Finite Horizon Linear Quadratic Gaussian Density Regulator with Wasserstein Terminal Cost

Abhishek Halder[†*] and Eric D.B. Wendel[‡*]

***Abstract*— We formulate and solve an optimal control problem where a finite dimensional linear time invariant (LTI) control system steers a given Gaussian probability density function (PDF) close to another in fixed time, while minimizing the trajectory-wise expected quadratic cost. We measure the "closeness" between the actual terminal PDF and the desired terminal PDF, as the squared Wasserstein distance between the two density functions, and penalize the lack of closeness as terminal cost. The resulting controller is termed as linear quadratic Gaussian density regulator. Our derivation for the necessary conditions of optimality finds that unlike the standard linear quadratic Gaussian (LQG) control problem, the Lyapunov matrix differential equation for covariance is coupled with the Riccati matrix differential equation for covariance costate, via nonlinear boundary conditions. We prove that the LQG control problem can be recovered as a special case of our density regulator problem. A numerical example is worked out to elucidate the formulation.**

I. Introduction

This paper considers continuous-time optimal control for linear time invariant (LTI) systems with fixed final time, where the initial and desired terminal states' probability density functions (PDFs) are prescribed Gaussians. These PDFs model the *concentration* [1] of initial and desired terminal states. For the "cost-to-go", we use the expected quadratic cost as in the standard LQG [2] problem. However, since the initial and desired terminal *state PDFs*, and not the initial and desired terminal *state vectors*, are specified in the problem statement (see Fig. 1), a terminal cost is required that penalizes the mismatch between the actual terminal PDF and the desired terminal PDF. In this paper, we use the squared Wasserstein distance as the terminal cost, and show that it serves as a natural generalization of the quadratic terminal cost that appears in the LQG problem.

The motivation behind path-wise linear quadratic control while respecting endpoint density specifications, arise naturally in engineering applications. For example, in robotics, there is a growing literature [3]–[5] on moving a swarm of robots from a given initial spatial configuration to another. In nuclear magnetic resonance (NMR) spectroscopy and imaging (MRI), it is of interest [6] to shape the bulk magnetization distribution. In process industry applications, the design objectives are often specified [7]–[9] in terms of particle size and shape densities.

The perspectives and approach of this work differ from that of the standard LQR (LQG) problems, which are de-

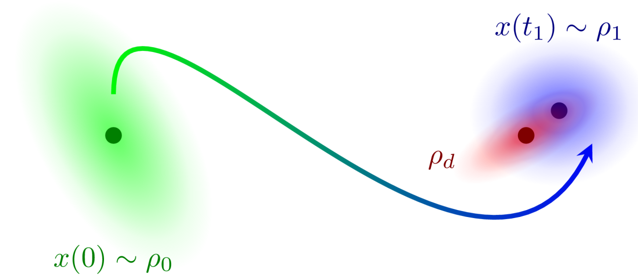

Fig. 1. We consider the linear quadratic control of state trajectories over fixed horizon $[0, t_1]$ such that the initial state $x(0) \sim \rho_0 = \mathcal{N}(\mu_0, S_0)$ (*green*) goes to the terminal state $x(t_1) \sim \rho_1$ (*blue*), where the PDF ρ_1 is "close" to a desired PDF $\rho_d = \mathcal{N}(\mu_d, S_d)$ (*red*). Here, the notation $x \sim \rho$ means that the random vector x has the joint PDF $\rho(x)$, and $\mathcal{N}(\mu, \Sigma)$ denotes Gaussian PDF with mean vector μ and covariance matrix Σ. The *filled circles* represent the respective mean vectors, and the shaded ellipses denote the respective covariance matrices. This is a relaxation of the classical LQG problem in the sense that instead of requiring the terminal state $x(t_1)$ stays close to a desired state, we require the terminal state statistics (ρ_1) to be close to a desired state statistics ρ_d. A typical trajectory is shown that goes from the *green ellipse* ρ_0 to the *blue ellipse* ρ_1.

terministic (stochastic) optimal control problems on finite dimensional state space, in that we consider an optimal control problem formulated on the manifold of PDFs. Our contributions, as we will show, apply to linear controllable systems with or without stochastic perturbations in their dynamics. On the other hand, if we take the zero covariance limit of the desired terminal Gaussian, then the problem considered in this paper reduces to the standard LQG problem with quadratic terminal cost. We will make this rigorous in Section III.B.

A. Related Work and Contributions of This Paper

In [10], minimum *energy* affine state feedback controller was derived for a stochastic linear system, that steers the state ensemble from a given initial PDF to a given terminal PDF in fixed time. Our work differs from [10] in two respects. *First*, our cost-to-go is quadratic in both state and control as in standard LQR/LQG problems. *Second*, instead of enforcing a *terminal constraint* $x(t_1) \sim \rho_1 = \rho_d = \mathcal{N}(\mu_d, S_d)$, we allow $\rho_1 \neq \rho_d = \mathcal{N}(\mu_d, S_d)$ (see Fig. 1), but incur a *terminal cost* when the "distance" between ρ_1 and ρ_d is large. Thus, our terminal cost must define a notion of distance, preferably a metric, on the space of PDFs.

[†]Department of Electrical and Computer Engineering, [‡]Department of Mathematics, Texas A&M University, College Station, TX 77843, USA, {ahalder,ericdbw}@tamu.edu. [*]denotes equal contribution.

Since the evolution of state PDFs follow either Liouville (for deterministic dynamics) or Fokker-Planck-Kolmogorov (for stochastic dynamics) partial differential equation (PDE), some recent papers [11]–[13] have investigated the optimal control of these PDEs to effect the optimal control of the state PDFs. In particular, for *controllable* LTI dynamics with affine state feedback, it has been proved that any initial mean-covariance pair (μ_0, S_0) can be steered to any terminal mean-covariance pair $(\mu(t_1), S(t_1)) = (\mu_d, S_d)$ in fixed time t_1, for both deterministic (Theorem 2 in [11]) and stochastic case (Theorem 2.10.5–6 in [12], Theorem 3 in [14]). The problem considered in this paper can be thought of as a relaxation of the requirement that the state statistics reaches an exact desired statistics, since we only require the terminal statistics close to a desired one.

Also related to our work is the dynamic formulation of optimal transport [15], which from a control-theoretic perspective, can be interpreted as the minimum energy state feedback for a vector of single integrators subject to the constraint that the initial PDF ρ_0 gets to the terminal PDF $\rho_1 = \rho_d$ in fixed time t_1.

To the best of the authors' knowledge, penalizing final density mismatch via terminal cost, while minimizing quadratic state and control cost-to-go, is novel with respect to the existing literature. Our main contribution is to show that by modeling the terminal cost through Wasserstein distance, we can derive and solve a two point boundary value problem, which unlike LQG, has nonlinear coupling through boundary conditions. Interestingly, we prove that by taking Dirac limit of the desired terminal density, our formulation recovers the LQG control problem.

B. Structure of the Paper

This paper is organized as follows. The problem formulation is detailed in Section II, followed by the main results in Section III. A numerical example is worked out in Section IV. Section V concludes the paper.

C. Notation and Preliminaries

The set of natural numbers is denoted as $\mathbb{N}$, the set of non-negative real numbers is $\mathbb{R}^+$, the trace of a matrix is denoted as $\operatorname{tr}(\cdot)$, and for $n \in \mathbb{N}$, I_n stands for the identity matrix of size $n \times n$. We use $^\top$ for transpose, $\otimes$ for Kronecker product, $\operatorname{spec}(\cdot)$ for spectrum, $\|\cdot\|_F$ for Frobenius norm, and $\circ$ for composition operators, respectively. The Kronecker sum of an $m \times m$ matrix A and an $n \times n$ matrix B, is denoted as $A \oplus B \triangleq A \otimes I_m + I_n \otimes B$.

We use $\mathbb{E}_y[\cdot]$ for expectation with respect to the random vector y. When there is no potential confusion, we drop the subscript and use $\mathbb{E}[\cdot]$. We use $\mathrm{d}(\cdot)$ for the differential, and $\mathrm{D}(\cdot)$ for the Jacobian operator. For taking derivatives of matrix valued functions, we utilize the Jacobian identification rules (p. 199, Table 2 in [16]). We use $\delta(x)$ to denote Dirac delta at the origin.

The symbol $\mathbf{S}_n$ denotes the space of $n \times n$ symmetric matrices; and $\mathbf{S}_n^+$, an open subset of $\mathbf{S}_n$, denotes the cone of $n \times n$ symmetric positive definite matrices. Notice that $\mathbf{S}_n^+$ is a smooth differentiable manifold with tangent space $T_A\mathbf{S}_n^+ = \mathbf{S}_n$, where $A \in \mathbf{S}_n^+$. Matrix inequalities like $A \succ B$ are to be understood in Loewner partial order, *i.e.*, $A \succ B \Leftrightarrow A - B \succ 0$, meaning the matrix $A - B$ is positive-definite. We denote $\mathbb{R}^{n\times n} = \mathbf{M}_n$ as the Hilbert space of $n \times n$ matrices equipped with Frobenius inner product $\langle A, B\rangle \triangleq \operatorname{tr}\left(A^\top B\right)$. For each $A \in \mathbf{S}_n^+$, if we define the left and right multiplication operators as $\mathcal{L}_A X \triangleq AX$, and $\mathcal{R}_A X \triangleq XA$ respectively, where $X \in \mathbf{M}_n$, then we can introduce a Riemannian metric $g_A(X, Y) \triangleq \langle X, (\mathcal{L}_A \circ \mathcal{R}_A)^{-1} Y\rangle = \operatorname{tr}\left(A^{-1}XA^{-1}Y\right)$. Given $X, Y \in \mathbf{S}_n^+$, any C^1 curve $\gamma : [0,1] \mapsto \mathbf{S}_n^+$, connecting $\gamma(0) = X$ and $\gamma(1) = Y$, has length (as measured in $g_A(X,Y)$) equal to $L(\gamma) = \int_0^1 \| \gamma^{-\frac{1}{2}}(t)\gamma'(t)\gamma^{-\frac{1}{2}}(t) \|_F \,\mathrm{d}t$. The (minimal) geodesic is the shortest path

$$\begin{aligned}\gamma^*(t) &= \underset{\gamma(t)\in C^1[0,1]}{\operatorname{arginf}} \{L(\gamma) : \gamma(0) = X, \gamma(1) = Y\} \\ &= X^{\frac{1}{2}} \left(X^{-\frac{1}{2}} Y X^{-\frac{1}{2}}\right)^t X^{\frac{1}{2}}, \qquad 0 \le t \le 1.\end{aligned}$$

II. Problem formulation

Consider the controlled stochastic LTI system

$$\mathrm{d}x(t) = Ax(t)\,\mathrm{d}t + Bu(t)\,\mathrm{d}t + F\,\mathrm{d}w(t) \tag{1}$$

for all $t \in [0, t_1]$, where the state vector $x(t) \in \mathbb{R}^n$, the control vector $u(t) \in \mathbb{R}^m$, and the standard Wiener process $w(t) \in \mathbb{R}^\ell$. We wish to find state feedback $u : \mathbb{R}^n \times [0, t_1] \mapsto \mathbb{R}^m$ that solves

Problem 1:

$$\begin{aligned}&\min_{u(\cdot)\in\mathcal{U}} \varphi(\rho_1, \rho_d) + \mathbb{E}_x\left[\int_0^{t_1} x(t)^\top Q x(t) + u(t)^\top R u(t)\right] \mathrm{d}t \\ &\qquad \text{s.t. (1)},\ x(0) \sim \rho_0 = \mathcal{N}(\mu_0, S_0),\ \rho_d = \mathcal{N}(\mu_d, S_d),\end{aligned}$$

where the final time t_1 is fixed, $\mathcal{U}$ is the space of admissible controls, $0 \preceq Q \in \mathbf{S}_n$, $R \in \mathbf{S}_m^+$, the terminal state $x(t_1) \sim \rho_1$, and the terminal cost $\varphi(\rho_1, \rho_d) \equiv W^2(\rho_1, \rho_d)$, *i.e.*, the squared Wasserstein distance, which we explain next.

Remark 1: Notice that the $\mathbb{E}_x[\cdot]$ in the cost function in **Problem 1** remains even if $F = 0$ in (1), *i.e.*, when the controlled dynamics is a deterministic LTI system. In that case, the expectation operator is due to initial condition uncertainties. For the stochastic LTI case, state uncertainties stem from both initial conditions and process noise.

A. Wasserstein Terminal cost

Denoting the desired terminal random state vector associated with ρ_d as x_d (*i.e.*, $x_d \sim \rho_d$), the squared Wasserstein distance of order two (hereafter, Wasserstein distance) between ρ_1 and ρ_d, is defined as the minimum mean square error between the random vectors $x(t_1)$ and x_d, *i.e.*,

$$W^2(\rho_1, \rho_d) \triangleq \inf_{\rho\in\mathcal{P}_2(\rho_1,\rho_d)} \mathbb{E}_y\left[\| x(t_1) - x_d \|_2^2\right], \tag{2}$$

where $y \triangleq (x(t_1), x_d)^\top$. The infimum in (2) is taken over all joint PDFs ρ supported over $\mathbb{R}^{2n}$ with finite second moment, whose marginals are ρ_1 and ρ_d, *i.e.*,

$$\begin{aligned}\mathcal{P}_2(\rho_1, \rho_d) \triangleq \Bigg\{\rho(y) : \int_{\mathbb{R}^{2n}} \| y \|_2^2\, \rho(y)\,\mathrm{d}y < \infty, \\ \int_{\mathbb{R}^n} \rho(y)\mathrm{d}x_d = \rho_1, \int_{\mathbb{R}^n} \rho(y)\mathrm{d}x(t_1) = \rho_d\Bigg\}.\end{aligned} \tag{3}$$

The value of the squared Wasserstein distance has the interpretation [1], [17] of the minimum amount of work needed to morph one PDF to the other, and can be shown to be a metric on the manifold of PDFs. For $\rho_1 = \mathcal{N}(\mu_1, S_1)$ and $\rho_d = \mathcal{N}(\mu_d, S_d)$, (2) can be computed [18] in closed form

$$W^2(\rho_1,\rho_d) = \| \mu_1 - \mu_d \|_2^2 + \operatorname{tr}\left(S_1 + S_d - 2\left(\sqrt{S_d}\, S_1\, \sqrt{S_d}\right)^{\frac{1}{2}}\right). \quad (4)$$

Thus, the terminal cost is a non-negative real-valued function $W^2 : \mathcal{N} \times \mathcal{N} \mapsto \mathbb{R}^+$, where $\mathcal{N}$ denotes the space of Gaussian PDFs.

B. Assumptions

Throughout the remainder of this work, we make the following assumptions.

1) In equation (1), the pair (A, B) is controllable.
2) Perfect state measurements are available.
3) The control is of the form $u(x,t) = K(t)x + v(t)$, where $K(t) \in \mathbb{R}^{m\times n}$ is the feedback gain, and $v(t) \in \mathbb{R}^m$ is the feedforward control.

Since we assume affine control structure, the controls are parameterized by the time-varying real matrix-vector pair $(K(t), v(t))$, and let $\mathcal{U} \triangleq \mathbb{R}^{m\times n} \times \mathbb{R}^m$ denote the set of (unconstrained) admissible controls.

III. MAIN RESULTS

Due to the affine state feedback assumption, the state transition matrix for (1) is an affine transformation acting on $x(0) \sim \rho_0 = \mathcal{N}(\mu_0, S_0)$, and hence the state vector $x(t) \sim \mathcal{N}(\mu(t), S(t))$. Thus, we can recast the *infinite dimensional* optimal control **Problem 1** as a *finite dimensional* optimal control problem on the mean-covariance sufficient statistics, as follows.

Problem 1a:

$$\min_{(K(t),v(t))\in\mathcal{U}} W^2(\rho_1,\rho_d) + \mathbb{E}_x\left[\int_0^{t_1} x(t)^\top Q x(t) + (K(t)x(t)+v(t))^\top R (K(t)x(t)+v(t))\right] \mathrm{d}t \quad (5a)$$

s.t.

$$\dot{\mu}(t) = (A + BK(t))\mu(t) + Bv(t), \quad (5b)$$

$$\dot{S}(t) = (A + BK(t))S(t) + S(t)(A + BK(t))^\top + FF^\top, \quad (5c)$$

where the terminal cost $W^2(\rho_1,\rho_d)$ is given by (4). **Problem 1a** is an optimal control problem on the space of Gaussian PDFs $\mathcal{N} = \mathbb{R}^n \times \mathbf{S}_n^+$, in Bolza form. The *linear quadratic Gaussian density regulator* (LQGDR) is the solution of the optimal control **Problem 1a**. We next derive the necessary conditions for optimality by applying Pontryagin's Maximum Principle (PMP) [19], [20].

Proposition 1: The optimal control solving **Problem 1a** is $u^o(x,t) = K^o(t)x + v^o(t)$, where

$$K^o(t) = R^{-1}B^\top P(t), \quad (6)$$

$$v^o(t) = R^{-1}B^\top\big(z(t) - P(t)\mu(t)\big), \quad (7)$$

are the optimal feedback gain matrix, and feedforward control vector. Furthermore, $P(t) \in \mathbf{S}_n$ and $z(t) \in \mathbb{R}^n$ are, respectively, the covariance costate matrix and the mean costate vector, satisfying the pair of decoupled Hamiltonian differential equations

$$\begin{pmatrix}\dot{\mu}(t)\\ \dot{z}(t)\end{pmatrix} = \begin{bmatrix} A & BR^{-1}B^\top \\ Q & -A^\top\end{bmatrix}\begin{pmatrix}\mu(t)\\ z(t)\end{pmatrix}, \quad (8)$$

$$\dot{S}(t) = (A + BK^o)S(t) + S(t)(A + BK^o)^\top + FF^\top, \quad (9)$$

$$\dot{P}(t) = -A^\top P(t) - P(t)A - P(t)BR^{-1}B^\top P(t) + Q, \quad (10)$$

with split boundary conditions

$$\mu(0) = \mu_0, \qquad z(t_1) = -\frac{1}{2}\frac{\partial W^2}{\partial \mu_1}, \quad (11)$$

$$S(0) = S_0, \qquad P(t_1) = -\frac{\partial W^2}{\partial S_1}. \quad (12)$$

Proof: The *augmented Lagrangian*, or *pre-Hamiltonian* for **Problem 1a** is a functional $h : \mathbb{R}^n \times \mathbf{S}_n \times \mathbb{R}^n \times \mathbf{S}_n^+ \times \mathcal{U} \mapsto \mathbb{R}$, given by

$$h(\bar{z}, P, \mu, S, K, v) = \langle \bar{z}, (A + BK)\mu + Bv\rangle + \langle P, (A + BK)S + S(A + BK)^\top + FF^\top\rangle - \mathbb{E}_x\left[x^\top Q x + (Kx + v)^\top R(Kx + v)\right],$$

where $\bar{z} = 2z$. The optimal control (6), (7) are obtained from

$$(K^o, v^o) = \underset{(K,v)\in\mathcal{U}}{\operatorname{argmax}}\ h(z, P, \mu, S, K, v),$$

and the maximized Hamiltonian, constant along trajectories of (8), (9) and (10), is simply

$$\begin{aligned} H(z, P, \mu, S) &= h(z, P, \mu, S, K^o, v^o) \\ &= z^\top(2A\mu + BR^{-1}B^\top z) \\ &\quad + \langle P, (2A + BR^{-1}B^\top P)S + FF^\top\rangle \\ &\quad - \operatorname{tr}((S + \mu\mu^\top)Q). \end{aligned} \quad (13)$$

The ordinary differential equation (ODE) (10) for $P(t)$ is obtained from $\dot{P} = -\partial h/\partial S$ and substituting the optimal feedback gain (6). Similarly, the ODE (8) for $z(t)$ is obtained from $\dot{z} = -\partial h/\partial \mu$ and by applying the scaling $z = \frac{1}{2}\bar{z}$, and then substituting optimal controls (6), (7).

The final boundary conditions (11), (12) are a consequence of the fact that there are no terminal constraints. The maximized Hamiltonian (13) is nonnegative along solutions of (8), (9), (10) satisfying the final boundary conditions. ■

Remark 2: Notice that the necessary conditions remain valid for $F = 0$, *i.e.*, the deterministic case corresponding to control of the propagation of uncertainty in normally distributed initial conditions, c.f [11], [12].

Till now, our derivation of necessary conditions have followed closely the same for the standard LQG problem, resulting the same set of matrix-vector differential equations (8), (9), (10). However, significant difference appears in final costate boundary conditions (11) and (12).

In the LQG problem, the terminal cost functional $\varphi(t_1) = \mathbb{E}_x\left[x(t_1)^\top M x(t_1)\right] = \operatorname{tr}\left(S_1 M + \mu_1^\top M \mu_1\right)$, for a given weight matrix $M \in \mathbf{S}_n$. This yields $P(t_1) = -M$, a constant matrix, for the LQG problem, making the Riccati ODE (10) decoupled from the Lyapunov ODE (9), which simplifies the LQG solution. As we will show next, our boundary condition (12) would result $P(t_1)$ as a nonlinear function of S_1, thereby giving a boundary coupled system of Riccati and Lyapunov matrix ODEs.

A. Gradients of W^2

We observe that

$$\frac{\partial W^2}{\partial \mu_1} = \frac{\partial}{\partial \mu_1}\left(\left(\mu_1 - \mu_d\right)^\top \left(\mu_1 - \mu_d\right)\right) = 2\left(\mu_1 - \mu_d\right), \quad (14)$$

and

$$\frac{\partial W^2}{\partial S_1} = I_n \,-\, 2\,\frac{\partial}{\partial S_1}\mathrm{tr}\left(\left(\sqrt{S_d}\,S_1\,\sqrt{S_d}\right)^{\frac{1}{2}}\right). \quad (15)$$

To proceed further, we need the following lemma whose proof is deferred to Appendix (subsection B). The proof illustrates an appealing connection with the solution of matrix Lyapunov equation.

Lemma 1: For all $S_1, S_d \in \mathbf{S}_n^+$,

$$\frac{\partial}{\partial S_1}\,\mathrm{tr}\left(\left(\sqrt{S_d}\,S_1\,\sqrt{S_d}\right)^{\frac{1}{2}}\right) = \frac{1}{2}S_d^{\frac{1}{2}}\left(S_d^{-\frac{1}{2}}S_1^{-1}S_d^{-\frac{1}{2}}\right)^{\frac{1}{2}}S_d^{\frac{1}{2}}. \quad (16)$$

Remark 3: **(Geometric interpretation)** Given $S_1, S_d \in \mathbf{S}_n^+$, recall that the unique geodesic $\gamma^* : [0,1] \mapsto \mathbf{S}_n^+$, connecting $S_d, S_1^{-1} \in \mathbf{S}_n^+$, associated with the Riemannian metric $g_A\left(S_d, S_1^{-1}\right) = \mathrm{tr}\left(A^{-1}S_dA^{-1}S_1^{-1}\right)$, is

$$\begin{aligned}\gamma^*(t) &= S_d \,\#_t\, S_1^{-1} = S_d^{\frac{1}{2}}\left(S_d^{-\frac{1}{2}}S_1^{-1}S_d^{-\frac{1}{2}}\right)^t S_d^{\frac{1}{2}},\\ &= S_1^{-1}\,\#_{1-t}\,S_d = S_1^{-\frac{1}{2}}\left(S_1^{\frac{1}{2}}S_dS_1^{\frac{1}{2}}\right)^{1-t}S_1^{-\frac{1}{2}}.\end{aligned}$$

The midpoint of this geodesic is defined as the *geometric mean* [21]–[23] between the endpoint matrices $\gamma(0) = S_d$ and $\gamma(1) = S_1^{-1}$, denoted as $S_d \,\#\, S_1^{-1} \triangleq S_d \,\#_{\frac{1}{2}}\, S_1^{-1} = S_1^{-1}\,\#_{\frac{1}{2}}\,S_d = \gamma(\frac{1}{2})$. Therefore, from Lemma 1 and (15), we have

$$\frac{\partial W^2}{\partial S_1} = I_n \,-\, S_d \,\#\, S_1^{-1}. \quad (17)$$

Remark 4: **(Simplification when S_1 and S_d commute)** In case S_1 and S_d commute, then from (4) $W^2 = \parallel \mu_1 - \mu_d \parallel_2^2 + \parallel S_1 - S_d \parallel_F^2$, and $\dfrac{\partial W^2}{\partial S_1} = 2\left(S_1 - S_d\right)$, where the last equality follows from Lemma 2 in Appendix. However, from a practical point of view, S_1 and S_d need not commute for density control, and hence we will not work with this algebraic simplification any further.

Using (14) and (17), we can now rewrite the boundary conditions (11) and (12) as

$$\mu(0) = \mu_0, \qquad z(t_1) = \mu_d - \mu_1, \quad (18)$$

$$S(0) = S_0, \qquad P(t_1) = S_d \,\#\, S_1^{-1} \,-\, I_n. \quad (19)$$

This nonlinear coupling at the final time between the covariance and its costate introduces significant challenges to either direct or indirect methods for solving the resulting 2PBVP. In Section IV we will numerically solve the two point boundary value problem (2PBVP) (8), (9), (10), (18), (19) via shooting method. Before proceeding to examples, we now demonstrate that the classical finite horizon LQG optimal controller can be recovered in the Dirac limit of our LQGDR.

B. LQG Controller is A Special Case of LQGDR

We would like to prove that in the limit $\rho_d = \mathcal{N}\left(\mu_d, S_d\right) \to \delta\left(x\right)$, the LQGDR reduces to the finite horizon LQG controller. To this end, we first generalize the terminal cost (2) as follows.

Definition 1: (**Weighted Wasserstein distance**) For a given matrix $M \in \mathbf{S}_n$, the *weighted Wasserstein distance* W_M between two PDFs ρ_1 and ρ_d, is defined as the minimum *weighted* mean square error between the corresponding random vectors $x\left(t_1\right)$ and x_d, *i.e.*,

$$W_M^2\left(\rho_1, \rho_d\right) \triangleq \inf_{\rho \in \mathcal{P}_2\left(\rho_1, \rho_d\right)} \mathbb{E}_y\left[\left(x\left(t_1\right) - x_d\right)^\top M\left(x\left(t_1\right) - x_d\right)\right],$$

where $y \triangleq \left(x\left(t_1\right), x_d\right)^\top$, and $\mathcal{P}_2\left(\rho_1, \rho_d\right)$ is defined in (3). Clearly, $W_M = W$ for $M = I_n$.

To intuitively see why our claim about LQG recovery is true, notice that in the limit $\rho_d \to \delta\left(x_d\right) \Rightarrow x_d = 0$ a.s. Consequently, the LQGDR cost function with weighted Wasserstein terminal cost

$$\begin{aligned}&\inf_{\rho \in \mathcal{P}_2\left(\rho_1, \rho_d\right)} \mathbb{E}_y\left[\left(x\left(t_1\right) - x_d\right)^\top M\left(x\left(t_1\right) - x_d\right)\right]\\ &\qquad + \mathbb{E}_x\left[\int_0^{t_1}\left(x(t)^\top Qx(t) + u(t)^\top Ru(t)\right)\mathrm{d}t\right]\end{aligned}$$

reduces to the LQG cost function

$$\mathbb{E}_x\left[x\left(t_1\right)^\top Mx\left(t_1\right) + \int_0^{t_1}\left(x(t)^\top Qx(t) + u(t)^\top Ru(t)\right)\mathrm{d}t\right],$$

since $\mathcal{P}_2\left(\rho_1, \delta(x_d)\right) = \{\rho_1\delta\left(x_d\right)\}$, and as a result the LQGDR terminal cost becomes

$$\begin{aligned}&\inf_{\rho \in \mathcal{P}_2 \in \left(\rho_1, \delta\left(x_d\right)\right)} \mathbb{E}_y\left[x\left(t_1\right)^\top Mx\left(t_1\right)\right]\\ =\;& \int_{\mathbb{R}^{2n}} x\left(t_1\right)^\top Mx\left(t_1\right)\rho_1(x(t_1))\delta(x_d)\,\mathrm{d}x(t_1)\mathrm{d}x_d\\ =\;& \int_{\mathbb{R}^n} x\left(t_1\right)^\top Mx\left(t_1\right)\rho_1(x(t_1))\,\mathrm{d}x(t_1)\\ =\;& \mathbb{E}_x\left[x\left(t_1\right)^\top Mx\left(t_1\right)\right], \qquad \text{a.s.}\end{aligned}$$

This establishes that the LQGDR *problem* reduces to the LQG *problem* in the limit $\rho_d \to \delta(x_d)$. In the following, we directly prove the *solution* equivalence.

Theorem 1: In the limit $\rho_d = \mathcal{N}\left(\mu_d, S_d\right) \to \delta\left(x_d\right)$, the 2PBVP for LQGDR with weighted Wasserstein terminal cost, is same as the 2PBVP for LQG, for fixed $M \in \mathbf{S}_n$.

Proof: It suffices to prove that in the said limit, $P_{\text{LQGDR}}\left(t_1\right) = P_{\text{LQG}}\left(t_1\right)$, and $z_{\text{LQGDR}}\left(t_1\right) = z_{\text{LQG}}\left(t_1\right)$. The LQG terminal cost $\varphi(t_1) = \mathrm{tr}\left(S_1M + \mu_1^\top M\mu_1\right)$ yields the well-known LQG costate boundary conditions $P_{\text{LQG}}\left(t_1\right) = -M$, and $z_{\text{LQG}}\left(t_1\right) = -M\mu_1 = P_{\text{LQG}}\left(t_1\right)\mu_1$. To derive the corresponding LQGDR costate boundary conditions, we need a closed-form expression for $W_M^2\left(\rho_1, \rho_d\right)$ akin to (4).

Consider the zero mean random vectors $\bar{x}_d \triangleq x_d - \mu_d$, and $\bar{x}_1 \triangleq x(t_1) - \mu_1$. Since $x\left(t_1\right) - x_d = \left(\bar{x}_1 - \bar{x}_d\right) + \left(\mu_1 - \mu_d\right)$, we have

$$\begin{aligned}
&\mathbb{E}\left[(x(t_1) - x_d)^\top M (x(t_1) - x_d)\right] \\
&= (\mu_1 - \mu_d)^\top M (\mu_1 - \mu_d) + \mathbb{E}[(\bar{x}_1 - \bar{x}_d)^\top M (\bar{x}_1 - \bar{x}_d)] \\
&= (\mu_1 - \mu_d)^\top M (\mu_1 - \mu_d) + \mathbb{E}[\mathrm{tr}\left((\bar{x}_1 - \bar{x}_d)(\bar{x}_1 - \bar{x}_d)^\top M\right)] \\
&= (\mu_1 - \mu_d)^\top M (\mu_1 - \mu_d) + \mathrm{tr}\left((S_1 + S_d - 2C) M\right), \qquad (20)
\end{aligned}$$

where $C \triangleq \mathbb{E}[\bar{x}_1 \bar{x}_d^\top]$. From Definition 1 and (20), we arrive at the optimization

$$\min_{C \in \mathbb{R}^{n \times n}} \mathrm{tr}\left((S_1 + S_d - 2C) M\right) \quad \text{s.t.} \quad \begin{bmatrix} S_1 & C \\ C^\top & S_d \end{bmatrix} \succeq 0.$$

Since $M \in \mathbf{S}_n$ is fixed, by Schur complement lemma, the above is equivalent to

$$\max_{C \in \mathbb{R}^{n \times n}} \mathrm{tr}(C) \qquad \text{s.t.} \qquad S_1 - C S_d^{-1} C^\top \succeq 0. \tag{21}$$

The optimiziation (21) has known [18], [24] maximizer $C^* = S_1 S_d^{\frac{1}{2}} \left(S_d^{\frac{1}{2}} S_1 S_d^{\frac{1}{2}}\right)^{-\frac{1}{2}} S_d^{\frac{1}{2}}$, and hence

$$\begin{aligned}
W_M^2 &= (\mu_1 - \mu_d)^\top M (\mu_1 - \mu_d) \\
&+ \mathrm{tr}\left(\left(S_1 + S_d - 2\left[\sqrt{S_d} S_1 \sqrt{S_d}\right]^{\frac{1}{2}}\right) M\right) \qquad (22)
\end{aligned}$$

From (22), we deduce that

$$\begin{aligned}
&\mathrm{d}\, \mathrm{tr}\left((\mu_1 - \mu_d)^\top M (\mu_1 - \mu_d)\right) \\
=\ & \mathrm{tr}\left[(\mathrm{d}\mu_1)^\top M (\mu_1 - \mu_d) + (\mu_1 - \mu_d)^\top M (\mathrm{d}\mu_1)\right] \\
=\ & 2\, \mathrm{tr}\left[(\mu_1 - \mu_d)^\top M (\mathrm{d}\mu_1)\right], \qquad (23)
\end{aligned}$$

that results $\dfrac{\partial W_M^2}{\partial \mu_1} = \left(2(\mu_1 - \mu_d)^\top M\right)^\top = 2M(\mu_1 - \mu_d)$, and hence

$$z_{\mathrm{LQGDR}}(t_1) = -\frac{1}{2} \frac{\partial W_M^2}{\partial \mu_1} = M(\mu_d - \mu_1), \tag{24}$$

$$\Rightarrow \lim_{(\mu_d, S_d) \to (0,0)} z_{\mathrm{LQGDR}}(t_1) = -M\mu_1 = z_{\mathrm{LQG}}(t_1). \tag{25}$$

On the other hand, we have

$$\begin{aligned}
&\mathrm{d}\, \mathrm{tr}\left(\left(S_1 + S_d - 2\left[\sqrt{S_d} S_1 \sqrt{S_d}\right]^{\frac{1}{2}}\right) M\right) \\
=\ & \mathrm{tr}\left(\left(\mathrm{d}\left(S_1 + S_d - 2\left[\sqrt{S_d} S_1 \sqrt{S_d}\right]^{\frac{1}{2}}\right)\right) M\right) \\
=\ & \mathrm{tr}\left(\mathrm{D}\left(S_1 + S_d - 2\left[\sqrt{S_d} S_1 \sqrt{S_d}\right]^{\frac{1}{2}}\right) (\mathrm{d}S_1) M\right) \\
=\ & \mathrm{tr}\left(M\, \mathrm{D}\left(S_1 + S_d - 2\left[\sqrt{S_d} S_1 \sqrt{S_d}\right]^{\frac{1}{2}}\right) (\mathrm{d}S_1)\right),
\end{aligned}$$

giving $\dfrac{\partial W_M^2}{\partial S_1} = \left(\mathrm{D}\left(S_1 + S_d - 2\left[\sqrt{S_d} S_1 \sqrt{S_d}\right]^{\frac{1}{2}}\right)\right)^\top M$.
From (17), we know $\left(\mathrm{D}\left(S_1 + S_d - 2\left[\sqrt{S_d} S_1 \sqrt{S_d}\right]^{\frac{1}{2}}\right)\right)^\top$ $= I_n - S_d \# S_1^{-1}$, and hence

$$P_{\mathrm{LQGDR}}(t_1) = -\frac{\partial W_M^2}{\partial S_1} = \left(S_d \# S_1^{-1} - I_n\right) M, \tag{26}$$

$$\Rightarrow \lim_{(\mu_d, S_d) \to (0,0)} P_{\mathrm{LQGDR}}(t_1) = 0 - M = P_{\mathrm{LQG}}(t_1). \tag{27}$$

Equations (25) and (27) conclude the proof. ∎

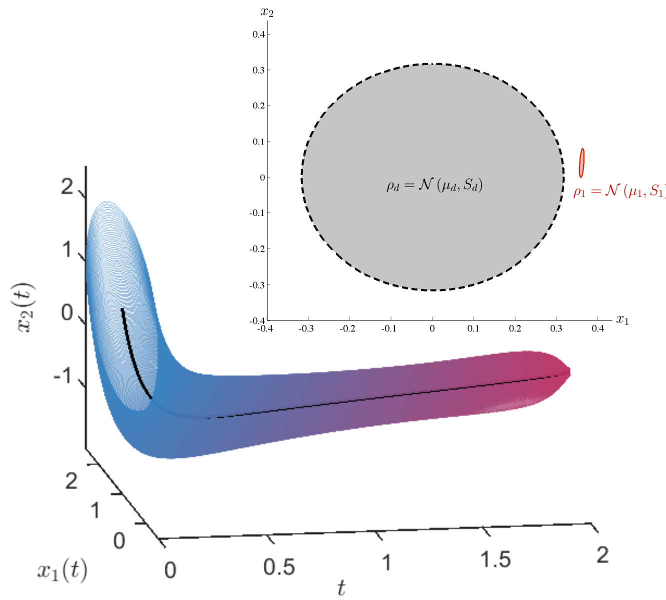

Fig. 2. The controlled evolution of the state statistics from the initial PDF $\rho_0 = \mathcal{N}\left((1,1)^\top, I_2\right)$ (*blue*) to the final PDF $\rho_1 = \mathcal{N}(\mu_1, S_1)$ (*red*) is plotted with the 1-σ covariance ellipses illustrating the evolution of the sufficient statistics $(\mu(t), S(t))$ over time $t \in [0, 2]$. The mean evolution is shown in *black*. The *inset plot* shows the desired (*dashed black boundary*) and actual (*solid red boundary*) terminal Gaussian PDFs' 1-σ covariance ellipses, showing the mismatch at $t = t_1$.

IV. Numerical Example

Consider the controllable linear stochastic system (1) with system matrices

$$A = \begin{bmatrix} 0 & 1 \\ 2 & -3 \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad F = \begin{bmatrix} 0.01 \\ 0.01 \end{bmatrix}, \tag{28}$$

and cost function weighting matrices $Q = 100\, I_2$, $R = 1$. We take the initial PDF to be normal $\rho_0 = \mathcal{N}\left((1,1)^\top, I_2\right)$, and the desired terminal Gaussian PDF $\rho_d = \mathcal{N}(0, 0.1\, I_2)$.

We use a shooting method to solve 2PBVP (9), (10), (19), in which the covariance costate $P(t)$ is integrated backwards in time, and then the covariance $S(t)$ is integrated forwards in time. The 2PBVP for the Hamiltonian system (8), (18) is solved independently.

As Figure 2 illustrates, the large values on the diagonal of Q ensure that the 1-σ error ellipses of the covariance converge with little "overshoot" to a covariance close to the desired, while the small desired covariance ($S_d = 0.1\, I_2$) ensures a small spread in the final covariance $S_1 = \left(\begin{smallmatrix} 3\text{e-}5 & 1\text{e-}4 \\ 1\text{e-}4 & 1.7\text{e-}3 \end{smallmatrix}\right)$ about mean $\mu_1 = (3.6\text{e-}1,\ 3.87\text{e-}2)^\top$. The maximized Hamiltonian (13) is $H = 0.1252$, which confirms that we have converged at least to a local optimum. The expected optimal control trajectory is shown in Figure 3.

V. Conclusions

In this paper, we have formulated and solved a generalization of the standard linear quadratic Gaussian (LQG) control problem, where instead of steering the terminal state close to the origin, we steered the state statistics close to a desired statistics. It is shown that for Gaussian initial and desired

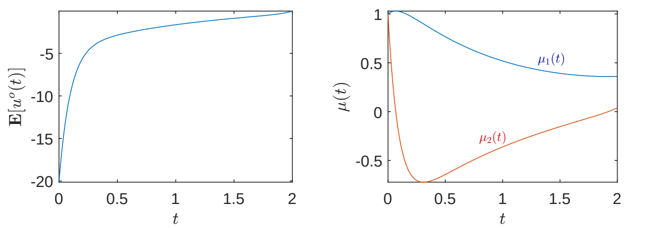

Fig. 3. The expected optimal control $\mathbb{E}[u^o(t)] = K^o\mu(t) + v^o(t)$ (*left*) and controlled mean evolution $\mu(t)$ (*right*) for system (28), under LQGDR proposed in this paper. The large initial value for the unconstrained optimal controls tapers off as the system approaches the desired mean (μ_d) and covariance (S_d).

terminal statistics, under affine state feedback, this problem can be cast as a finite dimensional optimal control problem with a terminal cost modeled through Wasserstein metric. We derived the resulting two point boundary value problem, which unlike the LQG case, leads to nonlinearly coupled boundary conditions between the covariance and covariance costate. It is shown that in the Dirac limit of desired terminal statistics, we recover the standard LQG control problem. A numerical example has been worked out to elucidate our formulation. Future work will address the optimality of the affine state feedback strategy. Another planned direction of investigation is the joint estimation-density control problem with noisy measurements.

References

[1] A. Halder, and R. Bhattacharya, "Geodesic Density Tracking with Applications to Data Driven Modeling". *Proceedings of the American Control Conference*, pp. 616–621, 2014.

[2] K.J. Åström, *Introduction to Stochastic Control Theory*. Academic Press, New York; 1970.

[3] S. Bandyopadhyay, Soon-Jo Chung, and F.Y. Hadaegh, "Probabilistic Swarm Guidance using Optimal Transport". *Proceedings of the IEEE Conference on Control Applications (CCA)*, pp. 498–505, 2014.

[4] B. Açıkmeşe, and D.S. Bayard, "Markov Chain Approach to Probabilistic Guidance for Swarms of Autonomous Agents". *Asian Journal of Control*, Vol. 17, No. 4, pp. 1105–1124, 2014.

[5] L.C.A. Pimenta, N. Michael, R.C. Mesquita, G.A.S. Pereira, and V. Kumar, "Control of Swarms Based on Hydrodynamic Models". *Proceedings of the IEEE International Conference on Robotics and Automation (ICRA)*, pp. 1948–1953, 2008.

[6] J.-S. Li, and N. Khaneja, "Ensemble Control of Bloch Equations". *IEEE Transactions on Automatic Control*, Vol. 54, No. 3, pp. 528–536, 2009.

[7] H. Wang, H. Baki, and P. Kabore, "Control of Bounded Dynamic Stochastic Distributions using Square Root Models: An Applicability Study in Papermaking Systems". *Transactions of the Institute of Measurement and Control*, Vol. 23, No. 1, pp. 51–68, 2001.

[8] R.D. Braatz, "Advanced Control of Crystallization Processes". *Annual Reviews in Control*, Vol. 26, No. 1, pp. 87–99, 2002.

[9] Y. Wang, and F.J. Doyle, "Reachability of Particle Size Distribution in Semibatch Emulsion Polymerization". *AIChE Journal*, Vol. 50, No. 12, pp. 3049–3059, 2004.

[10] Y. Chen, T. Geogiou, and M. Pavon, "Optimal Steering of A Linear Stochastic System to A Final Probability Distribution. Part I". *arXiv:1408:2222*, 2014.

[11] R.W. Brockett, "Optimal Control of the Liouville Equation". *AMS IP Studies in Advanced Mathematics*, Vol. 39, pp. 23–35, 2007.

[12] R.W. Brockett, "Notes on the Control of the Liouville Equation". *Control of Partial Differential Equations*, pp. 101–129, 2012.

[13] S.S. Mazurenko, "The Dynamic Programming Method in Systems with States in the Form of Distributions". *Moscow University Computational Mathematics and Cybernetics*, Vol. 35, No. 3, pp. 133–141, 2011.

[14] Y. Chen, T. Geogiou, and M. Pavon, "Optimal Steering of A Linear Stochastic System to A Final Probability Distribution. Part II". *arXiv:1410:3447*, 2014.

[15] J.D. Benamou, and Y. Brenier, "A Computational Fluid Mechanics Solution to the Monge-Kantorovich Mass Transfer Problem". *Numerische Mathematik*, Vol. 84, no. 3, pp. 375–393, 2000.

[16] J.R. Magnus, and H. Neudecker, *Matrix Differential Calculus with Applications in Statistics and Econometrics*. John Wiley & Sons, Third edition; 2007.

[17] C. Villani, *Topics in Optimal Transportation*. No. 58, American Mathematical Society, 2003.

[18] C.R. Givens, and R.M. Shortt, "A Class of Wasserstein Metrics for Probability Distributions". *The Michigan Mathematical Journal*, Vol. 31, No. 2, pp. 231–240, 1984.

[19] L.S. Pontryagin, V.G. Boltyanskii, R.V. Gamkrelidze, and E.F. Mischenko, *The Mathematical Theory of Optimal Processes*. John Wiley & Sons Inc., 1962.

[20] A.A. Agrachev, and Y. Sachkov, *Control Theory from the Geometric Viewpoint*. Springer, 2004.

[21] W. Pusz, and S.L. Woronowicz, "Functional Calculus for Sesquilinear Forms and the Purification Map". *Reports on Mathematical Physics*, Vol. 8, No. 2, pp. 159–170, 1975.

[22] T. Ando, C.K. Li, and R. Mathias, "Geometric Means". *Linear Algebra and Its Applications*, Vol. 385, pp. 305–334, 2004.

[23] R. Bhatia, *Positive Definite Matrices*. Princeton Series in Applied Mathematics. Princeton University Press, Princeton, NJ; 2007.

[24] S.T. Rachev, and L. Rüschendorf, *Mass Transportation Problems. Vol. 1: Theory*. Springer-Verlag; 1998.

[25] J.W. Brewer, "Kronecker Products and Matrix Calculus in System Theory". *IEEE Transactions on Circuits and Systems*, Vol. 25, No. 9, pp. 772–781, 1978.

[26] Daniel Liberzon. *Calculus of Variations and Optimal Control Theory: A Concise Introduction*. Princeton University Press, 2012.

[27] D.S. Bernstein, *Matrix Mathematics: Theory, Facts, and Formulas*. Princeton University Press, Second ed., 2009.

Appendix

A. Preparatory Lemmas

Lemma 2: $\dfrac{\partial}{\partial S_1}\text{tr}\left((S_1 - S_d)(S_1 - S_d)^\top\right) = 2\,(S_1 - S_d)$.

Proof: Since

$$\begin{aligned}
& \mathrm{d}\,\text{tr}\left((S_1 - S_d)^\top (S_1 - S_d)\right) \\
= \;& \text{tr}\left((\mathrm{d}\,(S_1 - S_d))^\top (S_1 - S_d) \;+\; (S_1 - S_d)^\top\; \mathrm{d}\,(S_1 - S_d)\right) \\
= \;& \text{tr}\left((\mathrm{d}S_1)^\top (S_1 - S_d)\right) \;+\; \text{tr}\left((S_1 - S_d)^\top\; \mathrm{d}S_1\right) \\
= \;& 2\,\text{tr}\left((S_1 - S_d)^\top\; \mathrm{d}S_1\right),
\end{aligned}$$

from the Jacobian identification rule, we have $\dfrac{\partial}{\partial S_1}\text{tr}\left((S_1 - S_d)(S_1 - S_d)^\top\right) = \left(2\,(S_1 - S_d)^\top\right)^\top$. ■

Lemma 3: Square root of a positive definite matrix is unique positive definite.

Proof: Since $M \succ 0$ iff its symmetric part $N \triangleq \frac{M+M^\top}{2} \succ 0$, hence we have to show that $M = AA$ implies $\frac{A+A^\top}{2} \succ 0$. This follows from the positive definiteness of $N = \frac{AA+A^\top A^\top}{2}$. The uniqueness can be proved by contradiction. We skip the details for brevity. ■

Lemma 4: Square root of a symmetric positive definite matrix is itself symmetric.

Proof: Consider $M \in \mathbf{S}_n^+$, which by Lemma 3, has unique square root $\sqrt{M} = A$ (say). Thus, $AA = M$. Taking transpose to both sides, we get $A^\top A^\top = M^\top = M$. Suppose $A^\top = B \neq A$, which implies $BB = M$, meaning B is also a square root of M, contradicting the uniqueness. As a result, $A = B = A^\top$. Hence the statement. ■

Lemma 5: For $X \in \mathbf{S}_n^+$, let $G(X) \triangleq \sqrt{X}$. Then $\mathrm{D}G(X) = \left(\sqrt{X} \oplus \sqrt{X}\right)^{-1}$.

Proof: We start with slightly general setting by taking arbitrary $X \succ 0$, not necessarily symmetric. Taking differential $\mathrm{d}\left(\cdot\right)$ to both sides of the equation $\sqrt{X}\sqrt{X} = X$ results a special case of Sylvester equation

$$\left(\mathrm{d}\sqrt{X}\right)\sqrt{X} \;+\; \sqrt{X}\left(\mathrm{d}\sqrt{X}\right) \;=\; \mathrm{d}X, \tag{29}$$

that can be solved for the differential matrix $\mathrm{d}\sqrt{X}$ as

$$\begin{aligned} \mathrm{vec}\left(\mathrm{d}\sqrt{X}\right) &= \left(\sqrt{X}^{\top} \oplus \sqrt{X}\right)^{-1} \mathrm{vec}\left(\mathrm{d}X\right) \\ \Rightarrow \mathrm{d}\,\mathrm{vec}\left(G(X)\right) &= \left(\sqrt{X}^{\top} \oplus \sqrt{X}\right)^{-1} \mathrm{d}\,\mathrm{vec}\left(X\right) \end{aligned} \tag{30}$$

Since $X \succ 0$, hence $\sqrt{X}$ is unique and $\succ 0$. Consequently, the Kronecker sum in (30) is $\succ 0$ (thus non-singular). From (30), the Jacobian identification rule results $\mathrm{D}G\left(X\right) = \left(\sqrt{X}^{\top} \oplus \sqrt{X}\right)^{-1}$, where the transpose can be dropped by specializing $X \in \mathbf{S}_n^+$. ■

Lemma 6: Let $F\left(X\right) \triangleq AXB$. Then $\mathrm{D}F\left(X\right) = B^{\top} \otimes A$.

Proof: $F\left(X\right) = AXB \Rightarrow \mathrm{d}F(X) = A\,\mathrm{d}X\,B$. Taking $\mathrm{vec}(\cdot)$ on both sides, and using the fact that $\mathrm{vec}(\cdot)$ and $\mathrm{d}(\cdot)$ operators commute, we get

$$\begin{aligned} \mathrm{vec}\left(\mathrm{d}\,F(X)\right) &= \mathrm{vec}\left(A\,\mathrm{d}X\,B\right) \\ \Rightarrow \mathrm{d}\,\mathrm{vec}\,F(X) &= \left(B^{\top} \otimes A\right)\,\mathrm{vec}\left(\mathrm{d}X\right) \qquad (31) \\ &= \left(B^{\top} \otimes A\right)\,\mathrm{d}\,\mathrm{vec}\left(X\right), \qquad (32) \end{aligned}$$

where the RHS of (31) follows from the identity $\mathrm{vec}\left(PQR\right) = \left(R^{\top} \otimes P\right)\,\mathrm{vec}(Q)$. The Jacobian identification rule applied on (32), results $\mathrm{D}F\left(X\right) = B^{\top} \otimes A$. ■

B. Proof of Lemma 1

Let us introduce $R_d \triangleq \sqrt{S_d}$, $H\left(S_1\right) \triangleq \left(R_d S_1 R_d\right)^{\frac{1}{2}} \triangleq G \circ F(S_1)$, where $G(S_1) \triangleq \sqrt{S_1}$, and $F(S_1) \triangleq R_d S_1 R_d$. Also, let $\phi(S_1) \triangleq \mathrm{tr}(H(S_1))$, and $Y \triangleq \frac{\partial \phi}{\partial S_1}$. Our objective is to compute Y. We start with the identity $\mathrm{tr}\left(A^{\top}B\right) = \left(\mathrm{vec}\left(A\right)\right)^{\top}\mathrm{vec}\left(B\right)$, wherein we set $A \equiv I_n$, $B \equiv \mathrm{d}H(S_1)$, to obtain

$$\begin{aligned} \mathrm{tr}\left(\mathrm{d}H(S_1)\right) &= \left(\mathrm{vec}\left(I_n\right)\right)^{\top}\mathrm{vec}\left(\mathrm{d}H(S_1)\right) \\ \Rightarrow \mathrm{d}\,\mathrm{tr}\left(H(S_1)\right) &= \left(\mathrm{vec}\left(I_n\right)\right)^{\top}\mathrm{d}\,\mathrm{vec}\left(H(S_1)\right) \\ \Rightarrow \mathrm{d}\phi\left(S_1\right) &= \left(\mathrm{vec}\left(I_n\right)\right)^{\top}\mathrm{D}H(S_1)\,\mathrm{d}\,\mathrm{vec}\left(S_1\right) \\ &= \left(\mathrm{vec}\left(I_n\right)\right)^{\top}\mathrm{D}G(F(S_1))\,\mathrm{D}F(S_1)\,\mathrm{d}\,\mathrm{vec}\left(S_1\right), \end{aligned}$$

where the last step is the chain rule for Jacobians. Using Lemma 5 and 6, the above yields

$$\mathrm{d}\phi(S_1) = \left(\mathrm{vec}\left(I_n\right)\right)^{\top}\left(\sqrt{R_d S_1 R_d} \oplus \sqrt{R_d S_1 R_d}\right)^{-1} \left(R_d \otimes R_d\right)\,\mathrm{d}\,\mathrm{vec}(S_1). \tag{33}$$

On the other hand, by virtue of the definition $Y \triangleq \dfrac{\partial \phi}{\partial S_1}$, we must have

$$\mathrm{d}\phi(S_1) = \left(\mathrm{vec}\left(Y\right)\right)^{\top}\,\mathrm{d}\,\mathrm{vec}\left(S_1\right). \tag{34}$$

Comparing the RHS of (33) and (34), and letting $Z \triangleq \sqrt{R_d S_1 R_d}$, we get

$$\begin{aligned} \mathrm{vec}\left(Y\right) &= \left(R_d \otimes R_d\right)\left(Z \oplus Z\right)^{-1}\mathrm{vec}\left(I_n\right) \\ \Rightarrow \left(R_d^{-1} \otimes R_d^{-1}\right)\mathrm{vec}\left(Y\right) &= \left(Z \oplus Z\right)^{-1}\mathrm{vec}\left(I_n\right), \end{aligned} \tag{35}$$

where we have used the fact [25] that inverse of Kronecker product is the Kronecker product of inverses. Next, invoking the identity $\left(C^{\top} \otimes A\right)\,\mathrm{vec}(B) = \mathrm{vec}\left(ABC\right)$, we now rewrite the LHS of (35) as $\mathrm{vec}\left(\Upsilon\right)$, where $\Upsilon \triangleq R_d^{-1} Y R_d^{-1}$. Thus, solving (35) for Y, reduces to solving

$$\mathrm{vec}\left(\Upsilon\right) = \left(Z \oplus Z\right)^{-1}\mathrm{vec}\left(I_n\right) \tag{36}$$

for Υ. However, equation (36) has one-to-one correspondence with the following special case of Sylvester equation

$$Z\Upsilon + \Upsilon Z = I_n, \tag{37}$$

and hence we can solve for Υ from the linear matrix equation (37), in lieu of the linear matrix-vector equation (36). At this point, we realize (37) is actually a special (self-adjoint) case of Lyapunov equation, which in turn, is a special case of Sylvester equation. Since $Z \succ 0$, and $-Z \prec 0$, we have $\mathrm{spec}\left(Z\right) \cap \mathrm{spec}\left(-Z\right) = \emptyset$, thus ensuring (p. 444, Corollary 7.2.5 in [27]) that (37) has a *unique* solution, given by the infinite horizon Grammian

$$\Upsilon = \int_0^{\infty} e^{-tZ}\,I_n\,e^{-tZ}\,\mathrm{d}t = \int_0^{\infty} e^{-2tZ}\,\mathrm{d}t = \left(2Z\right)^{-1}. \tag{38}$$

Reverting back to the original unknown Y, (38) yields $R_d^{-1} Y R_d^{-1} = \dfrac{1}{2}\left(R_d S_1 R_d\right)^{-\frac{1}{2}}$, which implies

$$Y = \frac{1}{2} R_d \left(R_d S_1 R_d\right)^{-\frac{1}{2}} R_d = \frac{1}{2} R_d \left(R_d^{-1} S_1^{-1} R_d^{-1}\right)^{\frac{1}{2}} R_d,$$

thus completing the proof. ■