A fixed-point characterization of the optimal costate in finite-horizon optimal control problems

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Abstract—A fixed-point characterization of the optimal costate in finite-horizon optimal control problems for non-linear systems is presented. It is shown that the *optimal* initial condition of the costate variable must be a fixed-point, for any time, of the composition of the forward and backward flows of the underlying Hamiltonian dynamics. Such an abstract property is then translated into a constructive condition by relying on a sequence of repeated Lie brackets involving the Hamiltonian dynamics and evaluated at a single point in the state-space. This leads to a system of algebraic equations in the unknown initial *optimal* costate that allows achieving a desired degree of accuracy of the approximation while always consisting of a number of equations equal to the dimension of the state of the underlying system, regardless of the achieved accuracy. A dual characterization of the optimal terminal value of the state is also discussed, together with a few computational aspects of the proposed strategy.

I. INTRODUCTION

One of the most classical control problem consists in steering the state of the underlying controlled plant from an initial condition - *e.g.* deriving from a perturbation of a nominal operating condition or from a prescribed shift of the corresponding working point for the system - to a desired final condition or equilibrium point. It is therefore natural that tools and strategies capable of achieving such a control objective in an *optimal* way would have attracted intensive research interest in the past decades, see *e.g.* [1], [2], [3], [4], [5], [6], [7]. The above control task can be naturally formulated as an *infinite-horizon optimal control* problem [8], provided the time available to perform the steering is sufficiently large, compared to the time-scales of the underlying plant. Interestingly, whenever it is instead crucial to complete the control task within a prescribed time interval, fixed *a priori*, while less attention is paid to the value of the state at the end of such an interval, the structure of the solution to such

a seemingly similar problem becomes notably different, being for instance intrinsically time-varying [5].

Despite such differences two main strategies, common to the so-called infinite-horizon and finite-horizon optimal control problems, have been introduced and deeply explored in the second half of the last century, *i.e.* Dynamic Programming (DP), see *e.g.* [2], [9], and Pontryagin's Minimum (or Maximum) Principle (PMP) [10].

The former approach characterizes the optimal feedback in terms of the solution to a certain quadratic partial differential equation (PDE), *i.e.* the so-called Hamilton-Jacobi-Bellman (HJB) equation [4]. Methods inspired by DP are particularly appealing since they provide necessary and sufficient conditions for optimality and permit the characterization of the optimal solution, as well as of the optimal cost, for any initial condition in the state-space. In the case of infinite-horizon control problems strategies to approximate the optimal control law have been envisioned, see *e.g.* [11], [12], [13], [14], [15], [16], [17], [18]. Along a different line to circumvent the computational issues arising in the solution of the HJB equation, an alternative (weaker) notion of solution has been proposed in the case of non-differentiable value functions, see *e.g.* [19], [20], introducing the notion of *viscosity solution* of the HJB equation. However, in the case of finite-horizon optimal control problems the task of determining a closed-form expression for the solution to the HJB PDE is further complicated by the intrinsic dependence of the value function on time.

On the other hand, methods based on the PMP provide - without additional conditions, such as convexity - only necessary conditions for optimality. As a consequence such strategies may be employed only to identify *candidate* optimal solutions or *extremals*. Moreover, the characterization of the optimal control law heavily relies on the knowledge of the initial condition of the state of the system even for infinite-horizon control problems, hence essentially leading to *open-loop* strategies. Nonetheless, the wide-spread use of such strategies is essentially motivated by the simplicity of the underlying conditions, provided in terms of *ordinary differential equations* (instead of partial differential equations) that should be satisfied by the optimal process together with an auxiliary variable (the *costate*). While in the case of infinite-horizon problems determining the correct boundary conditions for such a dynamical system essentially requires to compute an explicit solution to the HJB PDE, hence recovering the computational complexity of the DP approach, in the case of finite horizon optimal control problems it can be recast in

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terms of a *two-point boundary value problem* (TPBVP) for a nonlinear system.

As a consequence, intensive research efforts have been devoted to the design of efficient strategies to determine or approximate the solution to TPBVPs for linear or nonlinear systems. Indeed, by relying on the increasingly growing computational capabilities available in modern applications, the so-called *computational optimal control* has become a separate field of active research [21], [22], [23], [24], [25], [26], [27], [28]. Such efforts resulted in the development of several efficient tools and software devoted to the solution to TPBVPs, including *e.g.* GPOPS [29], ICLOCS2 [30], as well as the approaches in [31], [32], [33], [34], [35] among several others. Although diverse, the above methods share common features: they are based on a direct *transcription* of the underlying continuous-time optimal control problem into a *nonlinear programming problem* (NLP), which can be then solved with standard [36] or more dedicated approaches, *e.g.* IPOPT [37]. In particular, direct collocation methods rely on a discretization of the state and control at a collection of suitably defined points within the time interval of interest. In *h*-methods, the time interval is divided into a prescribed grid and the state is approximated by means of polynomials of fixed degree in each cell of the mesh, with convergence to the optimal solution achieved by increasing the number of collocated points. On the other hand, in *p*-methods convergence to the optimal solution is obtained by increasing the order of the polynomial. Recently, *hp*-methods [21] that combine the two previous approaches *adaptively* adjusting the dimension of the grid and the degree of the polynomial have been envisioned. As a common feature to all the previous approaches, the *transcription* of the continuous-time optimal control problem yields a sparse, although typically *very large*, NLP problem, hence a very large system of nonlinear algebraic equations.

The main contribution of this paper consists in proposing a design strategy to compute or approximate the *optimal* initial condition for the costate variable in finite-horizon optimal control problems by solving a system of n algebraic equations, regardless of the prescribed degree of accuracy. The result is achieved by first discussing a *fixed-point* characterization of the optimal costate, which is then translated into more constructive conditions by relying on a sequence of Lie brackets. These involve the underlying Hamiltonian vector field together with a suitably defined *projective* vector field. Such Lie brackets are then evaluated at the initial condition of the state variable, thus leading to a system of algebraic equations in the (unknown) costate initial condition. An identical strategy is then extended to the computation of the optimal terminal value of the state variable. Somewhat similar ideas are employed in [38] to construct solutions to infinite horizon optimal control problems. In particular, therein the key aspect consists in considering the composition of the flows of the (projected) Hamiltonian dynamics and that of the closed-loop optimal system in the original coordinates. Note that an identical strategy could not be straight-forwardly pursued in the context of finite horizon problems, since the latter vector field becomes time-varying, hence introducing challenges that can be only circumvented by considering instead the composition of the

forward and backward Hamiltonian system, as pursued herein. The rest of the paper is organized as follows. The definition of the finite-horizon optimal control problem dealt with is provided in Section II together with additional results and assumptions instrumental for the subsequent derivations. The main statements - consisting of a design strategy that allows to characterize or approximate the optimal initial condition of the costate variable - are presented in Section III. The specialization to the linear setting of the above results is instead the topic of Section IV, while the objective of Section V is to extend the previous machinery to compute (or approximate) also the value of the state variable at the end of the interval of interest, which is unknown, similarly to the costate initial condition. Finally, the paper is concluded by extensive discussions on several computational aspects of the approach in Section VI and further comments in Section VII.

Notation. $\mathbb{N}$ defines the set of positive integers, $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$, and $\mathbb{R}_{\geq 0}$ ($\mathbb{R}_{>0}$) defines the set of non-negative (positive) real numbers. $\sigma(A)$ denotes the spectrum of the matrix $A \in \mathbb{R}^{n \times n}$. Given a symmetric matrix $M = M^\top$, $M \succeq 0$, denotes a positive semi-definite matrix, namely such that $v^\top M v \geq 0$ for any vector v ; similarly $M \succ 0$ denotes a positive definite matrix. I_n denotes the identity matrix of dimension n . Given two vectors $x_1 \in \mathbb{R}^{n_1}$ and $x_2 \in \mathbb{R}^{n_2}$, (x_1, x_2) denotes the vector $\begin{bmatrix} x_1^\top & x_2^\top \end{bmatrix}^\top$. For a continuously differentiable function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $\nabla_x f$ denotes the column vector of the partial derivatives of f , namely $\nabla_x f = [\partial f(x)/\partial x_1, \dots, \partial f(x)/\partial x_n]^\top$. Given two vector fields $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$, the Lie bracket of f and g , denoted $[f, g](x)$, is defined as $[f, g](x) = (\nabla_x g)f(x) - (\nabla_x f)g(x)$. The repeated Lie bracket operation of a vector field g with the same vector field f is recursively defined as $\text{ad}_f^k g(x) = [f, \text{ad}_f^{k-1} g](x)$, with $\text{ad}_f^0 g(x) = g(x)$. Given an ordinary differential equation $\dot{x} = f(x)$ with boundary condition $x(0) = x_0$ and the vector field $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ sufficiently smooth, the mapping $\varphi_f : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ denotes the corresponding *flow* such that $\partial \varphi_f(t; x_0)/\partial t = f(\varphi_f(t; x_0))$ for any $t \geq 0$ and x_0 . The notation $\mathcal{C}^\kappa$ indicates the space of functions that possess continuous derivatives of order less than or equal to κ . A function $f : \mathcal{X} \rightarrow \mathbb{R}^n$ is analytic in the open set $\mathcal{X}$, denoted as $f \in \mathcal{C}^\omega(\mathcal{X})$, if for every $v \in \mathcal{X}$ there is a neighborhood $\mathcal{U}$ such that the Taylor series expansion centered at v converges pointwise to $f(x)$ for $x \in \mathcal{U}$. Given a function $f : \mathcal{X} \rightarrow \mathcal{X}$, a point c in the topological space $\mathcal{X}$ is a *fixed-point* of f if $f(c) = c$, namely if $(c, c) \in \text{graph } f$. $\mathbb{B}(\bar{x}, R)$ denotes the open ball of radius $R > 0$ centered at $\bar{x} \in \mathbb{R}^n$, *i.e.* $\mathbb{B}(\bar{x}, R) := \{x \in \mathbb{R}^n : |x - \bar{x}| < R\}$, whereas $\bar{\mathbb{B}}(\bar{x}, R)$ denotes the closure of $\mathbb{B}(\bar{x}, R)$.

II. PRELIMINARIES AND PROBLEM STATEMENT

Consider an optimal control problem defined over a finite horizon and described by

$$\min_u J_{t_0, x_0}(u) := \frac{1}{2} \int_{t_0}^T (q(x(\tau)) + \|u(\tau)\|^2) d\tau, \quad (1a)$$

$$\text{s.t. } \dot{x}(t) = f(x(t)) + g(x(t))u(t), \quad x(t_0) = x_0 \quad (1b)$$

with $x(t) \in \mathcal{X} \subseteq \mathbb{R}^n$, where $\mathcal{X}$ is a n -dimensional smooth manifold, and $u(t) \in \mathbb{R}^m$, $u \in \mathcal{C}^0([0, T])$, while $x_0 \in \mathcal{X}$ is a given initial condition of the differential equation (1b). It is worth observing that - even in the absence of additional requirements, e.g. *hard* constraints (saturation) on the control input - the optimal control problem formulated in (1a)-(1b) already exhibits the features and computational challenges that are addressed in this paper. In fact - as anticipated herein and briefly recalled in the rest of this section - it is well known that the problem (1a)-(1b) may be tackled either by relying on Pontryagin's Minimum Principle or on a Dynamic Programming approach, which however requires the computation of the explicit solution of the Hamilton-Jacobi-Bellman partial differential equation. While the latter can be seldom determined in practice, the former strategy yields typically a two-point boundary value problem defined with respect to the underlying (nonlinear) Hamiltonian dynamics. To address such a problem several methods have been proposed, including the so-called *collocation methods* [23] and *shooting methods* [39].

The main objective of this paper is to propose an approach alternative to the above mentioned methods, which hinges upon more abstract, geometric, properties of the optimal costate and for which - differently from the former methods - the number of algebraic equations does not grow with increasing accuracy of the approximation and remains equal to the dimension of the state. On the other hand, instead of considering the entire forward flow of an unstable system as in the latter strategies, herein the required conditions are obtained by characterizing the optimal costate by means of subsequent Lie brackets evaluated at a single time instant.

Assumption 1: The function $q : \mathbb{R}^n \rightarrow \mathbb{R}_{>0}$, $q(0) = 0$, and the vector fields $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $f(0) = 0$, and $g_i : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $g_i(0) = 0$, $i = 1, \dots, m$, are analytic at $x = 0$ with *radius of convergence* r_x such that $\mathcal{X} \subset \mathbb{B}(0, r_x)$. $\circ$

The function $V^* : \mathbb{R}_{\geq 0} \times \mathcal{X} \rightarrow \mathbb{R}_{\geq 0}$ defined as $V^*(t_0, x_0) = \min_u \{J_{t_0, x_0}(u)\}$ is referred to as the *value function* of the problem (1). Since the cost functional (1a) and the vector fields appearing in (1b) do not depend explicitly on the time t , in the following it is assumed that $t_0 = 0$ without loss of generality.

Remark 1: The presence of a terminal cost, $m(x(T))$, with $m : \mathcal{X} \rightarrow \mathbb{R}_{\geq 0}$ a real analytic function, on the state of the system (1b) in (1a) can be straight-forwardly encompassed into the framework of (1a) by replacing the terminal cost with an equivalent *Lagrangian* cost. In fact, since

$$m(x(T)) = m(x_0) + \int_0^T \frac{d}{dt} m(x(t)) dt, \quad (2)$$

and since $x(0) = x_0$ is a constant with respect to u , the terminal cost m can be included in the Lagrangian term by defining the modified running cost $\tilde{q}(x, u) = q(x) + 2(\nabla_x m(x))(f(x) + g(x)u)$, provided $\tilde{q}(x, u) + \|u\|^2$ remains positive definite with respect to x and u for consistency with the definition of (1a). $\blacktriangle$

Consider the underlying (minimized) Hamiltonian function $\mathbf{H} : T^*\mathcal{X} \rightarrow \mathbb{R}$, with $T^*\mathcal{X}$ denoting the cotangent bundle over

$\mathcal{X}$ with natural coordinates (x, λ) , defined as

$$\mathbf{H}(x, \lambda) := \frac{1}{2}q(x) + \lambda^\top f(x) - \frac{1}{2}\lambda^\top g(x)g(x)^\top \lambda. \quad (3)$$

The optimal process $(x^*(t), \lambda^*(t))$ then satisfies the Hamiltonian dynamics

$$\begin{bmatrix} \dot{x} \\ \dot{\lambda} \end{bmatrix} = J\nabla \mathbf{H}(x, \lambda) := X_{\mathbf{H}}(x, \lambda), \quad (4)$$

with

$$J := \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix} \quad (5)$$

and $X_{\mathbf{H}}$ denoting the Hamiltonian vector field, together with the *split* boundary conditions $(x(0), \lambda(T)) = (x_0, 0)$. Alternatively, the Hamiltonian dynamics (4) can be initialized at $(x(0), \lambda(0)) = (x_0, \nabla_x V^*(t_0, x_0))$, where the value function $V^*(t, x)$, $V^* : \mathbb{R} \times \mathcal{X} \rightarrow \mathbb{R}_{>0}$, satisfies the Hamilton-Jacobi-Bellman partial differential equation

$$-\frac{\partial V^*}{\partial t} = \frac{1}{2}q(x) + \frac{\partial V^*}{\partial x}f(x) - \frac{\partial V^*}{\partial x}g(x)g(x)^\top \left(\frac{\partial V^*}{\partial x}\right)^\top, \quad (6)$$

for all $x \in \mathcal{X}$ and $t \in [0, T]$, together with the boundary condition $V^*(T, x) = 0$ for any $x \in \mathcal{X}$. As a consequence, the computation of the value function constitutes a critical bottleneck for the solution of problem (1) regardless if one relies on the DP strategy or on PMP approach, since for any $x_0 \in \mathcal{X}$ the costate variable $\lambda(0)$ should be initialized at $\lambda_0^*(x_0) := \nabla_x V^*(0, x_0)$.

In the following it is assumed that, for given initial condition x_0 and terminal time $T > 0$, the optimal control problem (1) admits a solution that satisfies additional continuity properties, as detailed in the statement below.

Assumption 2: Given an initial condition $x_0 \in \mathcal{X}$ and a terminal time $T \in \mathbb{R}_{>0}$, there exists a unique smooth solution $V^* : \mathbb{R} \times \mathcal{X} \rightarrow \mathbb{R}_{>0}$ of (6), for $t \in [0, T]$ and for all $x \in \mathcal{X}$ together with the boundary condition $V^*(T, x) = 0$ for all $x \in \mathcal{X}$. $\circ$

Finally, introducing $z := (x, \lambda)$ and considering the Hamiltonian dynamics $\dot{z} = X_{\mathbf{H}}(z)$, $z_0 = (x_0, \lambda_0)$, let $\Phi_t^{X_{\mathbf{H}}} : \mathcal{X} \times \mathbb{R}^n \rightarrow \mathcal{X} \times \mathbb{R}^n$ denote the one-parameter group of local diffeomorphisms, under the operation of composition, that defines an integral curve of $X_{\mathbf{H}}$ for any $z \in T^*\mathcal{X}$, namely $\Phi_t^{X_{\mathbf{H}}}(z) = \varphi_{X_{\mathbf{H}}}(t; x_0, \lambda_0)$, where $\varphi_{X_{\mathbf{H}}} : \mathbb{R}_{\geq 0} \times \mathcal{X} \times \mathbb{R}^n \rightarrow \mathcal{X} \times \mathbb{R}^n$ defines the *flow* of the vector field $X_{\mathbf{H}}$. As a consequence of Assumption 2 the flow $\varphi_{X_{\mathbf{H}}}(t; x_0, \nabla_x V^*(0, x_0))$ is defined for all $t \in [0, T]$ and it satisfies $\lambda(t) = \nabla_x V^*(t, x(t))$, see for instance [10, Chapter 1]. Moreover, as a result of Assumption 1, the costate $\lambda : \mathbb{R} \rightarrow \mathbb{R}^n$ is an analytic function of time. Suppose, in addition, that the following requirement is satisfied on the radius of convergence for the analyticity property of the costate λ with respect to time.

Assumption 3: The flow $\varphi_{X_{\mathbf{H}}}(t; x_0, \lambda_0^*(x_0))$ is an analytic function at $t = 0$ with the property that its radius of convergence r_H satisfies $r_H > 2T$. $\circ$

III. A FIXED-POINT CHARACTERIZATION OF THE OPTIMAL COSTATE

Let $\pi : T^*\mathcal{X} \rightarrow \mathcal{X}$ denote the natural projection operator that maps an element of $T^*\mathcal{X}$ into the corresponding base point $x \in \mathcal{X}$. The following statement provides a *fixed-point* characterization of the optimal costate variable.

Theorem 1: Consider the finite-horizon optimal control problem (1). Let $x_0 \in \mathcal{X}$ and $T \in \mathbb{R}_{>0}$ be given and suppose that Assumptions 1-3 hold. Then a vector $\lambda_0 \in \mathbb{R}^n$ is such that $\lambda_0 = \nabla_x V^*(0, x_0)$ if and only if there exists a function $\lambda_a : [0, T] \rightarrow \mathbb{R}^n$, analytic at $t = 0$, with radius of convergence larger than T and such that $\lambda_a(T) = 0$, with the property that

$$\omega(t) := \varphi_{X_H}(-t; \pi \circ \varphi_{X_H}(t; x_0, \lambda_0), \lambda_a(t)) = (x_0, \lambda_0), \quad (7)$$

for all $t \in [0, T]$. $\diamond$

Proof: ($\Rightarrow$) Since the function $t \mapsto V^*(t, x(t))$ is smooth, hence at least twice continuously differentiable, it follows that the trajectory $x : \mathbb{R} \rightarrow \mathbb{R}^n$ yields the optimal time-evolution of the state variable only if it can be obtained as the projection on the x -coordinates of a trajectory of the Hamiltonian dynamics (4) and the costate variable verifies $\lambda(t) = \nabla_x V^*(t, x(t))$, for all $t \in [0, T]$, which is analytic by Assumptions 1 and 2. Moreover, recalling that the value function $V^*(t, x)$, $V^* : \mathbb{R} \times \mathcal{X} \rightarrow \mathbb{R}_{>0}$, satisfies the Hamilton-Jacobi-Bellman partial differential equation (6) for all $x \in \mathcal{X}$ and $t \in [0, T]$, together with the boundary condition $V^*(T, x) = 0$ for all $x \in \mathcal{X}$, it follows that $\nabla_x V^*(T, x) = 0$ for any $x \in \mathcal{X}$. Therefore, $\lambda_0 = \nabla_x V^*(0, x_0)$ verifies (7) together with the *feasible* selection $\lambda_a(\cdot) := \nabla_x V^*(\cdot, x(\cdot))$.

($\Leftarrow$) For any $x_0 \in \mathcal{X} \subset \mathbb{R}^n$, λ_0 yields the *optimal* initial condition of the costate variable if the composition of the *forward* flow (for t seconds) along the vector field X_H from (x_0, λ_0) with the *backward* flow (for t seconds) along the same vector field - considering the state component reached at time t and the costate component potentially *set* to the value of an analytic function $\lambda_a(t)$ - yields again (x_0, λ_0) , for all $t \geq 0$. Since the latter task alone may be accomplished by letting $\lambda_a(\cdot)$ be defined as any function $v(x(\cdot))$ such that the manifold $\{(x, \lambda) \in \mathcal{X} \times \mathbb{R}^n : \lambda = v(x)\}$ is invariant for (4), namely any $v : \mathcal{X} \rightarrow \mathbb{R}^n$ with the property that $(\frac{\partial v}{\partial x} \nabla_\lambda H(x, \lambda) + \nabla_x H(x, \lambda))|_{\lambda=v(x)} = 0$, for any $x \in \mathcal{X}$, sufficiency of (7) follows by additionally requiring that $\lambda_a(T) = 0$ and by uniqueness of the trajectories of (4). $\square$

Remark 2: The condition (7) entails that the mapping $(x_0, \lambda_0) \mapsto \varphi_{X_H}(-t; \pi \circ \varphi_{X_H}(t; x_0, \lambda_0), \lambda_a(t))$ possesses a *fixed-point* at $(x_0, \nabla_x V^*(0, x_0))$ for all $t \geq 0$, obtained by letting $\lambda_a(t) = \nabla_x V^*(t, x^*(t))$. Therefore, the operations of *flowing* along the vector field X_H forward for t seconds, projecting the reached composite state into $\mathcal{X}$, and flowing backward again along X_H for t seconds must yield the initial condition (x_0, λ_0) of the extended system, provided the costate component of X_H is suitably *set* to $\lambda_a(t)$ at time t . $\blacktriangle$

Let now $\text{id} : \mathcal{X} \times \mathbb{R}^n \rightarrow \mathcal{X} \times \mathbb{R}^n$ denote the *identity function*, namely $\text{id}(z) = z$, and define the *partial projective mapping*

Fig. 1. Graphical representation of the composition of the forward and backward flows of the Hamiltonian dynamics (4). The gray dashed vector describes the *distance* of (x_0, λ_0) from being a fixed-point of the composition in (7).

$p : \mathcal{X} \times \mathbb{R}^n \rightarrow \mathcal{X} \times \mathbb{R}^n$ as

$$p(z) = \begin{bmatrix} \pi \circ z \\ h(z) \end{bmatrix}, \quad (8)$$

where $h : \mathcal{X} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ is an arbitrary analytic function. Suppose that the following standing assumption holds.

Assumption 4: There exist positive constants $c_\ell \in \mathbb{R}_{>0}$ and $c_u \in \mathbb{R}_{>0}$ such that

$$\inf_{t \in [0, T], x \in \mathcal{X}} \sigma((\Phi_{-t}^{X_H})_*) \geq c_\ell, \quad (9a)$$

$$\sup_{t \in [0, T], x \in \mathcal{X}} \bar{\sigma}((\Phi_{-t}^{X_H})_*) \leq c_u, \quad (9b)$$

with $(\Phi_{-t}^{X_H})_*$ denoting the *differential* of $\Phi_{-t}^{X_H}$. $\circ$

Note that (9a) in particular implies that the differential of the flow $\Phi_{-t}^{X_H}$ is an invertible matrix for any $t \in [0, T]$.

Theorem 2: Consider the finite-horizon optimal control problem (1). Let $x_0 \in \mathcal{X}$ and $T \in \mathbb{R}_{>0}$ be given and suppose that Assumptions 1-4 hold. Then a vector $\lambda_0 \in \mathbb{R}^n$ is such that $\lambda_0 = \nabla_x V^*(0, x_0)$ if and only if there exist $\lambda_k := h_k(x_0, \lambda_0) \in \mathbb{R}^n$ with $h_k(z) := \langle \nabla h_{k-1}, X_H \rangle$, $k = 1, 2, \dots$ and $h_0(z) = h(z)$, with the properties that

$$\text{ad}_{X_H}^k p(x_0, \lambda_0) = \text{ad}_{X_H}^k \text{id}(x_0, \lambda_0), \quad (10)$$

for $k = 1, 2, \dots$, and $\sum_{k=0}^{\infty} \lambda_k \frac{T^k}{k!} = 0$. $\diamond$

Proof: Since the function $t \mapsto \omega(t)$ defined in the left-hand side of (7) is analytic at $t = 0$, the condition on the right-hand side of (7) is equivalent to requiring that $\omega(0) = (x_0, \lambda_0)$, which holds for any $(x_0, \lambda_0) \in \mathcal{X} \times \mathbb{R}^n$, and that $d^k \omega(t)/dt^k|_{t=0} = 0$. Define then the analytic function

$$W(t) = (\Phi_{-t}^{X_H})_* p(\Phi_t^{X_H}(z_0)) \quad (11)$$

with $z_0 = (x_0, \lambda_0)$ and the vector field p introduced in (8), and note that by the *Campbell-Baker-Hausdorff formula* $W : \mathbb{R} \rightarrow \mathbb{R}^{2n}$ can be expanded in the form [40]

$$W(t) = \sum_{k=0}^{\infty} \text{ad}_{X_H}^k p(z_0) \frac{t^k}{k!}, \quad (12)$$

namely such that

$$\left. \frac{d^k W(t)}{dt^k} \right|_{t=0} = \text{ad}_{X_H}^k p(z_0). \quad (13)$$

Moreover, by noting that ω may be written as $\omega(t) = \Phi_{-t}^{X_H} \circ p(\Phi_t^{X_H}(z_0))$ and by relying on (9a), it follows that $(\Phi_{-t}^{X_H})^{-1} W(t) = p(\Phi_t^{X_H}(z_0))$, hence

$$\omega(t) = \Phi_{-t}^{X_H} \left((\Phi_t^{X_H})^{-1} W(t) \right). \quad (14)$$

Therefore, $\omega(t) = (x_0, \lambda_0)$ for all $t \geq 0$ if and only if $W(t) = (\Phi_{-t}^{X_H})_* \Phi_t^{X_H}$ for all $t \geq 0$, which in turn is equivalent to

$$\text{ad}_{X_H}^k p(z_0) = \left(\left. \frac{d^k}{dt^k} (\Phi_{-t}^{X_H})_* \Phi_t^{X_H} \right) \right|_{t=0}. \quad (15)$$

The latter is then equivalent to (10) by applying again the *Campbell-Baker-Hausdorff formula* with p replaced by the identity function on $\mathcal{X} \times \mathbb{R}^n$. The proof is concluded then by noting that $h(z(T)) = 0$ by the summation requirement on λ_k and that $\lambda_a(t) = h(z(t)) = \sum_{k=0}^{\infty} \lambda_k (t^k/k!)$. $\square$

The conditions in (10) consist of a system of *algebraic* equations that are linear in the variables λ_i , $i = 1, 2, \dots$, although nonlinear in λ_0 . The following statement shows that the conditions (10) can be equivalently recast into a system of n equations in the variable λ_0 alone. To this end, consider first the definition of the operator $\mathcal{D}$, introduced in [38], as follows.

Definition 1: Given a smooth vector field $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$, consider the operator $\mathcal{D}_i(f)$ recursively defined as $\mathcal{D}_0(f) = f$ and

$$\mathcal{D}_i(f) = (\nabla \mathcal{D}_{i-1}(f)) \mathcal{D}_0(f), \quad (16)$$

for $i \in \mathbb{N}$, where ∇f denotes the Jacobian matrix of the vector-valued function f . $\circ$

Theorem 3: Consider the finite-horizon optimal control problem (1). Let $x_0 \in \mathcal{X}$ and $T \in \mathbb{R}_{>0}$ be given and suppose that Assumptions 1-4 hold. Then a vector $\lambda_0 \in \mathbb{R}^n$ is such that $\lambda_0 = \nabla_x V^*(0, x_0)$ if and only if

$$\mathcal{T}(\lambda_0) := \lambda_0 + N \sum_{i=1}^{\infty} \mathcal{D}_{i-1}(X_H(x_0, \lambda_0)) \frac{T^i}{i!} = 0, \quad (17)$$

with $N := \begin{bmatrix} 0 & I_n \end{bmatrix} \in \mathbb{R}^{n \times 2n}$ describing the natural projection $\pi_\lambda : \mathcal{X} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ on the λ -coordinates. $\diamond$

Proof: To begin with, note that, provided the first $k-1$ equations in (10) are satisfied, the k -th becomes

$$\begin{aligned} 0 &= (\nabla_z \text{ad}_{X_H}^{k-1} p(z_0)) X_H(z_0) - (\nabla_z X_H(z))^\top \text{ad}_{X_H}^{k-1} p(z_0) \\ &\quad - (\nabla_z \text{ad}_{X_H}^{k-1} z_0) X_H(z_0) + (\nabla_z X_H(z))^\top \text{ad}_{X_H}^{k-1} \text{id}(z_0) \\ &= \left(\nabla_z \text{ad}_{X_H}^{k-1} p(z_0) - \nabla_z \text{ad}_{X_H}^{k-1} z_0 \right) X_H(z_0) \\ &= \nabla_z \left(\text{ad}_{X_H}^{k-1} p(z_0) - \text{ad}_{X_H}^{k-1} z_0 \right) X_H(z_0). \end{aligned} \quad (18)$$

Then it can be shown by induction that

$$\begin{aligned} \nabla_z \left(\text{ad}_{X_H}^{k-1} p(z_0) - \text{ad}_{X_H}^{k-1} z_0 \right) X_H(z_0) &= -\mathcal{D}_{k-1}(X_H(z_0)) \\ &\quad + \left[\begin{array}{c} M \mathcal{D}_{k-1}(X_H(z_0)) \\ h_k(z_0) \end{array} \right], \end{aligned} \quad (19)$$

for any $k \geq 1$, with $M = \begin{bmatrix} I_n & 0 \end{bmatrix} \in \mathbb{R}^{n \times 2n}$. In fact, for $k=1$, one has

$$\begin{aligned} 0 &= [X_H, p](z_0) - [X_H, \text{id}](z_0) \\ &= \left(\left[\begin{array}{c} M \\ \nabla h(z) \end{array} \right] X_H(z) - (\nabla X_H(z))^\top \left[\begin{array}{c} Mz \\ h(z) \end{array} \right] \right) \Big|_{z=z_0} \\ &\quad - (X_H(z) - (\nabla X_H(z))^\top z) \Big|_{z=z_0} \\ &= \left[\begin{array}{c} M X_H(x_0, \lambda_0) \\ \lambda_1 \end{array} \right] - X_H(x_0, \lambda_0), \end{aligned} \quad (20)$$

where the last equality is obtained by noting that $Mz_0 = x_0$ and $h(z_0) = \lambda_0$. Then, assuming that (19) holds up to a certain index k , it can be shown that, for $k+1$,

$$\begin{aligned} \nabla_z \left(\text{ad}_{X_H}^{k+1} p(z) - \text{ad}_{X_H}^{k+1} z \right) X_H(z) &= \\ &= \nabla_z \left([X_H, \text{ad}_{X_H}^k p(z)] - [X_H, \text{ad}_{X_H}^k z] \right) X_H(z) = \\ &= \nabla_z \left(\nabla_z \left(\text{ad}_{X_H}^k p(z) - \text{ad}_{X_H}^k z \right) X_H(z) \right. \\ &\quad \left. + \nabla_z X_H \left(\underbrace{\text{ad}_{X_H}^k p(z) - \text{ad}_{X_H}^k z}_{=0, \text{ for } z=z_0} \right) X_H(z) \right), \end{aligned}$$

where the property that the previous k equations are satisfied at $z = z_0$ has been employed. Therefore,

$$\begin{aligned} \nabla_z \left(\text{ad}_{X_H}^{k+1} p(z_0) - \text{ad}_{X_H}^{k+1} z_0 \right) X_H(z_0) &= \\ &= \nabla_z \left(\left[\begin{array}{c} M \mathcal{D}_{k-1}(X_H(z_0)) \\ h_k(z_0) \end{array} \right] - \mathcal{D}_{k-1}(X_H(z_0)) \right) X_H(z_0) = \\ &= \left[\begin{array}{c} M \mathcal{D}_k(X_H(z_0)) \\ h_{k+1}(z_0) \end{array} \right] - \mathcal{D}_k(X_H(z_0)), \end{aligned} \quad (21)$$

where the first equality is obtained by the inductive hypothesis. As a straight-forward consequence of (21), it follows that $\lambda_i = \pi_\lambda \circ \mathcal{D}_{i-1}(X_H(z_0))$ and the claim, hence equation (17), is therefore shown by noting that the values λ_i describe the coefficients of the Taylor series of $\lambda_a(t)$ at $t=0$ and by imposing the terminal condition $\lambda_a(T) = 0$. $\square$

Remark 3: Equations identical to (10), and consequently to (18), can be obtained, in a more convoluted way, by directly considering the subsequent time derivatives of the function ω

Fig. 2. Graphical illustration of the sets Λ_{loc} (solid black line) and Λ (gray region) involved in the proof of Theorem 4.

introduced in (7). For instance, for $k = 1$,

$$\begin{aligned} \dot{\omega}(t) = & -\frac{\partial}{\partial t} \varphi_{X_{\mathbf{H}}}(-t; M \varphi_{X_{\mathbf{H}}}(t; x_0, \lambda_0), \lambda_a(t)) \\ & + \nabla_s \varphi_{X_{\mathbf{H}}}(-t; s) \left[\begin{array}{c} M \frac{\partial}{\partial t} \varphi_{X_{\mathbf{H}}}(t; x_0, \lambda_0) \\ \dot{\lambda}_a(t) \end{array} \right] \end{aligned} \quad (22)$$

which coincides with equation (20) for $t = 0$ recalling that $\nabla_s \varphi_{X_{\mathbf{H}}}(0; s) = I_n$ and letting $\lambda_1 := \dot{\lambda}_a(0)$. $\blacktriangle$

Before stating the following result we provide a definition. Given a vector-valued function $\sigma : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $\mathbb{V}(\sigma)$ denotes the *algebraic set* associated to σ , namely the set $\{x \in \mathbb{R}^n : \sigma(x) = 0\}$. Moreover, given a set $\mathcal{W}$ and a point v , $\mathbf{d}(\mathcal{W}, v)$ denotes the distance between a set and a point, namely

$$\mathbf{d}(\mathcal{W}, v) = \inf_{w \in \mathcal{W}} d(w, v). \quad (23)$$

Theorem 4: Consider the finite-horizon optimal control problem (1). Let $x_0 \in \mathcal{X}$ and $T \in \mathbb{R}_{>0}$ be given and suppose that Assumptions 1-4 hold. Let

$$\mathcal{T}_{\kappa}(\lambda_0) := \lambda_0 + N \sum_{i=1}^{\kappa} \mathcal{D}_{i-1}(X_{\mathbf{H}}(x_0, \lambda_0)) \frac{T^i}{i!} = 0. \quad (24)$$

Then for any $\varepsilon > 0$ there exist $\kappa(\varepsilon)$ and a compact set $\Lambda \subset \mathbb{R}^n$ containing $\nabla_x V^*(0, x_0)$ such that

$$\mathbf{d}(\mathcal{L}, \nabla_x V^*(0, x_0)) < \varepsilon, \quad (25)$$

with $\mathcal{L} := \mathbb{V}(\mathcal{T}_{\kappa}) \cap \Lambda$. $\diamond$

Proof: The claim is proved by showing that the difference between $\mathcal{T}_{\kappa}$ and $\mathcal{T}$ can be made arbitrarily small in a compact set containing λ_0^* . Since by Assumptions 2 and 3 the optimal costate $\lambda^* : \mathbb{R} \rightarrow \mathbb{R}^n$ is an analytic function at $t = 0$ such that the terminal time T belongs to the interior of the domain of convergence with the property that $\mathbb{B}(0, 2T) \subset \mathbb{B}(0, r_H)$, it follows that the Taylor series expansion in the left-hand side of (17) is absolutely, uniformly, convergent to $\lambda^*(T)$. As a consequence, by applying the Cauchy's integral formula to the complex extension of the analytic function $\lambda^*(\cdot)$, which is well-defined and analytic, and since, by (17), $\lambda^{(k)}(0) =$

$N \mathcal{D}_k(X_{\mathbf{H}}(x_0, \lambda_0))$, it follows that

$$\begin{aligned} |N \mathcal{D}_k(X_{\mathbf{H}}(x(s), \lambda(s)))| & \leq \frac{k!}{2\pi} \int_{\partial \mathbb{B}(s, \varrho)} \frac{|\lambda^*(w)|}{|w - s|^{k+1}} |dw| \\ & < c_{\lambda} \frac{k!}{2\pi} \frac{1}{\varrho^{k+1}} 2\pi \varrho = c_{\lambda} \frac{k!}{\varrho^k}, \end{aligned} \quad (26)$$

recalling that $\mathbb{B}(s, \varrho) \subset \mathbb{B}(0, r_H)$, for some $\varrho > T$ and for any $s \in [0, T]$, where $c_{\lambda} > \max_{w \in \mathbb{B}(0, r_H)} |\lambda^*(w)|$. Therefore,

$$|N \mathcal{D}_k(X_{\mathbf{H}}(\hat{x}, \hat{\lambda}))| < c_{\lambda} \frac{k!}{\varrho^k}, \quad (27)$$

for any $k \in \mathbb{N}$ and for all $(\hat{x}, \hat{\lambda})$ in the set $\Lambda_{\text{loc}} := \{(\hat{x}, \hat{\lambda}) \in \mathbb{R}^{2n} : \exists s \in [0, T], (\hat{x}, \hat{\lambda}) = \varphi_{X_{\mathbf{H}}}(s; x_0, \lambda_0^*(x_0))\}$. By considering now the Lagrange form of the remainder of the Taylor series expansion $\mathcal{T}_{\kappa}$ with respect to $\mathcal{T}$, it follows that the latter remainder in Λ_{loc} is given by

$$\mathcal{R}_{\kappa}(s) := N \mathcal{D}_{\kappa+1}(X_{\mathbf{H}}(x_{\xi}, \lambda_{\xi})) \frac{T^{\kappa+1}}{(\kappa+1)!}, \quad (28)$$

for any $s \in [0, T]$ and for some $(x_{\xi}, \lambda_{\xi}) \in \Lambda_{\text{loc}}$, by Taylor's theorem, hence such that $|\mathcal{T}_{\kappa}(\lambda) - \mathcal{T}(\lambda)| < |N \mathcal{D}_{\kappa+1}(X_{\mathbf{H}}(x_{\xi}, \lambda_{\xi}))| (T^{\kappa+1}) / ((\kappa+1)!) < c_{\lambda} T^{\kappa+1} / \varrho^{\kappa+1}$, for any $\lambda \in \Lambda_{\text{loc}}$. Thus, by smoothness of the Hamiltonian vector field $X_{\mathbf{H}}$ with respect to (x, λ) , there exists $\mu > 0$ such that

$$|\mathcal{T}_{\kappa}(\lambda) - \mathcal{T}(\lambda)| < c_{\lambda} \left(\frac{T}{\varrho} \right)^{\kappa+1}, \quad (29)$$

for all $\lambda \in \Lambda = \Lambda_{\text{loc}} + \mathbb{B}(\Lambda_{\text{loc}}, \mu)$. The right-hand side of (29) can be then made arbitrarily small by increasing κ and recalling that $T < \varrho$. $\square$

The intuition behind the statement of Theorem 4 is provided in the following discussion. By relying on Assumption 2, $\mathbb{V}(\mathcal{T})$ consists of a single point, namely $\lambda_0^*(x_0) = \nabla_x V^*(0, x_0)$. The truncation $\mathcal{T}_{\kappa}$ for finite κ may instead have multiple (real) roots such that $\mathcal{T}_{\kappa} = 0$. The conclusions of Theorem 4 guarantee that among such real solutions there is one that approaches $\lambda_0^*(x_0)$ for increasing values of κ .

Note that determining roots of $\mathcal{T}_{\kappa}(\lambda_0)$ coincides with computing solutions to the system (10) for $k = 1, \dots, \kappa$, with

$$\lambda_{\kappa}^{\kappa} = -\frac{\kappa!}{T^{\kappa}} \left(\lambda_0^{\kappa} + \lambda_1^{\kappa} T + \dots + \lambda_{\kappa-1}^{\kappa} (T^{\kappa-1} / (\kappa-1)!) \right), \quad (30)$$

where the superscript κ in the unknown vectors λ_i^{κ} hints at the finite truncation of (10).

Remark 4: In addition to the value of λ_0^{κ} that approximates $\nabla_x V^*(0, x_0)$ arbitrarily close, the statement of Theorem 4 entails that, instead of using such a value as the (approximate) initial condition of the unstable dynamics (4), the values λ_i^{κ} can be employed to compute a Taylor series expansion for $\lambda_a(t)$ as $\tilde{\lambda}(t) = \sum_{k=0}^{\kappa} \lambda_k(t^k/k!)$ and then implementing directly the feedforward control law $\tilde{u}(t) = -g(x(t))^{\top} \tilde{\lambda}(t)$. $\blacktriangle$

IV. INSIGHTS ON THE LINEAR CASE

The objective of this section consists in specializing the above results to the case of linear systems and quadratic cost functionals, namely

$$\min_u J_{x_0}(u) := \frac{1}{2} \int_0^T (x(\tau)^\top Q x(\tau) + \|u(\tau)\|^2) d\tau, \quad (31a)$$

$$\text{s.t. } \dot{x}(t) = Ax(t) + Bu(t), \quad x(0) = x_0, \quad (31b)$$

with $Q \succeq 0$. Under these structural assumptions the Hamiltonian dynamics are linear and described by the vector-field

$$X_H = \begin{bmatrix} A & -BB^\top \\ -Q & -A^\top \end{bmatrix} \begin{bmatrix} x \\ \lambda \end{bmatrix} := H \begin{bmatrix} x \\ \lambda \end{bmatrix}, \quad (32)$$

with $H \in \mathbb{R}^{2n \times 2n}$ referred to as the Hamiltonian matrix. In the context of Linear-Quadratic (LQ) optimal control, the computation of the optimal solution hinges upon the *Differential Riccati Equation* (DRE)

$$-\dot{P}(t) = Q + A^\top P(t) + P(t)A - P(t)BB^\top P(t), \quad (33)$$

$P(t) = P(t)^\top \in \mathbb{R}^{n \times n}$, with terminal boundary condition $P(T) = 0$, which is the linear counterpart of the HJB equation (6). The flow of the former Hamiltonian system then becomes $\varphi_{X_H}(t; z_0) = e^{Ht} z_0$. Therefore, the function $\omega(t)$ introduced in (7) reduces, in the linear case, to

$$\omega(t) = e^{-Ht} \begin{bmatrix} Me^{Ht} \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix} \\ \lambda_a(t) \end{bmatrix}. \quad (34)$$

As a result, a claim similar to that given in Theorem 4 in the nonlinear setting can be stated.

Proposition 1: Consider the finite-horizon optimal control problem (31). Let $x_0 \in \mathcal{X}$ be given. Then for any $\varepsilon > 0$ there exists $\kappa(\varepsilon)$ such that the solution λ_0^κ to

$$\begin{cases} H^i \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix} = \begin{bmatrix} MH^i \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix} \\ \lambda_i \end{bmatrix}, \quad i = 1, \dots, \kappa - 1 \\ H^\kappa \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix} = \begin{bmatrix} MH^\kappa \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix} \\ -\frac{\kappa!}{T^\kappa} \sum_{j=0}^{\kappa-1} \lambda_j (T^j/j!) \end{bmatrix} \end{cases} \quad (35)$$

satisfies

$$\|\lambda_0^\kappa - P(0)x_0\|_2^2 < \varepsilon. \quad (36)$$

◇

Proof: To begin with it is shown that a truncation of the equations (10) to the order κ reduces to (35) in the linear case. This is achieved by imposing that $\omega(t) = (x_0, \lambda_0)$ for any $t \geq 0$. Note that the latter condition is equivalent to requiring that

$$\varpi(t) := \begin{bmatrix} Me^{Ht} \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix} \\ \lambda_a(t) \end{bmatrix} - e^{Ht} \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix} = 0, \quad (37)$$

for all $t \geq 0$. This can be obtained by letting $\varpi^{(i)}(0) = 0$ for $i \in \mathbb{N}$, or approximated via a finite truncation with $i = 1, \dots, \kappa$. Therefore,

$$\varpi^{(i)}(t) := \begin{bmatrix} MH^i e^{Ht} \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix} \\ \lambda_a^{(i)}(t) \end{bmatrix} - H^i e^{Ht} \begin{bmatrix} x_0 \\ \lambda_0 \end{bmatrix},$$

which yields (35) together with the constraint $\sum_{i=0}^{\kappa} \lambda_a^{(i)}(0)(T^i/i!) = 0$. Finally, the inequality (36) is obtained by noting that (35) is a square linear system of equations admitting a unique solution λ_0^κ . □

Remark 5: In the case of LQ optimal control problems over finite-horizon, defining and partitioning the *transition matrix* associated to the Hamiltonian dynamics (32) according to

$$e^{Ht} := \Phi_H(T, 0) = \begin{bmatrix} \Phi_{11}(T, 0) & \Phi_{12}(T, 0) \\ \Phi_{21}(T, 0) & \Phi_{22}(T, 0) \end{bmatrix}, \quad (38)$$

yields that $\lambda_0^*(x_0) = -\Phi_{22}(T, 0)^{-1} \Phi_{21}(T, 0)x_0$, provided $\det(\Phi_{22}(T, 0)) \neq 0$. ▲

The following statement provides an insight on the structure and *sparsity* of the system of equations (35) by establishing a relation with the construction mentioned in Remark 5. To provide a concise statement, consider the partition

$$H^i := \begin{bmatrix} U_{11,i} & U_{12,i} \\ U_{21,i} & U_{22,i} \end{bmatrix}. \quad (39)$$

Proposition 2: Consider the finite-horizon optimal control problem (31). Let $x_0 \in \mathcal{X}$ be given. Then the solution λ_0^κ of (35) is given by

$$\lambda_0^\kappa = - \left(\sum_{i=0}^{\kappa} U_{22,i}^i (T^i/i!) \right)^{-1} \left(\sum_{j=1}^{\kappa} U_{21,j} (T^j/j!) \right) x_0 \quad (40)$$

provided the terminal time $T > 0$ is such that $\sum_{i=0}^{\kappa} U_{22,i}^i (T^i/i!)$ is non-singular. ◇

Proof: To begin with, considering the partition in (39) and noting that $MH^i = \begin{bmatrix} U_{11,i} & U_{12,i} \end{bmatrix}$, note that the i -th equation in (35) can be written as

$$\begin{bmatrix} U_{11,i}x_0 + U_{12,i}\lambda_0 \\ \lambda_i \end{bmatrix} = \begin{bmatrix} U_{11,i} \\ U_{21,i} \end{bmatrix} x_0 + \begin{bmatrix} U_{12,i} \\ U_{22,i} \end{bmatrix} \lambda_0,$$

hence

$$\begin{bmatrix} 0 \\ \lambda_i \end{bmatrix} = \begin{bmatrix} 0 \\ U_{21,i} \end{bmatrix} x_0 + \begin{bmatrix} 0 \\ U_{22,i} \end{bmatrix} \lambda_0,$$

which can be then compactly arranged, for $i = 1, \dots, \kappa$, as

$$\begin{bmatrix} -U_{22,1} & I & 0 & \dots & 0 \\ -U_{22,2} & 0 & I & \dots & 0 \\ \vdots & & & \ddots & \vdots \\ G_1 & \dots & & & G_\kappa \end{bmatrix} \begin{bmatrix} \lambda_0 \\ \lambda_1 \\ \vdots \\ \lambda_{\kappa-1} \end{bmatrix} = \begin{bmatrix} U_{21,1} \\ U_{21,2} \\ \vdots \\ U_{21,\kappa} \end{bmatrix} x_0, \quad (41)$$

Fig. 3. Graphical representation of the *dual* composition of the backward and forward flows of the Hamiltonian dynamics (4). The gray dashed vector describes the *distance* of $(x_T, 0)$ from being a fixed-point of the composition in (42).

with $G_1 = -(U_{22,\kappa} + (T^\kappa \kappa!)I)$ and $G_j = -(\frac{\kappa!}{j!} T^{j-\kappa})I$, for $j = 2, \dots, \kappa - 1$. The claim is then proven by noting that $\lambda_i = U_{22,i}\lambda_0 + U_{21,i}x_0$, $i = 1, \dots, \kappa - 1$, and replacing the latter into the last equation of (41). $\square$

V. THE DUAL CASE: FIXED-POINT CHARACTERIZATION OF THE OPTIMAL FINAL STATE

The fixed-point characterization of the optimal costate discussed in Theorem 1 relies on the property that the initial condition of the entire Hamiltonian dynamics (4) is only partially known, since $x(0) = x_0$ is fixed, while the value of the costate λ at time $t = 0$ must be determined. Such a consideration then leads to the characterization of the optimal costate as pursued in (7), which relies on the composition of Hamiltonian flows.

Interestingly, a somewhat *dual* strategy is also viable to directly compute the optimal final state by relying on the knowledge of the value of the optimal costate at the terminal time $t = T$, namely $\lambda(T) = 0$, and exploiting ideas fully similar to the composition in (7). This aspect is discussed in the following statement, the proof of which is a straightforward adaptation of that of Theorem 1, hence it is omitted.

Theorem 5: Consider the finite-horizon optimal control problem (1). Let $x_0 \in \mathcal{X}$ and $T \in \mathbb{R}_{>0}$ be given and suppose that Assumptions 1-3 hold. Then a vector $x_T \in \mathcal{X}$ is such that $x^*(T) = x_T$ if and only if there exists a function $x_a : [-T, 0] \rightarrow \mathcal{X}$, analytic at $t = 0$, with radius of convergence larger than T and such that $x_a(-T) = x_0$, with the property that

$$\omega_d(t) := \varphi_{X_H}(t; x_a(t), \pi_\lambda \circ \varphi_{X_H}(-t; x_T, 0)) = (x_T, 0), \quad (42)$$

for all $t \in [0, T]$. $\diamond$

By building on the fixed-point characterization (42) in Theorem 5, results identical to those in Section III can be stated and derived. Herein, an in-depth discussion is carried out explicitly in the somewhat explanatory case of linear systems, which allows to highlight the main differences with respect to the results above without any additional burden of notation.

To this end, similarly to (37), let

$$\varpi_d(t) := \begin{bmatrix} x_a(t) \\ N e^{-Ht} \begin{bmatrix} x_T \\ 0 \end{bmatrix} \end{bmatrix} - e^{-Ht} \begin{bmatrix} x_T \\ 0 \end{bmatrix}, \quad (43)$$

with $N = \begin{bmatrix} 0 & I_n \end{bmatrix} \in \mathbb{R}^{n \times 2n}$, which is equal to zero for any t if and only if $\omega_d(t)$ is equal to $(x_T, 0)$ for any t , as prescribed by (42) specialized to the linear case.

Proposition 3: Consider the finite-horizon optimal control problem (31). Let $x_0 \in \mathcal{X}$ be given. Then for any $\varepsilon > 0$ there exists $\kappa(\varepsilon)$ such that the solution x_T^κ to

$$\begin{cases} H^i \begin{bmatrix} x_T \\ 0 \end{bmatrix} = \begin{bmatrix} (-1)^i x_i \\ N H^i \begin{bmatrix} x_T \\ 0 \end{bmatrix} \end{bmatrix}, \quad i = 1, \dots, \kappa - 1 \\ H^\kappa \begin{bmatrix} x_T \\ 0 \end{bmatrix} = \begin{bmatrix} -\frac{\kappa!}{T^\kappa} \left(x_T - x_0 + \sum_{j=0}^{\kappa-1} (-1)^j x_j (T^j / j!) \right) \\ N H^\kappa \begin{bmatrix} x_T \\ 0 \end{bmatrix} \end{bmatrix} \end{cases} \quad (44)$$

satisfies

$$\|x_T^\kappa - x^*(T)\|_2^2 < \varepsilon. \quad (45)$$

$\diamond$

Proof: By following arguments identical to those employed in the proof of Proposition 1, consider subsequent time-derivatives up to the order κ of ϖ_d at $t = 0$, which immediately yields the first $\kappa - 1$ equations in (44) where x_i denotes the i -th derivative of $x_a(t)$ evaluated at $t = 0$. The last equation, instead, is obtained by additionally considering the constraint $x_a(-T) = x_0$. $\square$

Remark 6: By extending the discussion in Remark 4 to the *dual* case of the fixed-point characterization of the optimal final state, it may be possible to employ the vectors $x_i \in \mathbb{R}^n$, solutions to (44), to define a truncated Taylor series approximation of $x_a(t)$ according to

$$\tilde{x}(t) = x_T + x_1(t-T) + x_2 \frac{(t-T)^2}{2} + \dots + x_\kappa \frac{(t-T)^\kappa}{\kappa!}, \quad (46)$$

where $x_\kappa = -\frac{\kappa!}{T^\kappa} (x_T - x_0 + \sum_{j=0}^{\kappa-1} (-1)^j x_j (T^j / j!))$. $\blacktriangle$

VI. FURTHER DISCUSSIONS ON COMPUTATIONAL ASPECTS

The objective of this section is to expand the discussion concerning the computational aspects of the strategy introduced above. This is achieved, first, by pointing out drawbacks of the approach, mainly by means of a few numerical simulations, and then by suggesting possible ways of circumventing or mitigating such shortcomings.

Fig. 4. Time-histories of the optimal costate variable $\lambda^*(t)$, $t \in [0, 1]$ (solid black line) and of the approximation obtained via the truncation (24) (solid gray lines), for different values of κ .

A. Minimizing the time-derivatives of the approximate costate

By combining the discussion in Remark 4 with the equation (30), it appears that the coefficient λ_κ^κ alone - which dictates the κ -th derivative of the function $\tilde{\lambda}(t)$ at time $t = 0$ - is “in charge” of compensating for the remainder of the truncation of the Taylor expansion at $t = T$, namely of enforcing $\tilde{\lambda}(T) = 0$. This aspect is illustrated via the following numerical simulation.

Example 1: Consider the finite-horizon optimal control problem in (1) with $q(x) = x^2$, $f(x) = x^2$, $g(x) = 1$, $x(t) \in \mathbb{R}$, and $T = 1$. In this case, the Hamiltonian vector field $X_{\mathbf{H}}$ is given by

$$X_{\mathbf{H}}(x, \lambda) := \begin{bmatrix} x^2 - \lambda \\ -x - 2x\lambda \end{bmatrix}. \quad (47)$$

The latter vector field can be then employed to construct the function $\mathcal{T}_\kappa(\lambda_0)$ according to (24) with the recursive operator $\mathcal{D}$ introduced in Definition 1. In this case, then, the function $\mathcal{T}_\kappa(\lambda_0)$ is a *univariate* polynomial in λ_0 , for fixed $x_0 \in \mathbb{R}$. In the following numerical simulations let $x_0 = 0.5$. The time histories of Figure 4 clearly illustrates the discussion at the beginning of this section. In fact, while on one hand the convergence to the optimal value λ_0^* of a solution to $\mathcal{T}_\kappa(\lambda_0) = 0$ for increasing κ is evident, on the other hand it can be also appreciated that, for small values of κ , the major shortcoming of the approximate solution $\tilde{\lambda}(t)$ consists in the fact that such a solution - despite being correctly equal to zero at $t = T$ - intersects the value $\lambda = 0$ with higher-order derivatives much larger than those of the optimal costate λ^* , as expected in light of (30). $\circ$

To counteract the issue illustrated in the example above while maintaining the order κ to a reasonable value, it may

be possible to introduce and employ *correction functions*, as detailed below.

Definition 2: A function $\psi_\lambda : \mathbb{R} \rightarrow \mathbb{R}$ is said to be an *initial correction function* of order κ if it is such that $\psi_\lambda(T) = \psi_\lambda^{(1)}(T) = \dots = \psi_\lambda^{(\kappa)}(T) = 0$. A possible selection of $\psi_\lambda(t)$ is provided by

$$\psi_\lambda(t) = \alpha \frac{(t - T)^{\kappa+1}}{(\kappa + 1)!}, \quad (48)$$

with arbitrary $\alpha \in \mathbb{R}^n$. $\circ$

As it appears from Definition 2, the augmented estimate of the costate $\lambda_\psi(t) = \tilde{\lambda}(t) + \psi_\lambda(t)$ has the property that $\lambda_\psi(T) = 0$, while the estimate of the initial condition for the state is modified according to $\lambda_\psi(0) = \lambda_0^\kappa + \psi_\lambda(0)$. In addition, by resuming the discussion illustrated in the Example 1 above, the criterion on which the arbitrary vector α in (48) is selected is that of minimizing the norm of a specific time-derivative, e.g. the highest one, of the (modified) costate variable in the *proximity* of the terminal time T . More precisely, the choice of α must satisfy

$$\min_{\alpha} \mathcal{C}_i(\alpha, \gamma) := \left| \lambda_\psi^{(i)}(\gamma T) - \sum_{j=i+1}^{\kappa} \tilde{\lambda}^{(j)}(0) \frac{(\gamma T)^j}{j!} \right|^2, \quad (49)$$

for some $\gamma \in \mathbb{R}$, which prescribes the time at which the i -th order time derivative of λ_ψ is minimized. Interestingly, the criterion (49) can be easily minimized in closed form, yielding

$$\alpha^*(\gamma) := \arg \min_{\alpha} \mathcal{C}_i = - \frac{(\kappa + 1 - i)!}{((\gamma - 1)T)^{\kappa+1-i}} \mathcal{D}_{i-1}(X_{\mathbf{H}}(x_0, \lambda_0^\kappa)), \quad (50)$$

where λ_0^κ is obtained by solving the equation $\mathcal{T}_\kappa(\lambda) = 0$. The effect of the selection of the *scalar* coefficient γ , which constitutes the remaining degree of freedom, is illustrated by means of the following numerical simulation

Example 2: Consider the finite-horizon optimal control problem in (1) with $q(x) = x^\top x$, $f(x) = Ax$, $g(x) = B$, $x(t) \in \mathbb{R}^2$, and $T = 2$, where

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad (51)$$

namely the system (1b) exhibits double integrator dynamics. Consider then the solution λ_0^4 to (35) with $\kappa = 4$. Figure 5 depicts the phase plot of the optimal costate (solid black line) and of the approximation $\tilde{\lambda}$ (solid gray line) for $\kappa = 4$. Suppose then that an initial correction function ψ_λ as in (48) is introduced and the vector $\alpha \in \mathbb{R}^2$ is selected to minimize $\mathcal{C}_i(\alpha, \gamma)$ in (49) for $i = \kappa$, namely to minimize the norm of the highest derivative of λ_ψ at $t = \gamma T$. By inspecting the structure of the unique minimizer (50), one realizes that the selection of the parameter γ naturally leads to a *line-search* strategy along the direction of the highest derivative defined by the constant vector $\mathcal{D}_{\kappa-1}(X_{\mathbf{H}}(x_0, \lambda_0^\kappa))$, represented by the dotted gray line in Figure 5, which leaves the time history of the costate not altered towards the end of the interval $[0, T]$. The latter points are clearly illustrated by the gray dashed lines in Figure 5 that

Fig. 5. Phase plot of the optimal costate (solid black line) and of the approximate costate $\tilde{\lambda}$ (solid gray line) obtained with $\kappa = 4$ in (35), together with the augmented functions λ_ψ obtained for different values of the parameter γ (dashed gray lines). The dotted line describes the direction of the κ -th order time derivative of the approximate costate $\tilde{\lambda}$.

describe the augmented function λ_ψ for different values of the parameter γ . $\circ$

Therefore, in general, the choice of γ can be based on a *line-search algorithm* to determine - along the direction induced by minimizing the norm of a certain derivative of the approximate costate - the augmented estimate

$$\lambda_\psi(0) = \lambda_0^\kappa + \alpha^*(\gamma) \frac{(-T)^{\kappa+1}}{(\kappa+1)!} \quad (52)$$

that yields a minimal norm of the costate $\lambda_\psi(T)$ at the terminal time. Moreover, the above construction can be iterated by considering the minimization of the norm of different time derivatives of the augmented function $\lambda_\psi(t)$, with the sequence of such derivatives induced by the optimal *steps* $\alpha_k^*(\gamma_k^*)$ of the line-search algorithm. This aspect is illustrated by means of two consecutive steps of the algorithm in Figure 6, which completes the discussion of Example 2. Note that the simulation is limited to two steps to more clearly visualize the directions induced by the derivatives of the approximate costate $\tilde{\lambda}$ and that a longer sequence of iterations would converge to the exact value of λ_0^* , as it can be appreciated from Figure 7.

B. Time-scaling

The statements of Theorems 3 and 4 suggest that large values of the terminal time T may hinder the precision and reliability of the numerical operations involved in the computation of the estimate of the optimal costate. One may then envision a strategy that consists in *scaling* the time variable t with respect to which the system (1b) is defined in such a way that the finite-horizon problem can be written in the (scaled) time interval $[0, 1]$. However, while allowing

Fig. 6. Phase plot of the optimal costate (solid black line) and of the approximate costate $\tilde{\lambda}$ (solid gray line) obtained with $\kappa = 4$ in (35). The gray square depicts λ_0^4 , while the gray circles represent two steps of the line search algorithm obtained via (49) and the optimal selection of γ .

Fig. 7. Convergence of the line-search algorithm to λ_0^* with respect to the iteration number k .

to relax the requirements in Assumption 3 associated to a smaller interval, it can be shown that such an approach leads to numerical computations identical to those of the *unscaled* case.

To this end, define the *scaled* time $\tau(t)$ such that $\tau(0) = 0$ and $\tau(T) = 1$, e.g. consider the linearly scaled time $\tau = t/T$. According to this definition, it is easy to see that the scaled dynamics become

$$\frac{dx}{d\tau} = \frac{dx}{dt} \frac{dt}{d\tau} = T f(x(\tau)) + T g(x(\tau)) u(\tau), \quad (53)$$

and that the cost functional is similarly scaled as

$$\frac{1}{2} \int_0^1 (Tq(x(\tau)) + T\|u(\tau)\|^2) d\tau. \quad (54)$$

It is then not difficult to see that the scaled Hamiltonian vector field $X_{\mathbf{H}}^s(x, \lambda)$ is related to the unscaled one according to $X_{\mathbf{H}}^s(x, \lambda) = TX_{\mathbf{H}}(x, \lambda)$. Therefore, to approximate the initial condition of the optimal costate in the setting of the scaled formulation, one should solve the equations

$$\begin{aligned} 0 &= \lambda_0 + N \sum_{i=1}^{\kappa} \mathcal{D}_{i-1}(X_{\mathbf{H}}^s(x_0, \lambda_0)) \frac{1}{i!} \\ &= \lambda_0 + N \sum_{i=1}^{\kappa} \mathcal{D}_{i-1}(TX_{\mathbf{H}}(x_0, \lambda_0)) \frac{1}{i!} \\ &= \lambda_0 + N \sum_{i=1}^{\kappa} T^i \mathcal{D}_{i-1}(X_{\mathbf{H}}(x_0, \lambda_0)) \frac{1}{i!}, \end{aligned} \quad (55)$$

where the last equality is obtained by definition of the operator $\mathcal{D}_i$, which coincides with (24). Finally, in the case of nonlinearly scaled time according to $\tau = \sigma(t)$, with $\sigma(0) = 0$ and $\sigma(T) = 1$, the scaled dynamics becomes *time-varying* as $dx/d\tau = \dot{\sigma}(\sigma^{-1}(\tau))(f(x(\tau)) + g(x(\tau))u(\tau))$.

C. Minimizing the “gap” between approximate state and costate

With the aim of combining ideas similar to those introduced in Section VI-A with the *dual* characterization of the optimal state as in Section V, and in particular in Remark 6, consider the following statement that extends Definition 2.

Definition 3: A function $\psi_x : \mathbb{R} \rightarrow \mathbb{R}$ is said to be a *terminal correction function* of order κ if it is such that $\psi_x(0) = \psi_x^{(1)}(0) = \dots = \psi_x^{(\kappa)}(0) = 0$. A possible selection of $\psi_x(t)$ is provided by

$$\psi_x(t) = \beta \frac{t^{\kappa+1}}{(\kappa+1)!}, \quad (56)$$

with arbitrary $\beta \in \mathbb{R}^n$. $\diamond$

Clearly, the modified approximate state $x_{\psi}(t) = \tilde{x}(t) + \psi_x(t)$ still verifies $x_{\psi}(0) = x_0$. Along the same lines of what has been discussed above, the initial and terminal correction functions may be employed to provide a more accurate approximation of the optimal state and costate without increasing the complexity of the algebraic equation (24). This objective can be achieved by selecting the parameters α and β according to the criterion

$$\min_{\alpha, \beta} \left\| \begin{bmatrix} \dot{\tilde{x}}(\bar{t}) + \dot{\psi}_x(\bar{t}) \\ \dot{\tilde{\lambda}}(\bar{t}) + \dot{\psi}_{\lambda}(\bar{t}) \end{bmatrix} - X_{\mathbf{H}}(\tilde{x}(\bar{t}) + \psi_x(\bar{t}), \tilde{\lambda}(\bar{t}) + \psi_{\lambda}(\bar{t})) \right\|^2, \quad (57)$$

namely such that the distance between the actual time derivatives of the approximate state and costate - obtained according to the (distinct) strategies discussed in Sections III and V - and the corresponding value of the Hamiltonian vector field, at a specific time $\bar{t} \in [0, T]$, is minimized.

To conclude this section two notable cases of interest in the linear setting are discussed in detail. These consist in the

selection of the available parameters α and β to improve, on one hand, the approximation of the costate initial condition - obtained by minimizing (57) at $\bar{t} = 0$ or, on the other hand, the approximation of the state terminal condition obtained by minimizing (57) at $\bar{t} = T$. Such cases are discussed in the following two statements, respectively.

Proposition 4: Consider the finite-horizon optimal control problem (31). Fix $\kappa > 0$ and consider the solutions λ_0^{κ} , λ_i and x_T , x_i , with $i = 1, \dots, \kappa$, to (35) and (44), respectively. Suppose that $\{(\kappa+1)/T\} \cap \sigma(A) = \emptyset$. Then

$$\alpha^* := -(G_2^{\top} G_2 + G_4^{\top} G_4)^{-1} (G_2^{\top} G_1 + G_4^{\top} G_3), \quad (58)$$

with

$$G_1 := \sum_{j=1}^{\kappa} x_j \frac{(-T)^{i-1}}{(i-1)!} - Ax_0 + BR^{-1}B^{\top} \lambda_0^{\kappa}, \quad (59a)$$

$$G_2 := BR^{-1}B^{\top} (-T)^{\kappa+1}/(\kappa+1)!, \quad (59b)$$

$$G_3 := \lambda_1 + Qx_0 + A^{\top} \lambda_0^{\kappa}, \quad (59c)$$

$$G_4 := \frac{(-T)^{\kappa}}{\kappa!} I + \frac{(-T)^{\kappa+1}}{(\kappa+1)!} A^{\top}, \quad (59d)$$

is the unique minimizer of (57) at $\bar{t} = 0$. $\diamond$

Proof: The claim is easily proven by noting that in the case of system (31b) the Hamiltonian vector field $X_{\mathbf{H}}$ is linear and that, by construction $\tilde{x}(0) + \psi_x(0) = x_0$, $\tilde{\lambda}(0) + \psi_{\lambda}(0) = \lambda_0^{\kappa} + \alpha(-T)^{\kappa+1}/(\kappa+1)!$, while $\dot{\tilde{x}}(0) + \dot{\psi}_x(0) = \sum_{i=1}^{\kappa} x_i(-T)^{i-1}/(i-1)!$ and $\dot{\tilde{\lambda}}(0) + \dot{\psi}_{\lambda}(0) = \lambda_1 + \alpha(-T)^{\kappa}/(\kappa!)$. Therefore, the minimization in (57) becomes

$$\min_{\alpha} \left\| \begin{bmatrix} G_1 + G_2 \alpha \\ G_3 + G_4 \alpha \end{bmatrix} \right\|^2, \quad (60)$$

which depends only on the vector α , and where the matrices G_j , $j = 1, \dots, 4$ are defined in (59). The proof is then concluded provided it is shown that the positive semi-definite matrix $G_2^{\top} G_2 + G_4^{\top} G_4$ is invertible. To this end, note that $G_4 = (-1)^{\kappa} \frac{T^{\kappa}}{\kappa!} \left(I - \frac{T}{\kappa+1} A^{\top} \right)$ is non-singular by the assumption on the spectrum of the matrix A . $\square$

A similar result can be stated in the case in which the solution to (57) is employed to improve the approximation of the terminal value of the state $\tilde{x}$, namely at $\bar{t} = T$.

Proposition 5: Consider the finite-horizon optimal control problem (31). Fix $\kappa > 0$ and consider the solutions λ_0^{κ} , λ_i and x_T , x_i , with $i = 1, \dots, \kappa$, to (35) and (44), respectively. Suppose that $\{(\kappa+1)/T\} \cap \sigma(A) = \emptyset$. Then

$$\beta^* := -(G_2^{\top} G_2 + G_4^{\top} G_4)^{-1} (G_2^{\top} G_1 + G_4^{\top} G_3), \quad (61)$$

with

$$G_1 := x_1 - Ax_T, \quad (62a)$$

$$G_2 := \frac{T^\kappa}{\kappa!} I - \frac{T^{\kappa+1}}{(\kappa+1)!} A, \quad (62b)$$

$$G_3 := \sum_{j=1}^{\kappa} \lambda_j \frac{T^{i-1}}{(i-1)!} + Qx_T, \quad (62c)$$

$$G_4 := \frac{T^{\kappa+1}}{(\kappa+1)!} Q, \quad (62d)$$

is the unique minimizer of (57) at $\bar{t} = T$. $\diamond$

The proof of Proposition 5 follows arguments identical to those employed in the proof of Proposition 4, hence it is omitted.

VII. CONCLUSIONS AND FURTHER DISCUSSIONS

In this paper a fixed-point characterization of the optimal costate variable in finite-horizon optimal control problems has been proposed for linear and nonlinear systems. In particular, the main idea revolves around the property that the *optimal* initial condition of the Hamiltonian dynamics must verify, together with an auxiliary function that replicates the time-evolution of the costate itself, a fixed-point condition with respect to the composition of a forward and backward flows of the Hamiltonian vector field. Due to the presence of time in the above condition, although rather insightful such a characterization is however not particularly practical and amenable to numerical computations. Therefore, it has been shown that the above property can be cast in more constructive requirements by relying on the notion of (repeated) Lie brackets, which involve the Hamiltonian vector field and a suitably defined projective vector field and which are evaluated at a single point in the state-space. This strategy then yields a system of algebraic equations in the costate initial condition, the number of which always matches the dimension of the state of the underlying system regardless of the prescribed degree of accuracy for the approximation.

As further developments concerning the computation of the optimal costate, it would be of interest to expand the discussion about the main computational features of the algorithm. The final outreach is to envision and develop computationally efficient routines to compute or approximate the optimal costate. Moreover, the idea of deriving algebraic conditions from fixed-point characterizations in composition of flows seems appealing in diverse fields of application, in additional to optimal control, such as the computation of invariant sets, periodic orbits of nonlinear systems as well as concepts related to nonlinear reachability and controllability. Finally, similar abstract, geometric considerations may be extended also to the class of continuous-time stochastic systems by relying on an adapted formulation of the Hamiltonian dynamics, in which the backward evolution must be suitably defined to avoid violating nonanticipativeness of the solutions [41].

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