin{pmatrix} P_p \\ \vdots \\ 0 \end{pmatrix} \right\rangle \begin{pmatrix} P_p \\ \vdots \\ 0 \end{pmatrix} + \dots + \left\langle x(t,\cdot), \begin{pmatrix} 0 \\ \vdots \\ P_p \end{pmatrix} \right\rangle \begin{pmatrix} 0 \\ \vdots \\ P_p \end{pmatrix} \right),$$

which can be reformulated into the more compact form

$$x(t,\cdot) = \sum_{p=0}^{\infty} \begin{pmatrix} \int_a^b x_1(t,\theta) P_p(\theta)\,\mathrm{d}\theta \\ \vdots \\ \int_a^b x_n(t,\theta) P_p(\theta)\,\mathrm{d}\theta \end{pmatrix} P_p = \sum_{p=0}^{\infty} \underbrace{\left(\int_a^b P_p(\theta) x(t,\theta)\,\mathrm{d}\theta \right)}_{=\eta_p(t,u)} P_p.$$

Now, due to the expansion in an *orthonormal basis*, we have Parseval's identity

$$\|x(t,\cdot)\|_{L^2([a,b],\mathbb{R}^n)} = \sum_{p=0}^{\infty} \left\langle x(t,\cdot), \begin{pmatrix} P_p \\ \vdots \\ 0 \end{pmatrix} \right\rangle^2 + \dots + \left\langle x(t,\cdot), \begin{pmatrix} 0 \\ \vdots \\ P_p \end{pmatrix} \right\rangle^2,$$

i.e., the norm of the original function $x(t,\cdot)$ is equal to the norm of its Fourier coefficients resulting from an expansion in an orthonormal basis. Now we can rewrite

$$\begin{aligned} \|x(t,\cdot)\|^2_{L^2([a,b],\mathbb{R}^n)} &= \sum_{p=0}^{\infty} \left\langle x(t,\cdot), \begin{pmatrix} P_p \\ \vdots \\ 0 \end{pmatrix} \right\rangle^2 + \dots + \left\langle x(t,\cdot), \begin{pmatrix} 0 \\ \vdots \\ P_p \end{pmatrix} \right\rangle^2 \\ &= \sum_{p=0}^{\infty} \Big(\int_a^b x_1(t,\theta) P_p(\theta)\,\mathrm{d}\theta \Big)^2 \\ &\qquad + \dots + \Big(\int_a^b x_n(t,\theta) P_p(\theta)\,\mathrm{d}\theta \Big)^2 \\ &= \sum_{p=0}^{\infty} \left\| \begin{pmatrix} \int_a^b x_1(t,\theta) P_p(\theta)\,\mathrm{d}\theta \\ \vdots \\ \int_a^b x_n(t,\theta) P_p(\theta)\,\mathrm{d}\theta \end{pmatrix} \right\|^2 \\ &= \sum_{p=0}^{\infty} \|\eta_p(t,u)\|^2 = \|\eta(t,u)\|^2_{\ell^2(\mathbb{R}^n)}. \end{aligned}$$

In particular, this shows that the Legendre moment sequence $\eta(t,u)$ is square-summable. In a similar manner, again using Parseval's identity, we can also assert that

$$\|x(T,\cdot) - x_T^\star\|_{L^2([a,b],\mathbb{R}^n)} = \|\eta(T,u) - \eta^\star\|_{\ell^2(\mathbb{R}^n)}, \tag{8}$$

i.e., the L^2-norm of the difference between the actual configuration $x(T,\cdot)$ and the target configuration $x_T^\star$ is equal to the ℓ^2-norm of the difference of the corresponding Fourier coefficients viewed as a sequence of vectors in $\mathbb{R}^n$. Based on this insight, we can thus shift our attention to controlling the Fourier coefficients $(\eta_p^\star)_{p\in\mathbb{N}_0}$, as steering the Fourier coefficients of an ensemble state close to the Fourier coefficients of the target state results in steering the ensemble state close to the target state by virtue of (8).

The major difficulty we face when working with moments with respect to Legendre polynomials is the less obvious structure of the Legendre moment dynamics in contrast to the structure of the monomial moment dynamics, which has been very favorable. The main result we will establish in the course of our analysis will be an equivalence of L^2-ensemble controllability, moment controllability with respect to monomials, and moment controllability with respect to Legendre polynomials, as well as some more concrete tests based on A and B of the ensemble system.

4. Equivalence of the introduced ensemble controllability notions

In the remainder, we will set $x_0(\cdot) = 0$ for a simpler presentation. In doing so, there is no loss of generality because steering an ensemble from a non-zero initial configuration

$$x(T,\theta) = e^{\theta AT} x_0(\theta) + \int_0^T e^{\theta A(T-t)} Bu(t)\,\mathrm{d}t.$$

can be easily seen to be the steering of $x_0(\cdot) = 0$ to the terminal configuration $\theta \mapsto x(T,\theta) - e^{\theta AT} x_0(\theta)$ by virtue of

$$x(T,\theta) - e^{\theta AT} x_0(\theta) = \int_0^T e^{\theta A(T-t)} Bu(t)\,\mathrm{d}t.$$

We first observe that by considering the derivation

$$\xi_p(T,u) = \int_a^b \theta^p \int_0^T e^{\theta A(T-t)} Bu(t)\,\mathrm{d}t\,\mathrm{d}\theta$$
$$= \int_a^b \theta^p \int_0^T \sum_{k=0}^{\infty} \theta^k \frac{(T-t)^k}{k!} A^k Bu(t)\,\mathrm{d}t\,\mathrm{d}\theta \tag{9}$$
$$= \sum_{k=0}^{\infty} \Big(\int_a^b \theta^{k+p}\,\mathrm{d}\theta \Big) A^k B \Big(\int_0^T \frac{(T-t)^k}{k!} u(t)\,\mathrm{d}t \Big).$$

and associating to the series expansion of $\xi_p(T,u)$ in (9) the "infinite row"

$$K_p = \begin{pmatrix} \mu_p B & \mu_{p+1} AB & \mu_{p+2} A^2 B & \dots \end{pmatrix},$$

where $\mu_p := \int_a^b \theta^p\,\mathrm{d}\theta$, we directly recover the reachable set of the pth order moment of the ensemble configuration in terms of the range space of K_p. Stacking all moments up to degree M we find that associated to the expansion of the stacked vector of $\xi_0(T), \dots, \xi_M(T)$ yields nothing but the "column-infinite Kalman matrix" (7). This integral-based derivation (in contrast to the derivation based on the differential viewpoint), allows us to obtain the "infinite Kalman matrix" of the dynamics of the moments with respect to Legendre polynomials without having to first find the operators $\mathcal{A}_\eta : \ell^2(\mathbb{R}^n) \to \ell^2(\mathbb{R}^n)$ and $\mathcal{B}_\eta : \mathbb{R}^m \to \ell^2(\mathbb{R}^n)$ of $\dot\eta = \mathcal{A}_\eta \eta + B_\eta u$ and then having to form $K_\eta = (\mathcal{B}_\eta, \mathcal{A}_\eta \mathcal{B}_\eta, \mathcal{A}_\eta^2 \mathcal{B}_\eta, \dots)$.

Indeed, analogously to the foregoing derivation for the monomial moments, in the case of Legendre moments we have

$$\eta_p(T,u) = \int_a^b P_p(\theta) \int_0^T e^{\theta A(T-t)} Bu(t)\,\mathrm{d}t\,\mathrm{d}\theta$$
$$= \int_a^b P_p(\theta) \int_0^T \sum_{k=0}^{\infty} \theta^k \frac{(T-t)^k}{k!} A^k Bu(t)\,\mathrm{d}t\,\mathrm{d}\theta$$
$$= \sum_{k=0}^{\infty} \Big(\int_a^b P_p(\theta)\theta^k\,\mathrm{d}\theta \Big) A^k B \Big(\int_0^T \frac{(T-t)^k}{k!} u(t)\,\mathrm{d}t \Big).$$

With the definition

$$\nu_{p,k} := \int_a^b P_p(\theta)\theta^k\,\mathrm{d}\theta. \tag{10}$$

and the stacking of $\eta_0(T), \dots, \eta_M(T)$, we immediately obtain the truncated "infinite Kalman matrix" K_η

$$K_\eta^{(M)} = \begin{pmatrix} \nu_{0,0}B & \nu_{0,1}AB & \nu_{0,2}A^2B & \dots \\ \nu_{1,0}B & \nu_{1,1}AB & \nu_{1,2}A^2B & \dots \\ \vdots & \vdots & \vdots & \\ \nu_{M,0}B & \nu_{M,1}AB & \nu_{M,2}A^2B & \dots \end{pmatrix}, \tag{11}$$

without having had to go through the more tedious route in the dynamic approach. This immediately yields the test for controllability of the Legendre moment dynamics in terms of the columns of each truncation $K_\eta^{(M)}$ with $M \in \mathbb{N}_0$ to span $\mathbb{R}^{n(M+1)}$. With the two purely algebraic tests for checking the controllability of the dynamics of both monomial moments and Legendre moments, it is now possible to show the equivalence of the two moment-controllability notions by algebraically manipulations of the truncated Kalman matrices.

Definition 5 (*Moment-Controllability with Respect to Legendre Polynomials*)**.** A linear ensemble

$$\frac{\partial}{\partial t} x(t,\theta) = \theta A x(t,\theta) + Bu(t), \qquad \theta \in [a,b]$$

is said to be moment-controllable with respect to Legendre polynomials if the dynamics of the Legendre moments $\eta_p(t,u) = \int_a^b P_p(\theta)x(t,\theta)\,\mathrm{d}\theta$, with $(P_p)_{p\in\mathbb{N}_0}$ forming an orthonormal basis for $L^2([a,b],\mathbb{R}^n)$, evolving in $\ell^2(\mathbb{R}^n)$ is approximately controllable, or, equivalently, if for all $M \in \mathbb{N}_0$ the column-infinite "matrices"

$$K_\eta^{(M)} = \begin{pmatrix} \nu_{0,0}B & \nu_{0,1}AB & \nu_{0,2}A^2B & \dots \\ \nu_{1,0}B & \nu_{1,1}AB & \nu_{1,2}A^2B & \dots \\ \vdots & \vdots & \vdots & \\ \nu_{M,0}B & \nu_{M,1}AB & \nu_{M,2}A^2B & \dots \end{pmatrix},$$

contain columns that span the whole ambient space.

With the Hilbert space argument in the previous section, in particular (8), we have the following result.

Theorem 6. *A linear ensemble*

$$\frac{\partial}{\partial t} x(t,\theta) = \theta A x(t,\theta) + Bu(t), \qquad \theta \in [a,b]$$

is L^2-ensemble controllable if and only if it is moment-controllable with respect to Legendre polynomials.

In the following we reveal how the study of the more general Kalman matrix involving different $\nu_{p,k}$ can be in fact simply reduced to the simpler case involving the simpler Kalman matrix for moment-controllability with respect to monomials. By performing purely linear algebraic manipulations on the row truncations of the "infinite Kalman matrix" of the Legendre moment dynamics, we show that for all $M \in \mathbb{N}_0$, the column spaces are the same for $K^{(M)}$ associated with monomial moments and $K_\eta^{(M)}$ associated with Legendre moments. This shows the equivalence between the two moment-controllability notions, and as a result an equivalence of L^2-ensemble controllability and moment-controllability with respect to monomials, which has not been obvious before.

Theorem 7. *Consider a linear ensemble of the form*

$$\frac{\partial}{\partial t} x(t,\theta) = \theta A x(t,\theta) + Bu(t), \qquad \theta \in [a,b] \subset [-1,1].$$

The ensemble is L^2-ensemble controllable if and only if it is moment-controllable with respect to monomials.

Proof. The equivalence between L^2-ensemble controllability and moment-controllability *with respect to Legendre polynomials* P_p is clear by virtue of the aforementioned standard inner product space argument. We will now show that moment-controllability with respect to Legendre polynomials is in fact equivalent to moment-controllability with respect to monomials, which admits a more favorable structure for the associated Kalman matrices. First, we recall that a linear ensemble of the form $\frac{\partial}{\partial t}x(t,\theta) = \theta A x(t,\theta) + Bu(t)$ is moment-controllable with respect to Legendre polynomials if for any $\eta_0, \dots, \eta_M \in \mathbb{R}^n$, where M is arbitrary fixed, the equation

$$\begin{pmatrix} \eta_0 \\ \eta_1 \\ \vdots \\ \eta_M \end{pmatrix} = \begin{pmatrix} \nu_{0,0}B & \nu_{0,1}AB & \nu_{0,2}A^2B & \dots \\ \nu_{1,0}B & \nu_{1,1}AB & \nu_{1,2}A^2B & \dots \\ \vdots & \vdots & \vdots & \\ \nu_{M,0}B & \nu_{M,1}AB & \nu_{M,2}A^2B & \dots \end{pmatrix} \begin{pmatrix} \bar u_0 \\ \bar u_1 \\ \bar u_2 \\ \vdots \end{pmatrix}$$

admits a solution $(\bar u_k)_{k\in\mathbb{N}_0}$. The solvability of this equation can be analyzed by purely algebraic means, i.e., by studying the above row rank of the column-infinite (but row-finite) Kalman matrix. Recalling the definition $\nu_{p,k} := \int_a^b P_p(\theta)\theta^k\,\mathrm{d}\theta$ and writing $P_p(\theta) = \sum_{d=0}^{p} a_d \theta^d$ for the (orthogonal) polynomials introduced in view of an L^2-based analysis, we can conclude that

$$\nu_{p,k} = \int_a^b P_p(\theta)\theta^k\,\mathrm{d}\theta = \int_a^b \sum_{d=0}^{p} a_d \theta^{d+k} \mathrm{d}\theta = \sum_{d=0}^{p} a_d \mu_{d+k},$$

i.e., the occurring factors in the above Kalman matrix can be written as linear combinations of the factors μ_k from the moment-controllability analysis. More specifically, we note that $\nu_{0,k} = \mu_k$ for all $k \in \mathbb{N}$, i.e. the first row of the above Kalman matrix exactly admits the factors $\mu_0, \mu_1, \mu_2, \ldots$.

Given this particular special structure of the Kalman matrix for moment-controllability with respect to Legendre polynomials, one can verify (in a rather elementary exercise) that by applying suitable *(block) row manipulations* (that involve the coefficients a_d), the study of the row rank of the matrix in (11) can be directly boiled down to the study of the Kalman matrix (7) for moment-controllability with respect to monomials. This shows the claimed equivalence between L^2-ensemble controllability and moment-controllability of the ensemble, which concludes the proof. □

Theorem 7 establishes the equivalence between L^2-ensemble controllability and moment-controllability with respect to monomials, which was conjectured in [16]. Compared to the Kalman matrix (11) for moment-controllability with respect to Legendre polynomials, the Kalman matrix (7) admits a simpler and more evident structure. The next important step to come closer to a general and easily verifiable sufficient condition for L^2-ensemble controllability is then to formulate a condition on the pair (A, B) so that (7) has full row rank for each of the infinitely many truncations. While [16] already provided some strong evidence and hints in this direction, the long sought after sufficient condition based on (A, B) has not been formulated until now.

Now unlike in the classical controllability problem for a linear system $\dot{x} = Ax + Bu$, the strategy is not to leverage the Cayley–Hamilton theorem to reduce the consideration entirely to the finite family of matrices $B, AB, \ldots, A^{n-1}B$. Rather, the additional higher powers are in fact necessary for achieving a full row rank for the matrices $K^{(M)}$ with growing size. However, to arrive at simple reading results, we have to be able to handle the non-closure. The following result highlights an important case in which handling non-closure is feasible.

Theorem 8. *Consider a linear ensemble of the form*

$$\frac{\partial}{\partial t}x(t,\theta) = \theta A x(t,\theta) + Bu(t),$$

where $\theta \in [0, 1]$. *Assume there exist* $q \in \mathbb{N}$ *and* $\lambda \in \mathbb{R}\backslash\{0\}$ *such that* $A^q = \lambda I$. *Then, if* (A, B) *is controllable, the ensemble is moment-controllable with respect to monomials, and hence also* L^2*-ensemble controllable.*

Remark. We note that the imposed condition that for some $p \in \mathbb{N}$ and some $\lambda \neq 0$, one has $A^p = \lambda I$, which appears somewhat peculiar, is rather adequate. In fact, all the existing examples of L^2-ensemble controllable systems considered in the literature with non-invertible B (see e.g. the examples in [15]) happen to fall into this special class of systems, so that it is fair to claim that the results obtained in this paper are of sufficient generality. Furthermore, the recent structure-focused study of the general nonlinear ensemble control formulation in [19] provides further evidence pertaining to the relevance of this class of linear ensembles.

Proof. By virtue of the equivalency of L^2-ensemble controllability and moment-controllability with respect to monomials formulated in Theorem 7, it is sufficient to show moment-controllability with respect to monomials for the given class of linear ensemble systems. To this end, we need to show that for all $M \in \mathbb{N}_0$, the columns of $K^{(M)}$ span $\mathbb{R}^{n(M+1)}$, or, equivalently, that for any vectors $\eta_0, \ldots, \eta_M$, where M is arbitrary fixed, there exists a sequence $(\bar{u}_k)_{k\in\mathbb{N}_0}$ so that

$$\begin{pmatrix} \eta_0 \\ \eta_1 \\ \vdots \\ \eta_M \end{pmatrix} = \begin{pmatrix} \mu_0 B & \mu_1 AB & \mu_2 A^2 B & \ldots \\ \mu_1 B & \mu_2 AB & \mu_3 A^2 B & \ldots \\ \vdots & \vdots & \vdots & \\ \mu_M B & \mu_{M+1} AB & \mu_{M+2} A^2 B & \ldots \end{pmatrix} \begin{pmatrix} \bar{u}_0 \\ \bar{u}_1 \\ \bar{u}_2 \\ \vdots \end{pmatrix}.$$

Clearly, for a fixed $p \in \{0, \ldots, M\}$, we have

$$\eta_p = \sum_{k=0}^{\infty} \mu_{p+k} A^k B \bar{u}_k.$$

In anticipation of leveraging the special property of A, we now may carry out the summation in packets associated to $B, AB, \ldots A^{q-1}B$, by which

$$\eta_p = \sum_{m=0}^{\infty}\sum_{\ell=0}^{q-1} \mu_{p+(\ell+mq)} A^{\ell+mq} B \bar{u}_{\ell+mq}.$$

Now, exploiting the special structure of A, we have $A^{\ell+mq} = A^{\ell}(A^q)^m = \lambda^m A^{\ell}$, so that

$$\begin{aligned}\eta_p &= \sum_{\ell=0}^{q-1} A^{\ell} B \Big(\sum_{m=0}^{\infty} \mu_{p+(\ell+mq)} \lambda^m \bar{u}_{\ell+mq} \Big) \\ &=: \sum_{\ell=0}^{q-1} A^{\ell} B \Big(\sum_{m=0}^{\infty} \mu_{p+(\ell+mq)} \tilde{u}_{\ell+mq} \Big) =: \sum_{\ell=0}^{q-1} A^{\ell} B \alpha_{p,\ell},\end{aligned}$$

in which we changed variables $\tilde{u}_{\ell+mq} := \lambda^m \bar{u}_{\ell+mq}$, which is reversible due to $\lambda \neq 0$, and furthermore introduced

$$\alpha_{p,\ell} = \sum_{m=0}^{\infty} \mu_{p+(\ell+mq)} \tilde{u}_{\ell+mq}.$$

Now, without loss of generality, we can assume $q \geq n$, as otherwise we would rescale $\tilde{q} = aq$ with some $a \in \mathbb{N}$ so that $\tilde{q} \geq n$, in which case we have

$$A^{\tilde{q}} = A^{aq} = (A^q)^a = (\lambda I)^a = \lambda^a I,$$

so that we would also rescale $\tilde{\lambda} = \lambda^a$. Since (A, B) is furthermore controllable, the problem boils down to choosing $\tilde{u}_0, \tilde{u}_1, \ldots$ so that the coefficients $\alpha_{p,\ell}$ are such that any vector consisting of $\eta_0, \ldots, \eta_M$ can be attained.

Fix some $\varrho \in \{0, 1, \ldots, q-1\}$ and observe that

$$\begin{pmatrix} \alpha_{0,\varrho} \\ \alpha_{1,\varrho} \\ \vdots \\ \alpha_{M,\varrho} \end{pmatrix} = \begin{pmatrix} \mu_{\varrho} & \mu_{\varrho+q} & \ldots & \mu_{\varrho+qM} \\ \mu_{\varrho+1} & \mu_{\varrho+q+1} & \ldots & \mu_{\varrho+qM+1} \\ \vdots & \vdots & \ldots & \vdots \\ \mu_{\varrho+M} & \mu_{\varrho+q+M} & \ldots & \mu_{\varrho+qM+M} \end{pmatrix} \begin{pmatrix} \tilde{u}_{\varrho} \\ \tilde{u}_{\varrho+q} \\ \vdots \\ \tilde{u}_{\varrho+qM} \end{pmatrix}. \tag{12}$$

Now, in the case that $\theta \in [0, 1]$, we have the more explicit representation

$$\mu_p = \int_0^1 \theta^p \, d\theta = \frac{1}{p+1},$$

so that (12) can be written as

$$\begin{pmatrix} \alpha_{0,\varrho} \\ \alpha_{1,\varrho} \\ \vdots \\ \alpha_{M,\varrho} \end{pmatrix} = \begin{pmatrix} \frac{1}{\varrho+1} & \frac{1}{\varrho+q+1} & \frac{1}{\varrho+2q+1} & \ldots \\ \frac{1}{\varrho+2} & \frac{1}{\varrho+q+2} & \frac{1}{\varrho+2q+2} & \ldots \\ \frac{1}{\varrho+3} & \frac{1}{\varrho+q+3} & \frac{1}{\varrho+2q+3} & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \tilde{u}_{\varrho} \\ \tilde{u}_{\varrho+q} \\ \vdots \\ \tilde{u}_{\varrho+qM} \end{pmatrix},$$

in which we can recognize the matrix as a *Cauchy matrix* (cf. the illustrative examples of Cauchy and Hilbert matrices, as well as their relevance, in [16]), which is always invertible. Since this argument holds for arbitrary ϱ, this shows that we can find $\tilde{u} \in \ell^2$ and hence $u \in \ell^2$ such that any moments configuration $\eta_0, \ldots, \eta_M$ can be achieved. Since the overall argument, in turn, also holds for arbitrary $M \in \mathbb{N}$, this shows moment-controllability of the ensemble and hence also L^2-controllability by virtue of Theorem 7. □

While the formulation of Theorem 8 explicitly refers to the model case $\theta \in [0, 1]$, it provides a characterization for ensemble controllability in all cases where the origin is not an interior point of the parameter interval, cf. the result on scaling invariance of the parameter interval in Proposition 3. In the more difficult case when the considered parameter interval covers the origin, as frequently considered upon the identification of this more delicate case [16], we can formulate the following also very comprehensive result.

Theorem 9. *Consider an ensemble*

$$\frac{\partial}{\partial t}x(t,\theta) = \theta A x(t,\theta) + Bu(t),$$

where $\theta \in [-1, 1]$ and suppose there exists $q \in \mathbb{N}$ and $\lambda \in \mathbb{R}\backslash\{0\}$ such that $A^q = \lambda I$. Then, if (A^2, B) is controllable, the ensemble is L^2-ensemble controllable.

In other words, the sufficient condition for ensemble controllability of an ensemble $(\theta A, B)$ for $\theta \in [-1, 1]$, is equivalent to the sufficient condition for L^2-ensemble controllability of the pair $(\theta A^2, B)$ over $\theta \in [0, 1]$.

Proof. As in the proof of the first theorem, we have

$$\eta_p = \sum_{\ell=0}^{q-1} A^\ell B \Big(\sum_{m=0}^{\infty} \mu_{p+\ell+mq} \tilde{u}_{\ell+mq} \Big) =: \sum_{\ell=0}^{q-1} A^\ell B \alpha_{p,\ell},$$

As before, the coefficients $\alpha_{p,\ell}$ are essentially related to the values $\tilde{u}_0, \tilde{u}_1, \ldots$ via (12). The problem in the case that $\theta \in [-1, 1]$ is that due to the fact that $\int_{-1}^{1} \theta^p \, d\theta = 0$ for even numbers p, certain entries of the matrix in (12) may now be vanishing. This is, however, always occurring in an alternating fashion, which is the reason why one splits the consideration into the two cases in which $B, A^2B, \ldots, A^{2(n-1)}B$ and $AB, \ldots, A^{2(n-1)}(AB)$ have to be used separately for spanning the respective vectors η_p. In order to guarantee that this is always possible, we need (A^2, B) and (A^2, AB) to be controllable. By pulling out A to the left in the controllability matrix of (A^2, B) we see that the controllability for the pair (A^2, AB) follows from the controllability of the pair (A^2, B) and the fact that A^2 is invertible, the latter of which is a consequence of the assumption that $A^q = \lambda I$. Since in each of the two separate cases, the corresponding coefficients are each given by a Cauchy matrix relation similar to that in the proof of the foregoing theorem, the result follows. □

Example 10. Consider the canonical example of an ensemble of harmonic oscillators with heterogeneous frequencies, i.e.

$$A(\theta) = \begin{pmatrix} 0 & \theta \\ -\theta & 0 \end{pmatrix} = \theta \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} =: \theta A.$$

We have $A^2 = -I$, so that we may conclude that harmonic oscillators fall into the class of systems specified in the two previous theorems. Now if the parameter interval of interest is given by $\theta \in [0, 1]$, we can conclude from the first theorem that the ensemble is controllable with any non-zero column vector B, as (A, B) is controllable with any non-zero column vector B.

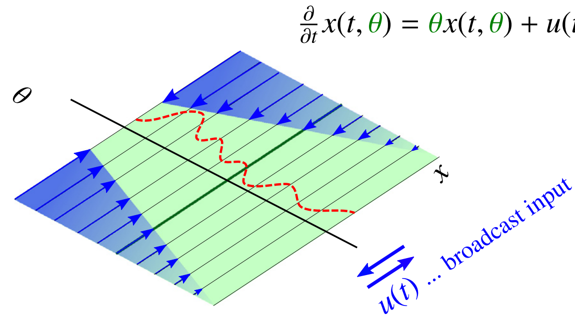

Fig. 1. Illustration of the ensemble control setup for the case of a scalar linear ensemble.

In the case that $\theta \in [-1, 1]$, we would need to consider the controllability of $(A^2, B) = (-I, B)$, which is not controllable using a single-input. This is in perfect accordance with previous observations regarding this example.

5. The computational ensemble control problem

In the previous section, we have introduced an (integral) operator theoretic framework in which the longstanding quest to find a general and succinct condition for L^2-ensemble controllability could be resolved. In this section, we turn towards the practical problem of computing steering policies for ensembles of linear systems [26–28] and show that the same operator theoretic framework provides novel insights as well as a novel computational framework, which in particular provides a unification and generalization of the approaches described in [26].

Our benchmark example will be the deceptively simple looking scalar ensemble

$$\frac{\partial}{\partial t}x(t,\theta) = \theta x(t,\theta) + u(t), \qquad \theta \in [-1, 0],$$

which may be depicted as in Fig. 1.

There we illustrate a portion of the real line, and a given parameter range for θ. Attached to each θ is a scalar linear system, which has an initial state, a drift vector field, and a control vector field (which is the same for all individual systems in the ensemble). Since this is the case for every $\theta \in [-1, 0]$, the ensemble state is a curve over the parameter θ. The drift for the whole ensemble admits a linear dependency on θ.

Now even though for each fixed $\theta \in [-1, 0]$, we have a simple first order lead element at hand, when considered as an ensemble combined with the premise of broadcast signaling, great challenges from both a practical as well as a theoretical perspective begin to appear. The ensemble control task to be considered will consist of steering this stable ensemble from a state of rest, i.e. $x(0, \theta) = 0$ for all $\theta \in [-1, 0]$ to the desired terminal state in which all values $x(T, \theta)$ are as close as possible to 1. The addition "as close as possible" is included to reflect the fact that an exact steering may not always be possible, but we will see that the ensemble can be steered to an arbitrary neighborhood of the desired terminal state. We now turn towards describing the computational approach linked to the theoretical considerations of this paper.

Given a linear operator $R : U \to X$ between two normed infinite-dimensional vector spaces U and X, it is indeed quite natural to discretize both spaces U and X by finite-dimensional vector spaces U_N and X_M and to consider the operator restricted to the discretized spaces. In this way an infinite-dimensional problem is naturally reduced to a finite-dimensional approximation of it, which can then be tackled by means of computational methods.

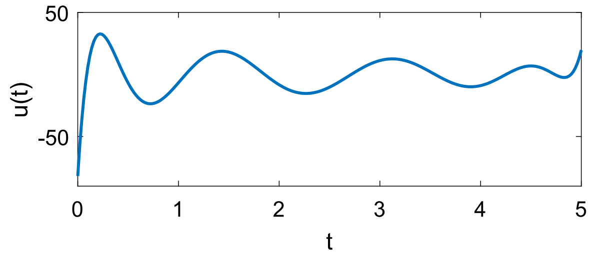

Fig. 2. The input signal obtained from solving the discretized version of the integral equation using the first ten Legendre polynomials as the orthonormal basis.

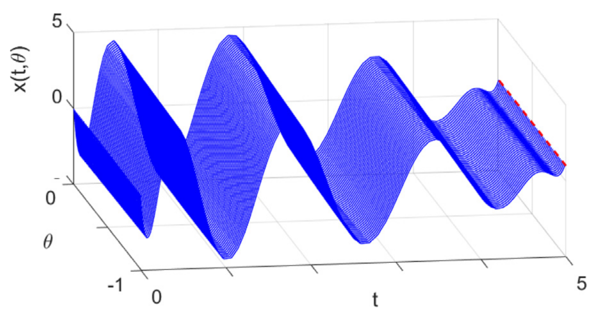

Fig. 3. The evolution of the ensemble state when applying the synthesized input signal illustrated in Fig. 2. The state appears to be very level throughout the application of the input signal.

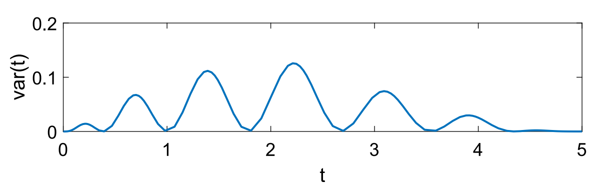

Fig. 4. The variance of the ensemble plotted over time. While this plot shows that the variance at the end point is close to zero, we also find that the variance is very low throughout the application of the input, which, in contrast to the final time point $t = T$, was not explicitly specified.

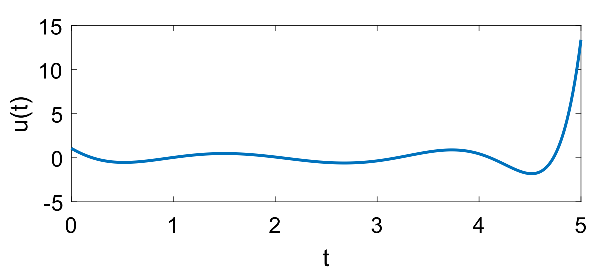

Fig. 5. The input signal obtained from solving the discretized and regularized version of the integral equation using the first ten Legendre polynomials as the orthonormal basis and the regularization parameter $\lambda = 10^{-13}$.

To this end, we first introduce a finite family of orthonormal vectors $P_1, \ldots, P_N$ on U and, similarly, a finite family of orthonormal vectors $Q_1, \ldots, Q_M$ on X. We denote the spans of these vectors by U_N and X_M respectively and consider the two corresponding orthogonal projections given by

$$P_{U_N} u = \sum_{i=1}^{N} \langle u, P_i \rangle P_i, \qquad P_{X_M} x = \sum_{i=1}^{M} \langle x, Q_i \rangle Q_i.$$

It is a well-known fact that for any $u \in U$, the orthogonal projection $P_{U_N} u$ is the element in the finite-dimensional subspace U_N that is the closest to u, and for any $x \in X$, the orthogonal projection $P_{X_M} x$ is the element in the finite-dimensional subspace X_M that is the closest to x.

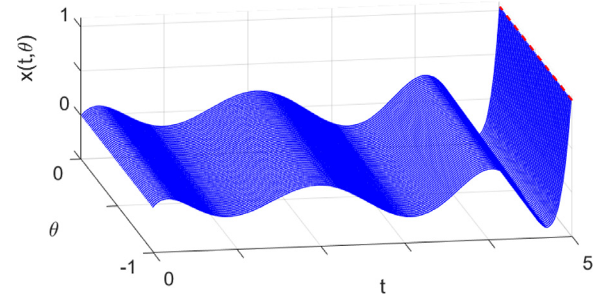

Fig. 6. The evolution of the ensemble state when applying the synthesized input signal illustrated in Fig. 5.

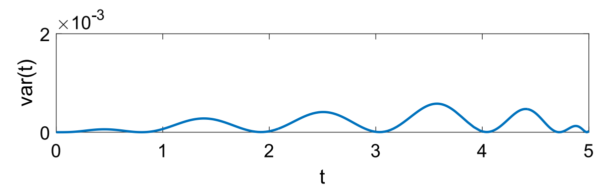

Fig. 7. The variance of the ensemble is significantly lower compared to the variance of the ensemble steered with the input obtained from the formulation without regularization.

Then we introduce a linear mapping $R_{M,N} : U_N \rightarrow X_M$ (between finite-dimensional spaces!) as the linear operator $P_{X_M} R$ whose domain is restricted to the subspace U_N. To progress towards a computational solution to the original reachability problem of finding a solution u which satisfies $Ru = x$, the idea is to project $x \in X$ on X_M to obtain $x_M = P_{X_M} x$, and to then find a least squares solution $u_N \in U_N$ to the problem of minimizing $\|R_{M,N} u_N - x_M\|^2$.

This is justified by the following consideration. Let $h' := x - x_M$, and define $\epsilon_x := \|h'\|$. Then, we have

$$\|R_{M,N} u_N - x\| = \|R_{M,N} u_N - (P_{X_M} x + h')\| \leq \|R_{M,N} u_N - P_{X_M} x\| + \epsilon_x.$$

Thus, the strategy for the practical problem would be to minimize the first term on the right-hand side, as the second term is dictated only by the choice of discretization. One can also further derive a theoretical bound for the error that results from the discretization. We observe that

$$\|R_{M,N} u_N - P_{X_M} x\| = \|P_{X_M}(R u_N - x)\| \leq \|R u_N - x\|.$$

To proceed, we recall that under the assumption of ensemble controllability (see e.g. [10]), the range space of R is dense in X, so that for any $\epsilon > 0$ one can find a $u^\star \in U$ so that $\|Ru^\star - x\| < \epsilon$. Given such $u^\star$, define $u_N^\star := P_{U_N} u^\star$, $h'' := u_N^\star - u^\star$ and $\epsilon_{u^\star} := \|h''\|$. Then one has $Ru_N^\star = Ru^\star + Rh''$. Inserting this in the above inequality, we arrive at a bound for the total error given by

$$\inf_{u_N \in U_N} \|R_{M,N} u_N - x\| \leq \|R\| \epsilon_{u^\star} + \epsilon_x.$$

Thus, with a sufficiently rich choice of basis vectors for U_N and X_M, one can expect the discretization errors $\epsilon_{u^\star}$ and ϵ_x to be sufficiently small, so that the finite-dimensional approximation provides a suitably accurate solution.

More explicitly, the discretization of the range operator $R_T : L^2([0, T], \mathbb{R}^m) \rightarrow L^2([a, b], \mathbb{R}^n)$, which can be represented in terms of an $M \times N$ matrix, denoted in the following by $R^\Delta := R_{M,N}$, can

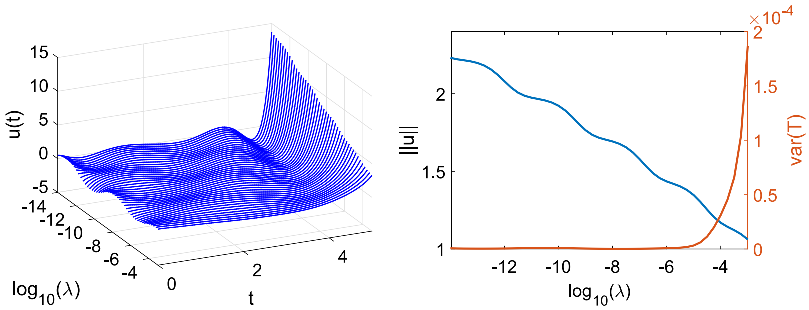

Fig. 8. Left: This plot illustrates the effect of the regularization parameter λ on the synthesized input signal. Right: This plot illustrates the dependency of the norm of the input signal and the variance in the terminal state on the parameter λ. In both plots a logarithmic scale is chosen for the λ-axis.

be directly specified by its entries, which can be computed as

$$R_{ij}^{\Delta} = \int_a^b \left(\int_0^T e^{A(\theta)(T-t)} B(\theta) P_j(t)\, \mathrm{d}t \right) Q_i(\theta)\, \mathrm{d}\theta \tag{13}$$

for $i = 1, \ldots, M$ and $j = 1, \ldots, N$.

Regarding this approach, we will only discuss two cases, which appear to be the most natural and also relevant ones to be considered in this context. This includes the case in which U is discretized by means of Legendre polynomials and X is discretized by indicator functions defined on intervals of constant length, and the case in which both U and X are discretized by indicator functions.

In the first case, we choose the first ten Legendre polynomials as the basis for U_N and 100 linearly independent indicator functions as the basis for X_M. We then compute the matrix representation of the truncated range operator R^{Δ} via (13) and attempt to solve the corresponding linear system of equations $R^{\Delta} u_N = x_M$, where $x_M = \sqrt{M/T} e$ with e denoting the all-ones vector. Having obtained a solution

$$u_N = (a_1 \ \cdots \ a_N)^{\top},$$

we construct the input signal as

$$u(t) = \sum_{i=1}^{N} a_i P_i(t).$$

Fig. 2 illustrates the input signal for $T = 5$ and Fig. 3 shows the resulting evolution of the ensemble when applying this input signal.

While we only explicitly specified the ensemble state to be perfectly level at the end time, namely all individual scalar ensembles to be as close to 1 as possible, we find that the ensemble satisfies this property at all times when applying the specific input signal. This is verified by plotting the variance of the ensemble over time, as shown in Fig. 4. As we will see in the subsequent studies of the example of scalar ensembles, this appears to be a somewhat more general principle.

While the first solution obtained through discretizing the range operator and solving a system of linear equations solved the steering task specified in the beginning, we must, however, also note that the steering is rather aggressive, leading to significant overshooting of the ensemble state before the target is hit. It would certainly be desirable if the task could also be solved in a more economical way. A quite natural way of how this may be achieved is to *regularize* the ill-conditioned inverse problem by considering the minimization problem

$$\text{minimize } \|R^{\Delta} u_N - x_M\|^2 + \lambda \|u_N\|^2, \tag{14}$$

where λ is the regularization parameter. The solution to this regularized problem is simply given by

$$u_N = ((R^{\Delta})^{\top} R^{\Delta} + \lambda I)^{-1} (R^{\Delta})^{\top} x_M.$$

From a control theoretic point of view, the regularized formulation corresponds to the very natural idea of introducing a penalty term for the input signal. From a numerical mathematics perspective, this is also a very well-known and prominent technique known as Tikhonov regularization.

Choosing for example $\lambda = 10^{-13}$ and solving the regularized problem, we obtain the input signal illustrated in Fig. 5, the evolution of the steered ensemble with this input is illustrated in Fig. 6, as well as the evolution of the ensemble variance illustrated in Fig. 7. The input signal obtained from the regularized formulation appears significantly more economic than the input signal obtained from the unregularized solution, being able to achieve the same goal in a much more calculated, subtle manner.

To illustrate the effect of the regularization in a more encompassing manner, in Fig. 8 we depict a family of different input signals associated to different choices of λ, as well as the dependence of both $\|u_N\|$ and the terminal variance on the parameter λ.

6. Conclusions

We revisited the classical least squares ensemble control problem, and showed how the recently introduced moment-based framework can be leveraged to settle the longstanding problem of establishing a general, concise, and easily verifiable condition for L^2-ensemble controllability. The starting point was to directly tackle the ensemble controllability problem through its integral operator theoretic formulation. This led to novel insights into the systems theoretic mechanisms of ensemble controllability in the case of linear ensembles with linear parameter variation. In the second part of the paper, the same integral geometric framework was taken to study the practical problem of constructing control signals that steer ensembles between desired states in a practically acceptable manner. We have presented a novel computational framework that allows for a systematic design of finely orchestrated and robust control inputs for ensembles of linear systems, and furthermore unifies previous computational approaches in a comprehensive way.

CRediT authorship contribution statement

Shen Zeng: Conceptualization, Methodology, Software, Visualization, Investigation, Reviewing and Editing. **Jr-Shin Li:** Conceptualization, Methodology, Software, Visualization, Investigation, Reviewing and Editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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