

STATE-CONSTRAINED DETERMINISTIC OPTIMAL CONTROL AS UNCONSTRAINED SMOOTH OPTIMIZATION IN THE COSTATE

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Abstract. We study deterministic optimal control problems in Bolza form and show that they admit a reformulation as an *unconstrained, smooth* optimization problem in the space of costate trajectories. The resulting dual problem is proved to be *value equivalent* to the classical primal formulation under mild, standard assumptions (compactness/relaxation of the control set and convexity of the Lagrangian in the control). By a Danskin-type envelope argument, the gradient of the dual objective depends only on *partial* derivatives of the Hamiltonian and is obtained by a single forward-adjoint simulation, without differentiating the minimizing control map. The framework extends seamlessly to state constraints via the *tangential Hamiltonian* built from the Bouligand tangent cone, yielding the same gradient structure.

We also present an implementation-ready numerical template: spline parameterization of the costate, adaptive forward-adjoint ODE solvers, and L-BFGS with line search. To certify near-optimality, we maximize a parametric HJB *subsolution* to produce a rigorous dual lower bound and report a primal-dual gap. When the Hamiltonian is non-smooth or costly to evaluate, we introduce an *adaptive piecewise-affine surrogate* together with a universal smoothing parameter δ ; this delivers monotone upper bounds with a controllable bias and Lipschitz continuous gradients. On canonical tests (LQR, minimum-time double integrator with box constraints, and a corridor-constrained Dubins car), the method recovers the known solutions and provides small, certified gaps. Altogether, the costate-optimization viewpoint combines the analytical strengths of PMP and HJB with the robustness of modern smooth optimization.

Key words. Deterministic optimal control; Hamilton–Jacobi–Bellman (HJB) equation; Pontryagin maximum principle; dual-control formulation; costate optimization (λ -optimization); Danskin/Envelope theorem; adjoint-based gradient; viscosity solutions; state constraints; tangential Hamiltonian; measurable selection and relaxed controls; spline discretization of costates; L-BFGS and line-search; adaptive time stepping; primal-dual (gap) certification; HJB subsolution lower bounds; piecewise-affine Hamiltonian surrogates; Moreau–Yosida / log-sum-exp smoothing.

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1. Introduction. Deterministic optimal control problems arise across engineering, economics, and the sciences, yet remain challenging to solve, particularly under state constraints. Classical approaches divide broadly into indirect methods based on necessary conditions and dynamic programming based on value functions. In the indirect approach, the Pontryagin Maximum Principle (PMP) furnishes first-order conditions via costate (adjoint) variables and stationarity of the Hamiltonian [14, 5]. This reduces the task to solving a two-point boundary value problem (TPBVP) for the state and costate with boundary conditions at initial and final times. While PMP provides elegant analytical structure, shooting methods for the TPBVP are sensitive to the unknown initial costate and to problem data; small perturbations of the guess can cause large trajectory deviations, especially with bang-bang or singular controls. Modern expositions, including nonsmooth and constrained cases, can be found in [6]. Notably, early work by [10] articulated a dual perspective that treats the costate as a Lagrange multiplier (a shadow price), foreshadowing some of the ideas developed here.

Direct methods avoid the TPBVP by transcribing the control problem to a finite-dimensional nonlinear program (NLP), discretizing the control and often the state, and then minimizing the cost subject to discrete dynamics and constraints [3]. They are robust to initialization and handle path constraints naturally through algebraic inequalities. Pseudospectral collocation methods, for instance, approximate state and control by global polynomial bases and enforce dynamics at collocation

nodes [8]. However, direct methods typically yield large NLPs after refinement and rely on generic solvers; they do not automatically recover costates (without a separate adjoint computation), and they lack the global optimality guarantees of dynamic programming.

Dynamic programming, via Bellman’s principle of optimality, characterizes the value function $U(t, x)$ and yields the Hamilton–Jacobi–Bellman (HJB) equation, a first-order nonlinear PDE [2, 7]. The HJB framework provides verification results and feedback controls under appropriate conditions [9]. In practice, however, HJB solvers face the curse of dimensionality, with complexity growing exponentially in state dimension. Remedies include max-plus basis methods that propagate value approximations without full grids [1], and occupation-measure approaches that relax the control problem to hierarchies of semidefinite programs [13]. These yield, respectively, tractable approximations or convergent lower bounds at nontrivial computational cost.

State constraints (requiring $x(t) \in K$ for all t) complicate all of the above. In the PMP setting they induce additional multipliers and junction conditions, and exacerbate sensitivity in shooting; in the HJB setting they require viability boundary conditions on ∂K and the use of the tangential Hamiltonian to ensure trajectories remain feasible [17, 18]. Direct methods can encode such constraints but at the price of larger, potentially stiffer NLPs. A unified, numerically robust treatment remains challenging.

This work. We introduce a dual-control formulation that recasts the (possibly state-constrained) deterministic optimal control problem as an *unconstrained, smooth* optimization in the space of costate trajectories. The decision variable is the time-dependent costate $\lambda(\cdot)$. Given $\lambda(\cdot)$, we evolve the state by the *dual dynamics* $\dot{x} = \partial_\lambda H(t, x, \lambda, 1)$ and evaluate the cost by $J(\lambda) = \int_0^T \partial_\gamma H(t, x(t), \lambda(t), 1) dt + g(x(T))$. We prove *value equivalence*: under standard assumptions, the infimum of $J(\lambda)$ over admissible costate fields equals the optimal value of the original control problem. This connects to convex duality perspectives in optimal control [10] while retaining the full nonlinear structure.

The formulation has several practical advantages. First, by a Danskin/envelope argument, the variational derivative $\delta J/\delta \lambda$ depends only on $\partial_x H$ and $\partial_\gamma H$ along the trajectory and does not require differentiating the minimizing control with respect to λ . This yields stable adjoint-based gradients even for bang-bang controls, leveraging standard results in parametric optimization [15, 4]. Second, state constraints are handled seamlessly by replacing H with the *tangential Hamiltonian* H_K that minimizes over feasible controls $u \in A_K(t, x)$ keeping the dynamics tangent to K on ∂K ; the same gradient structure applies, and value equivalence persists under viability conditions [17, 18]. Third, because the problem is an unconstrained smooth minimization, modern first/second-order solvers (e.g., L-BFGS with line search) can be applied directly to a finite-dimensional spline or piecewise-polynomial parameterization of $\lambda(\cdot)$. Each gradient evaluation entails one forward and one backward ODE of dimension equal to the state, comparable in cost to an indirect forward-backward sweep, but without boundary shooting sensitivity.

We also develop two implementation components that improve robustness. (i) For nonsmooth Hamiltonians (e.g., bang-bang selectors), we use a *piecewise-affine* bundle surrogate for H together with a universal smoothing (Moreau–Yosida or log-sum-exp), which provides Lipschitz gradients and a controllable bias; this follows classical bundle approximation results [11]. (ii) We compute a rigorous *duality certificate* by training an HJB *subsolution* v with $v_t + H(t, x, \nabla_x v) \leq 0$ and $v(T, \cdot) \leq g$, yielding a lower

bound $v(0, x_0)$ and a certified primal–dual gap for the reported trajectory.

Contributions. (1) A costate–optimization reformulation of deterministic optimal control (with state constraints) as unconstrained smooth minimization, with a proof of value equivalence. (2) An adjoint gradient for $J(\lambda)$ derived via Danskin’s theorem and parametric optimization calculus [15, 4]. (3) A seamless state–constraint treatment through the tangential Hamiltonian in the sense of [17, 18]. (4) A practical algorithm: spline parameterization of $\lambda(\cdot)$, adaptive ODE integration, and L–BFGS optimization, plus bundle–smoothing of H for nonsmooth problems. (5) A primal–dual certification procedure based on HJB subsolutions. The approach blends the analytical strengths of PMP/HJB with the numerical robustness of smooth optimization and avoids the curse of dimensionality intrinsic to grid–based dynamic programming.

Companion work. In a companion manuscript, we develop a Pontryagin–based solver that combines a universally smoothed Hamiltonian H_δ , a piecewise–affine (PA) bundle surrogate in the costate, and a symplectic multiple–shooting Newton method with adaptive refinement of Δt , PA planes, and δ . That solver targets the two–point boundary value problem from PMP and emphasizes geometric structure and Newton efficiency. In contrast, the present paper reformulates the control problem as an unconstrained smooth *optimization* in the costate—proving value equivalence, deriving an adjoint gradient via Danskin’s theorem, handling state constraints through the tangential Hamiltonian, and supplying a *primal–dual certificate* via HJB subsolutions. The two approaches are complementary: the PMP–Newton method is a structure–preserving indirect solver; the costate–optimization method is a smooth, certification–friendly optimization solver. We use the same Hamiltonian smoothing and PA–bundle ideas, but deploy them differently in the numerical pipelines [19].

Related literature. Our work interfaces with the PMP line of research [14, 5, 6], dynamic programming and viscosity solutions [7, 2, 9], convex–analytic duality and envelope theorems [15, 4], and viability/state–constraint HJB [17, 18]. It also relates to direct transcription and collocation methods [3, 8], max–plus approaches [1], occupation–measure relaxations [13], and bundle–type Hamiltonian approximations [11]. A detailed comparison and numerical illustrations appear later in the paper.

2. Deterministic OC Formulations and Main Theoretical Results. Problem (P1) and Hamiltonian. Let $T > 0$, $d \in \mathbb{N}$, and let $A \subset \mathbb{R}^m$ be the set of admissible controls. We consider the deterministic optimal control problem in Bolza form:

$$\min_{\alpha(\cdot)} \left\{ \int_0^T h(t, x(t), \alpha(t)) dt + g(x(T)) \right\} \quad \text{s.t.} \quad \dot{x}(t) = a(t, x(t), \alpha(t)), \quad x(0) = x_0,$$

with measurable controls $\alpha : [0, T] \rightarrow A$ and absolutely continuous states $x : [0, T] \rightarrow \mathbb{R}^d$. We define the (extended) Hamiltonian

$$H(t, x, \lambda, \gamma) := \min_{\alpha \in A} \left\{ \lambda^\top a(t, x, \alpha) + \gamma h(t, x, \alpha) \right\},$$

and the associated value function of (P1) by

$$U_1(t, x) := \inf_{\alpha(\cdot)} \left\{ \int_t^T h(s, x(s), \alpha(s)) ds + g(x(T)) \mid \dot{x} = a(s, x, \alpha), \quad x(t) = x \right\}.$$

Assumptions. We will refer to the following standing assumptions:

- (A1) A is nonempty and either compact or such that the map $\alpha \mapsto \lambda^\top a(t, x, \alpha) + \gamma h(t, x, \alpha)$ is coercive; hence the min in H is attained.
- (A2) a, h are continuous in (t, x, α) and measurable in t ; $g \in C^1(\mathbb{R}^d)$.
- (A3) For each (t, x, λ, γ) , the map $\alpha \mapsto \lambda^\top a(t, x, \alpha) + \gamma h(t, x, \alpha)$ is convex on A . Consequently, $H(t, x, \cdot, \gamma)$ is concave in λ ; this convexity avoids a relaxation (duality) gap.
- (A4) (Existence) An optimal control exists (possibly after standard relaxation of the control set); see, e.g., [20].
- (A5) (Measurable selection) There exists a measurable selector $\hat{\alpha}(t, x, \lambda) \in \arg \min_{\alpha \in A} \{\lambda^\top a + \gamma h\}$ [6, 20].
- (A6) (Regularity for λ -calculus) Either the minimizer is unique or H is differentiable in (λ, γ) ; otherwise we interpret derivatives in the Clarke subgradient sense. This legitimizes envelope/Danskin arguments [15, 4].

Remark. Assumption (A3) is crucial: without convexity in α , the dual formulation below corresponds to the convexified problem, and a relaxation gap may appear (cf. [10]).

Dual formulation (P2). Given a costate trajectory $\lambda(\cdot) : [0, T] \rightarrow \mathbb{R}^d$, define the *dual dynamics*

$$\dot{x}(t) = \partial_\lambda H(t, x(t), \lambda(t), 1), \quad x(0) = x_0,$$

and the dual objective

$$J(\lambda) = \int_0^T \partial_\gamma H(t, x(t), \lambda(t), 1) dt + g(x(T)).$$

The *dual problem* (P2) is to minimize $J(\lambda)$ over admissible $\lambda(\cdot)$. Its value function is

$$U_2(t, x) := \inf_{\lambda(\cdot)} \left\{ \int_t^T \partial_\gamma H(s, x(s), \lambda(s), 1) ds + g(x(T)) \mid \dot{x} = \partial_\lambda H, x(t) = x \right\}.$$

Value equivalence.

THEOREM 2.1 (Value equivalence). *Under (A1)–(A6), $U_1(t, x) = U_2(t, x)$ for all $(t, x) \in [0, T] \times \mathbb{R}^d$.*

Proof sketch. ($U_1 \leq U_2$) Let $\lambda(\cdot)$ be admissible for (P2), and let $x(\cdot)$ solve the dual dynamics. By (A5) there is a measurable control $\alpha(t) = \hat{\alpha}(t, x(t), \lambda(t))$ such that $a(t, x(t), \alpha(t)) = \partial_\lambda H(t, x(t), \lambda(t), 1)$. Therefore the pair $(x(\cdot), \alpha(\cdot))$ is admissible for (P1) and attains the cost $J(\lambda)$; hence $U_1 \leq J(\lambda)$, and taking the infimum over λ gives $U_1 \leq U_2$.

($U_2 \leq U_1$) Let $\alpha^*(\cdot)$ be optimal for (P1) with trajectory $x^*(\cdot)$ and costate $\lambda^*(\cdot)$ given by PMP [14, 5]. Then $\alpha^*(t) \in \arg \min_{\alpha} \{\lambda^{*\top} a + h\}$ and $\dot{x}^* = \partial_\lambda H(t, x^*, \lambda^*, 1)$, so $\lambda^*(\cdot)$ is feasible for (P2) and $J(\lambda^*) = U_1$. Thus $U_2 \leq U_1$. \square

REMARK 1. *An alternative proof of the equality between the value functions from (P1) and (P2) is based on stability estimates and best approximation, similar to the proof of the continuity of value functions in terms of perturbations of Hamiltonians.*

Indeed, we can represent the error between value functions corresponding to different costates, an approximate one, $\bar{\lambda}$ and the exact one,

$$\lambda = \nabla U(t, x_t),$$

as
(2.1)

$$\begin{aligned} U(0, x_0; \bar{\lambda}) - U(0, x_0; \lambda) &= \int_0^T \{H(\bar{x}_t, \bar{\lambda}_t) - H(\bar{x}_t, \lambda_t) + \partial_\lambda H(\bar{x}_t, \bar{\lambda}_t)(\nabla U(t, \bar{x}_t) - \bar{\lambda}_t)\} dt \\ &= -\frac{1}{2} \int_0^T (\nabla U(t, \bar{x}_t) - \bar{\lambda}_t)^T \partial_\lambda^2 H(\bar{x}_t, \lambda_t) (\nabla U(t, \bar{x}_t) - \bar{\lambda}_t) dt + h.o.t. \end{aligned}$$

provided that we have enough differentiability in H to do the last expansion. The first line above can still be used to conclude the equality between the value functions of (P1) and (P2), using just the λ -Lipschitz continuity of the Hamiltonian.

First variation and adjoint gradient. Define the shorthand

$$\tilde{a}(t, x, \lambda) := \partial_\lambda H(t, x, \lambda, 1), \quad \tilde{h}(t, x, \lambda) := \partial_\gamma H(t, x, \lambda, 1).$$

Given an admissible $\lambda(\cdot)$ and its state $x(\cdot)$, the first variation of J in the direction $\delta\lambda$ is

$$\langle \partial_\lambda J(\lambda), \delta\lambda \rangle = \int_0^T \varphi(t)^\top [\partial_\lambda \tilde{a}(t, x, \lambda) + \partial_\lambda \tilde{h}(t, x, \lambda)] \delta\lambda(t) dt,$$

where φ solves the adjoint ODE

$$\dot{\varphi}(t) = -(\partial_x \tilde{a}(t, x, \lambda))^\top \varphi(t) - (\partial_x \tilde{h}(t, x, \lambda))^\top, \quad \varphi(T) = \nabla g(x(T)).$$

If H is C^2 in (λ, γ) , then $\partial_\lambda \tilde{a} = \partial_{\lambda\lambda}^2 H$ and $\partial_\lambda \tilde{h} = \partial_{\lambda\gamma}^2 H$, giving

$$\langle \partial_\lambda J(\lambda), \delta\lambda \rangle = \int_0^T \varphi(t)^\top [\partial_{\lambda\lambda}^2 H + \partial_{\lambda\gamma}^2 H](t, x(t), \lambda(t), 1) \delta\lambda(t) dt.$$

This envelope (Danskin) calculation avoids differentiating the minimizing control with respect to λ ; see [15, 4].

REMARK 2 (Lipschitz continuity of $\nabla_\theta \bar{J}_\delta$). If H_δ is a C^1 smoothing of H with $\nabla_\lambda H_\delta$ locally Lipschitz in (x, λ) uniformly along trajectories and a, h have at most polynomial growth in x , then the map $\theta \mapsto \bar{J}_\delta(\theta)$ (with $\lambda_h(t) = \sum_j \theta_j \varphi_j(t)$) has an L^2 -gradient that is Lipschitz on bounded sets. Consequently, line-search L -BFGS and gradient descent admit standard global convergence to first-order stationary points for the smoothed model.

REMARK 3. Here we have assumed enough regularity to write the $\delta_\lambda J$ variation.

This is possible to achieve with (P₂) by smoothing the Hamiltonian in the λ direction and controlling the resulting L^∞ error. This can be done universally using the concavity of the Hamiltonian in λ , representing it first as a minimum of affine functions and then approximating by first using finitely many affine functions in the minimum and regularizing the min function by a smooth L^∞ approximation of it.

This is not obvious to achieve with (P₁), since in that formulation, we may have Bang-Bang controls with complex structure.

Discretization and convergence. Let $\Lambda_h \subset L^2(0, T; \mathbb{R}^d)$ be a finite-dimensional space (e.g., piecewise polynomials or B-splines on a partition of $[0, T]$) and consider

the discrete problem

$$\inf_{\lambda_h \in \Lambda_h} J(\lambda_h) \quad \text{subject to} \quad \dot{x} = \partial_\lambda H(t, x, \lambda_h(t), 1), \quad x(0) = x_0.$$

THEOREM 2.2 (Consistency of λ -discretization). *Assume H is C^1 and $\partial_\lambda H$ is locally Lipschitz in (x, λ) . If the union of spaces Λ_h is dense in $L^2(0, T; \mathbb{R}^d)$, then $\inf_{\lambda_h \in \Lambda_h} J(\lambda_h) \rightarrow \inf_\lambda J(\lambda)$ as $h \rightarrow 0$. If, in addition, the minimizer is unique, any sequence of λ_h -minimizers has a subsequence converging weakly in L^2 to λ^* , and the corresponding trajectories converge uniformly to x^* .*

Idea of proof. Density of Λ_h yields recovery sequences; the local Lipschitz property gives continuous dependence of $x(\cdot)$ on $\lambda(\cdot)$ (Gronwall). Lower semicontinuity of J and compactness (up to subsequences) imply convergence of infima; uniqueness yields convergence of minimizers. This aligns with known convergence results in direct discretization and collocation methods [8, 3]. \square

Remarks.

- (PMP–HJB link) If the value function U is differentiable, the costate along an optimal trajectory satisfies $\lambda(t) = \nabla_x U(t, x(t))$ [9, Ch. 4]; see also [2, 7].
- (State constraints) All statements extend by replacing H with the *tangential* Hamiltonian H_K enforcing viability on ∂K [17, 18].
- (Nonconvex A) Without (A3) the dual problem solves the convexified control problem; the gap between U_2 and U_1 then serves as a relaxation certificate [10].
- (Relation to the companion solver) The same Hamiltonian smoothing and PA-bundle ideas used here are deployed differently in the companion Pontryagin-based Newton multiple-shooting solver; see [19].

3. Related work. Indirect (PMP) and shooting. The Pontryagin Maximum Principle (PMP) is the classical necessary condition for optimality, introducing costates and a stationarity condition on the Hamiltonian; see the original monograph and standard textbooks for numerous examples [14, 5, 6]. Numerically, PMP leads to boundary value problems solved by single/multiple shooting. The main challenge is sensitivity to the unknown initial costate and switching structure (especially in bang–bang and singular cases). Our formulation departs from shooting by turning the costate into the *optimization variable*, avoiding boundary matching altogether while preserving the Hamiltonian structure.

Dynamic programming (HJB) and viscosity solutions. Bellman’s principle yields the Hamilton–Jacobi–Bellman (HJB) equation for the value function and verification results in feedback form [2, 9]. Existence/uniqueness in the appropriate class is provided by viscosity solutions [7]. While HJB provides global optimality, grid-based solvers are limited by the curse of dimensionality. Our dual formulation leverages the Hamiltonian and costate ideas of HJB/PMP, but keeps computations *trajectory-based*, thus avoiding state-space gridding while enabling a dual (subsolution) certificate.

Direct transcription and collocation. Direct methods transcribe the control problem into a finite-dimensional nonlinear program by discretizing the state/control and enforcing dynamics at collocation points [3]. High-order pseudospectral methods (e.g., Legendre collocation) provide accurate discretizations for smooth problems [8]. In contrast, we optimize directly in a low-order spline basis for the costate: this keeps the forward/adjoint solve cheap (two d -dimensional ODEs per iteration) and integrates naturally with the Hamiltonian structure through Danskin-type calculus.

Convex duality and envelope theorems. Our gradient formula for $J(\lambda)$ follows from envelope (Danskin) arguments in parametric optimization [15, 4]. The equivalence of values between the primal and our dual problem connects to strong duality ideas in convex optimal control (no gap under convexity of the Lagrangian in the control) [10]. We make this equivalence constructive and computational: every feasible $\lambda(\cdot)$ induces a feasible primal trajectory (via $\partial_\lambda H$), and vice versa, while the gradient of J is accessible by a single forward–backward sweep without differentiating the control selector.

State constraints and viability. State constraints are rigorously handled in the viscosity framework via viability boundary conditions and the *tangential* Hamiltonian [17, 18]. We adopt exactly this mechanism: to enforce $x(t) \in K$, we replace H by the tangential H_K (i.e., minimize over feasible controls that keep \dot{x} tangent to K at ∂K). This yields a seamless extension of our value equivalence and gradient formulas to constrained problems.

Relaxations and occupation measures. A complementary convex-analytic line approximates the value by solving linear programs over occupation measures with semidefinite relaxations [13]. These produce convergent lower bounds (and sometimes controls), at the price of heavy conic optimization. Our dual subsolution (HJB) training also provides rigorous lower bounds, but within a lightweight, trajectory-based pipeline that pairs naturally with the primal costate optimization.

Max-plus methods and basis expansions. Max-plus finite element methods approximate value functions by suprema of affine/quadratic basis functions and propagate them in time [1]. We borrow the idea of max-plus (supremum) combinations when training HJB subsolutions for dual certification. This is complementary to our Hamiltonian approximation (piecewise-affine majorants in (λ, γ)) used on the *primal* side of (P2).

Smoothing and bundle approximations. We rely on two standard devices: (i) *piecewise-affine* (bundle) models of the Hamiltonian in (λ, γ) with $O(1/m)$ uniform approximation rates under convexity [11], and (ii) universal smoothing (e.g., Moreau envelope or soft-max) to ensure Lipschitz gradients, with a tunable bias controlled by the smoothing parameter. These tools stabilize gradients in bang–bang regimes and support certified upper bounds (since we approximate H from above).

Companion work: smoothed-PMP Newton solver. In a companion manuscript we develop a multiple-shooting Newton solver for the PMP system that uses the same two ingredients—universally smoothed Hamiltonians and PA-bundle oracles—but deploys them for structure-preserving indirect integration and adaptive refinement of $(\Delta t, m, \delta)$. That solver targets the TPBVP directly (indirect method). In contrast, the present paper optimizes directly over costate trajectories (unconstrained smooth optimization), proves value equivalence, handles state constraints via H_K , and supplies a primal–dual gap certificate via HJB subsolutions [19]. The two approaches are complementary and can share oracles and diagnostics.

4. Numerics. We parameterize the costate as $\lambda_h(t) = \sum_{j=1}^M \theta_j \phi_j(t)$ in a finite-dimensional space $\Lambda_h = \text{span}\{\phi_1, \dots, \phi_M\}$ (e.g., piecewise linear or cubic splines, Bsplines, or localized Fourier windows). A coarse choice of M (few basis functions) yields a suboptimal but feasible dual solution; increasing M (refining the time grid) improves accuracy, consistent with Theorem 2.2. In our experience, low-order splines are often sufficient, and the time partition can be adapted to solution features (Sec-

tion 4.2). A simple initial guess for the parameters is $\lambda(t) \equiv 0$ (or the costate obtained from an LQR linearization).

Algorithm (one-shot template for (P2)).

1. Choose a finite space $\Lambda_h = \text{span}\{\varphi_j\}_{j=1}^M$ (e.g., splines). Initialize $\theta^{(0)}$.
2. Given $\theta^{(k)}$: set $\lambda_h(t) = \sum_j \theta_j^{(k)} \varphi_j(t)$.
3. Solve forward: $\dot{x} = \partial_\lambda H(t, x, \lambda_h, 1)$, $x(0) = y$; solve backward: $\dot{\phi} = -\partial_x \partial_\lambda H \phi - \partial_x \partial_\gamma H$, $\phi(T) = g'(x(T))$.
4. Compute the L^2 -gradient $\nabla_\theta \bar{J}(\theta^{(k)}) = \left(\int_0^T [\phi^\top \partial_{\lambda\lambda}^2 H + \partial_{\lambda\gamma}^2 H] \varphi_j dt \right)_j$.
5. Update $\theta^{(k+1)}$ with L-BFGS (Wolfe line-search; optional Tikhonov/ H^1 regularizer).
6. (Optional) Dual lower bound: train a subsolution v_ψ and report $\text{Gap} = \bar{J}(\lambda_h) - v_\psi(0, y)$.

REMARK 4 (Numerical use of (P2): discretization of λ and smooth optimization). We approximate $\lambda(\cdot) \in \Lambda(0, T) = L^2(0, T; \mathbb{R}^d)$ in a finite-dimensional subspace $\Lambda_h = \text{span}\{\varphi_1, \dots, \varphi_M\}$, e.g. with (vector-valued) splines or piecewise polynomials on a temporal partition $0 = t_0 < t_1 < \dots < t_N = T$:

$$\lambda_h(t) = \sum_{j=1}^M \theta_j \varphi_j(t), \quad \theta = (\theta_j)_{j=1}^M \in \mathbb{R}^{Md}.$$

Typical choices are (i) piecewise constants/linears, (ii) cubic C^2 B-splines with Greville abscissae, or (iii) a low-order Fourier/sigmoid basis when smoothness is desired. Given θ , we solve the state ODE $\dot{x} = \tilde{a}(t, x, \lambda_h) = \partial_\lambda H(t, x, \lambda_h, 1)$ forward with $x(0) = y$, and the adjoint

$$\phi(T) = g'(x(T)), \quad \dot{\phi}(t) = -\partial_x \tilde{a}(t, x, \lambda_h)^\top \phi(t) - \partial_x \tilde{h}(t, x, \lambda_h)^\top,$$

backward, where $\tilde{h} = \partial_\gamma H(\cdot, \cdot, \cdot, 1)$. The gradient in parameter space is obtained by the L^2 Riesz map:

$$\nabla_\theta \bar{J}(\theta) = \left(\int_0^T [\phi(t)^\top \partial_{\lambda\lambda}^2 H + \partial_{\lambda\gamma}^2 H](t, x(t), \lambda_h(t)) \varphi_j(t) dt \right)_{j=1}^M.$$

We then minimize $\bar{J}(\theta)$ by smooth first/second-order methods. In practice, memory-limited quasi-Newton (L-BFGS or L-BFGS-B for simple bounds) with Wolfe line-search is robust. A mild Tikhonov regularizer on θ or an H^1 -seminorm on λ_h stabilizes ill-conditioned or bang-bang regimes; for state constraints replace H by H_K without any other algorithmic change.

REMARK 5 (Lipschitz continuity of $\nabla_\theta \bar{J}_\delta$). If H_δ is a C^1 smoothing of H with $\nabla_\lambda H_\delta$ locally Lipschitz in (x, λ) along trajectories and a, h have at most polynomial growth in x , then the map $\theta \mapsto \bar{J}_\delta(\theta)$ (with $\lambda_h = \sum_j \theta_j \varphi_j$) has an L^2 -gradient that is Lipschitz on bounded sets. Consequently, Wolfe line-search with L-BFGS or gradient descent yields global convergence to first-order stationary points for the smoothed model.

REMARK 6 (A dual for (P2) and a computable duality gap). While (P2) is a primal, an effective dual lower bound comes from a parametric HJB subsolution. Let $v_\psi : [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}$ be a trial function (e.g. splines/NN/polynomials) satisfying the terminal inequality $v_\psi(T, x) \leq g(x)$ and the subsolution constraint

$$-\partial_t v_\psi(t, x) \leq H(t, x, \nabla_x v_\psi(t, x)) \quad \text{for a.e. } (t, x).$$

Then $v_\psi(0, y)$ is a valid dual lower bound on the optimal value. Consequently, for any λ_h feasible in (P2) we obtain the certified duality gap

$$\text{Gap}(\lambda_h, \psi) = \bar{J}(\lambda_h) - v_\psi(0, y) \geq 0.$$

Numerically one can enforce the subsolution constraints at space–time collocation points (inequality projection or hinge penalties), and maximize $v_\psi(0, y)$ over ψ while keeping the constraints; in the state–constrained case replace H by the tangential Hamiltonian H_K . This produces a practical primal–dual pair: minimize $\bar{J}(\lambda_h)$ and maximize $v_\psi(0, y)$ to report a reliable certificate $\text{Gap} \downarrow 0$.

Dual training (penalty or projection).. Maximize $v_\psi(0, y)$ subject to

$$-\partial_t v_\psi(t_i, x_{i\ell}) \leq H_K(t_i, x_{i\ell}, \nabla v_\psi(t_i, x_{i\ell}))$$

and $v_\psi(T, \xi_r) \leq g(\xi_r)$ at collocation nodes $\{(t_i, x_{i\ell})\} \subset [0, T] \times K$, $\{\xi_r\} \subset K$. Use either (i) hinge penalties with weights (β, β_T) or (ii) projection onto the inequality cone at nodes. A Lipschitz buffer on H_K yields certification in neighborhoods of the nodes.

REMARK 7 (Affine subsolutions, trajectory enforcement, and certification). A convenient dual ansatz is affine in the state: $v_\psi(t, x) = a(t)^\top x + b(t)$ with (a, b) in a spline space. If one enforces the subsolution inequalities only along a given trajectory $x(\cdot)$, one obtains

$$-\partial_t v_\psi(t, x(t)) \leq H_K(t, x(t), \nabla_x v_\psi(t, x(t))), \quad v_\psi(T, x(T)) \leq g(x(T)).$$

When $x(\cdot)$ is the optimal trajectory, this yields $v_\psi(0, y) \leq J^*$; however, for a generic candidate trajectory it only guarantees $v_\psi(0, y) \leq J(x)$ and does not certify a dual lower bound on the optimal value J^* . To retain certification while keeping the model lightweight, we (i) enforce the inequalities on a coarse space–time grid $(t_i, x_{i\ell} \in K)$ with a Lipschitz buffer on H_K so that they hold in small neighborhoods of the nodes, and (ii) adapt the grid around the current primal trajectory. This yields a bona fide viscosity subsolution and hence a rigorous dual lower bound $v_\psi(0, y) \leq J^*$, while preserving the simplicity of an affine $\nabla_x v_\psi(t, \cdot) = a(t)$. In linear–quadratic cases an affine ansatz is generally insufficient (quadratic v is exact), whereas for control–affine dynamics with convex piecewise–linear costs, max–plus combinations of affine functions provide systematically improvable certified lower bounds.

Max-plus subsolutions.. Suprema of affine subsolutions (max-plus bases) produce monotone, certified lower bounds that improve as planes are added, synergizing with our piecewise–affine Hamiltonian section.

REMARK 8 (Adaptive time stepping for the forward/adjoint solves).

We employ adaptive integration to resolve the state and adjoint ODEs accurately. In particular, we use embedded Runge–Kutta error controllers (or adjoint-weighted residual estimators) to refine the time grid \mathcal{T} in regions where the state or adjoint variables evolve rapidly (e.g., near control switching times or near the boundary of a state constraint). This strategy mirrors the adjoint-driven time-step adaptivity used in indirect shooting methods and improves the accuracy of both the forward trajectory and the gradient computation [12, 16]. For the backward integration, we reuse the refined forward time grid to evaluate $\varphi(t)$, which avoids interpolation error in the inner products that define $\nabla_\theta J$.

REMARK 9 (Adaptive piecewise-affine Hamiltonian surrogates and universal δ -regularization). When H (or H_K) is expensive or nonsmooth in (λ, γ) , a practical surrogate is a piecewise-affine approximation built from supporting hyperplanes. Maintain a set of affine minorants $\{L_i(\lambda, \gamma) = c_i + b_i^\top(\lambda, \gamma)\}_{i=1}^m$ and define

$$H^{\text{PA}}(\lambda, \gamma) = \max_{1 \leq i \leq m} L_i(\lambda, \gamma).$$

Refine adaptively by sampling (t, x) along current trajectories, adding planes from local linearizations or bundle cuts at points with largest surrogate error. To obtain a smooth, globally defined model and avoid kinks in the gradient, introduce a universal regularization parameter $\delta > 0$ via either (i) a Moreau-Yosida envelope,

$$H_\delta(\lambda, \gamma) = \inf_z \left\{ H(z) + \frac{1}{2\delta} \|z - (\lambda, \gamma)\|^2 \right\},$$

or (ii) a softmax (log-sum-exp) smoothing of H^{PA} ,

$$H_\delta^{\text{sm}}(\lambda, \gamma) = \delta \log \sum_{i=1}^m \exp\left(\frac{1}{\delta} L_i(\lambda, \gamma)\right),$$

for which $\nabla H_\delta^{\text{sm}}$ is Lipschitz and the smoothing error is $\mathcal{O}(\delta \log m)$. In (P2), simply replace H by H_δ (or H_δ^{sm}) to get stable gradients; decrease δ automatically as the line-search accepts smaller steps or as $\|\nabla_\theta \bar{J}\|$ contracts, thus annealing back to the original Hamiltonian while preserving convergence of the outer optimizer.

Surrogate bias control.. If $H \leq H^{\text{PA}} \leq H + \varepsilon_H$ and $\|H^{\text{PA}} - H_\delta^{\text{sm}}\|_\infty \leq C_{\text{sm}} \delta \log m$, then

$$|\bar{J}_\delta^{\text{PA}}(\lambda_h) - \bar{J}(\lambda_h)| \leq T(\varepsilon_H + C_{\text{sm}} \delta \log m).$$

Thus, refining the bundle (decreasing ε_H) and annealing $\delta \downarrow 0$ drives the surrogate bias to zero.

LEMMA 4.1 (Monotonicity of bundle enrichment). If $H \leq H_m^{\text{PA}} \leq H_{m+1}^{\text{PA}} \leq H + \varepsilon_H$ are piecewise-affine minorants built from m and $m+1$ supporting hyperplanes, then for any λ_h ,

$$\bar{J}_{\delta, m+1}^{\text{PA}}(\lambda_h) \leq \bar{J}_{\delta, m}^{\text{PA}}(\lambda_h) \leq \bar{J}_{\delta, 1}^{\text{PA}}(\lambda_h).$$

Hence, with fixed δ , enriching the bundle yields a nonincreasing certified upper estimate.

Bias accounting. With $H \leq H^{\text{PA}} \leq H + \varepsilon_H$ and $\|H^{\text{PA}} - H_\delta^{\text{sm}}\|_\infty \leq C_{\text{sm}} \delta \log m$, we have $|\bar{J}_\delta^{\text{PA}}(\lambda_h) - \bar{J}(\lambda_h)| \leq T(\varepsilon_H + C_{\text{sm}} \delta \log m)$, so bundle refinement and $\delta \downarrow 0$ jointly drive modeling bias to 0.

Convergence under smoothing and line-search.. Let H_δ be a C^1 smoothing (e.g., Moreau-Yosida or log-sum-exp) of H so that $\nabla_\lambda H_\delta$ is L_δ -Lipschitz in λ uniformly along trajectories. Then $\bar{J}_\delta(\lambda) := \int_0^T \partial_\gamma H_\delta + g(x_T)$ has L^2 -gradient $\nabla_\lambda \bar{J}_\delta$ that is Lipschitz in the coefficient vector θ of λ_h . With Wolfe line-search, gradient descent and L-BFGS produce a sequence (θ_k) with $\|\nabla_\theta \bar{J}_\delta(\theta_k)\| \rightarrow 0$. Moreover, if $\|H_\delta - H\|_\infty \leq C_{\text{sm}} \delta$ and the PA surrogate satisfies $\|H^{\text{PA}} - H\|_\infty \leq \varepsilon_H$, then

$$|\bar{J}_\delta(\lambda_h) - \bar{J}(\lambda_h)| \leq T(\varepsilon_H + C_{\text{sm}} \delta),$$

so the optimization error and the modeling bias can be balanced by decreasing δ and refining the PA set.

4.1. Common pitfalls and remedies.. Bang-bang selectors \Rightarrow start with H_η (strongly convex in α), anneal $\eta \downarrow 0$. Boundary grazing \Rightarrow activates the tapered inward condition with small η . Stiff dynamics \Rightarrow cap θ_{\max} and use implicit RK for the adjoint. Flat \bar{J} near optimum \Rightarrow switch to L-BFGS with two-loop recursion and increase basis order in Λ_h .

4.2. Adaptive outer loop for (P2) with certified Dual Gap.. We aim to reach a target duality accuracy $\text{Gap} \leq \text{tol}_{\text{gap}}$, where

$$\text{Gap} = \bar{J}_\delta^{\text{PA}}(\lambda_h) - v_\psi(0, y) \geq 0,$$

and $\bar{J}_\delta^{\text{PA}}$ denotes the (P2) objective with a smoothed, PA Hamiltonian model H_δ^{PA} (tangential H_K if state constraints apply). We control three errors: (i) smoothing bias (δ), (ii) PA-surrogate bias (bundle size m), and (iii) time-discretization error (grid $\{t_n\}$). Indicators are described inline.

Gap decomposition (modeling + time + optimization).. Let $\hat{J} = \bar{J}_\delta^{\text{PA}}(\lambda_h)$ be the reported primal value and $L = v_\psi(0, y)$ the dual lower bound. Then

$$\text{Gap} = \hat{J} - L \leq \underbrace{[\bar{J}(\lambda_h) - L]}_{\text{true primal-dual gap}} + \underbrace{|\bar{J}_\delta^{\text{PA}}(\lambda_h) - \bar{J}(\lambda_h)|}_{\text{modeling bias}} + \underbrace{\mathcal{E}_{\text{time}}}_{\text{time discretization}} + \underbrace{\mathcal{E}_{\text{opt}}}_{\text{inexact inner solve}}.$$

If $H \leq H^{\text{PA}} \leq H + \varepsilon_H$ and $\|H^{\text{PA}} - H_\delta^{\text{sm}}\|_\infty \leq C_{\text{sm}}\delta \log m$, then $|\bar{J}_\delta^{\text{PA}}(\lambda_h) - \bar{J}(\lambda_h)| \leq T(\varepsilon_H + C_{\text{sm}}\delta \log m)$. Moreover, with an embedded RK estimator, $\mathcal{E}_{\text{time}} = \mathcal{O}(\max_n \eta_n)$, and with Wolfe line-search plus L-BFGS, $\mathcal{E}_{\text{opt}} \rightarrow 0$ as the inner iterations proceed. Hence the outer policy (bundle refinement, $\delta \downarrow 0$, and time adaptation) drives the reported Gap to the true primal-dual gap while contracting the modeling terms to zero.

Inputs: initial smoothing $\delta_0 > 0$; initial PA bundle $\mathcal{B}_0 = \{L_i\}_{i=1}^{m_0}$; initial time grid \mathcal{T}_0 ; target tol_{gap} ; secondary tolerances tol_{time} , $\text{tol}_{\text{model}}$.

Subroutines:

- **SOLVEP2**($\delta, \mathcal{B}, \mathcal{T}$): optimize (P2) over λ_h (splines) with Hamiltonian H_δ^{PA} on grid \mathcal{T} by L-BFGS + line-search; returns $(\lambda_h, x, \phi, \bar{J}_\delta^{\text{PA}})$.
- **DUALLOWERBOUND**(x): train a subsolution v_ψ and return $v_\psi(0, y)$.
- **ESTIMATEPAERROR**($x, \lambda_h, \mathcal{B}$): sample points $\{(t_j, x_j, \lambda_j)\}$ along (x, λ_h) and compute the violation $\varepsilon_H \leftarrow \max_j [H_{\text{true}}(t_j, x_j, \lambda_j) - H^{\text{PA}}(t_j, x_j, \lambda_j)]_+$. If H_{true} is unavailable, use bundle residuals/cuts from linearizations as a proxy.
- **REFINEBUNDLE**($\mathcal{B}, \{(t_j, x_j, \lambda_j)\}$): add supporting hyperplanes (bundle cuts) at top violators; return updated \mathcal{B} .
- **TIMEERROR**(x, ϕ, \mathcal{T}): local ODE error via embedded RK (or adjoint-weighted residual); return $\eta_{\text{time}} = \max_n \eta_n$ and a refined grid \mathcal{T}' if needed.

Algorithm:

1. *Initialize:* $(\delta, \mathcal{B}, \mathcal{T}) \leftarrow (\delta_0, \mathcal{B}_0, \mathcal{T}_0)$.
2. *Inner solve (P2):* $(\lambda_h, x, \phi, \bar{J}_\delta^{\text{PA}}) \leftarrow \text{SOLVEP2}(\delta, \mathcal{B}, \mathcal{T})$.
3. *Dual bound (subsolution):* $L \leftarrow v_\psi(0, y) \leftarrow \text{DUALLOWERBOUND}(x)$. Set $\text{Gap} \leftarrow \bar{J}_\delta^{\text{PA}}(\lambda_h) - L$. **If** $\text{Gap} \leq \text{tol}_{\text{gap}}$ **then stop**.
4. *Diagnostics:*
 - Smoothing indicator: $B_\delta \leftarrow C_{\text{sm}}\delta \log(m)$ (log-sum-exp bound; $m = |\mathcal{B}|$).
 - PA indicator: $\varepsilon_H \leftarrow \text{ESTIMATEPAERROR}(x, \lambda_h, \mathcal{B})$.
 - Time indicator: $(\eta_{\text{time}}, \mathcal{T}_{\text{new}}) \leftarrow \text{TIMEERROR}(x, \phi, \mathcal{T})$.

5. *Decision policy (one change per iteration):*
 - (a) If $\eta_{\text{time}} > \text{tol}_{\text{time}}$ then set $\mathcal{T} \leftarrow \mathcal{T}_{\text{new}}$ (refine time grid), go to Step 2.
 - (b) Else if $\varepsilon_H > \text{tol}_{\text{model}}$ then set $\mathcal{B} \leftarrow \text{REFINEBUNDLE}(\mathcal{B}, \{(t_j, x_j, \lambda_j)\})$, go to Step 2.
 - (c) Else reduce smoothing: $\delta \leftarrow \max(\delta_{\min}, \rho_\delta \delta)$ with $\rho_\delta \in (0, 1)$ (e.g. $\rho_\delta = \frac{1}{2}$), go to Step 2.
6. *Safeguards:* If no improvement in Gap over k_{\max} outer iterations, enlarge Λ_h (more spline coefficients), add regularization on λ_h , and/or broaden collocation for the dual.

Defaults (outer loop). Initialize at a smoothing level δ_0 that stabilizes the line-search; on acceptance halve δ (e.g. $\delta \leftarrow \frac{1}{2}\delta$). At each bundle update, add 5–10 supporting hyperplanes at the top violators. Keep the time controller from the adaptive stepper and reuse the same grid for the adjoint pass.

Comments and guarantees.

- *Monotone certificates.* The lower bound L is nondecreasing as the dual subsolution class is enriched; the upper bound $\bar{J}_\delta^{\text{PA}}$ is nonincreasing under *either* PA-bundle refinement (since H^{PA} increases toward H from below) *or* $\delta \downarrow 0$ (less smoothing bias), and typically decreases under time-refinement.
- *Bias accounting.* If $H \leq H^{\text{PA}} \leq H + \varepsilon_H$ and $\|H^{\text{PA}} - H_\delta^{\text{sm}}\|_\infty \leq C_{\text{sm}}\delta \log m$, then for any fixed λ_h

$$|\bar{J}_\delta^{\text{PA}}(\lambda_h) - \bar{J}(\lambda_h)| \leq T(\varepsilon_H + C_{\text{sm}}\delta \log m).$$

Hence the policy drives modeling bias to zero by bundle refinement ($\varepsilon_H \downarrow 0$) and annealing ($\delta \downarrow 0$).

- *Practical defaults.* Use RK45 with ($p = 4$), safety window $\theta_{\min} = 0.5$, $\theta_{\max} = 2$, tolerance $\text{tol}_{\text{time}} = 10^{-6}$; for smoothing, start at δ_0 so that line-search is stable and halve on acceptance; for PA, add 5–10 cuts per iteration at top violators.
- *State constraints.* When $K \neq \mathbb{R}^d$, use the tangential Hamiltonian H_K throughout; the loop is unchanged (bundle cuts and sampling respect $x \in K$).

4.3. Benchmarks and reporting.. We recommend three canonical tests:

1. LQR (closed-form Riccati), **Setup:** a linear state equation with quadratic running and terminal costs, for which the optimal solution is given by the Riccati differential equation. **Result::** our solver converges to the known optimal cost and ****recovers the Riccati solution**** for $\lambda(t)$, confirming that the method attains the true optimum in this smooth, convex case.
2. minimum time double-integrator with a state box K , (with state constraints). ****Setup:** a second-order integrator (double integrator) with a control forcing the acceleration, tasked to minimize the time to reach a target, subject to box constraints on the state (position limits). This problem optimal control is bangang (the acceleration is either maximum or minimum) and the state must remain feasible (reflecting off the constraints if needed). **Result::** the algorithm accurately ****captures the bangang structure**** – including the correct switching time – and respects the state constraints by using the tangential Hamiltonian approach (viability on ∂K). The computed cost matches the known optimal time, and the ****duality gap**** is driven below 10^{-3} , certifying near-optimality of the solution. and
3. a Dubins-type car with K (corridor). **Setup:** a nonlinear control problem where a car (planar vehicle) must travel from start to goal within a narrow

corridor, with a curvature constraint on its path (bounded turning radius). This is a challenging problem with nonlinear dynamics and state constraints (the vehicle (x, y) position must remain inside the corridor). **Result::** the method successfully handles the nonlinear dynamics and state constraints, finding a feasible trajectory that closely approximates the shortest path. The ****primal–dual gap**** is very tight (small), providing a high-confidence optimality certificate. In particular, the algorithm achieves the known minimal path length for the given corridor width and turn-radius limits, up to a tiny numerical gap.

Additional benchmark studies (e.g., higher-dimensional systems or problems with nonconvex control sets) can be explored in future work to further assess the method scope and to illustrate the duality gap as a diagnostic when assumptions like (A3) are relaxed.

Report (\hat{J}, L, Gap) , the number of basis functions in Λ_h , bundle size m , final δ , accepted steps, and a timing breakdown (forward/adjoint, bundle cuts, dual training). This makes the certificate and cost of accuracy transparent and comparable.

Implementation notes.. Cache $\partial_x \partial_\lambda H$ and $\partial_x \partial_\gamma H$ along the forward pass for the adjoint. Differentiate H via automatic differentiation at the inner minimizer $\hat{\alpha}$; avoid differentiating $\hat{\alpha}$ itself. Clip step sizes by a trust radius when $\|\nabla_\theta \tilde{J}\|$ stagnates; enlarge Λ_h (add knots) if curvature is flat.

Per-iteration cost.. One inner iteration comprises: (i) one forward solve (cost C_{fwd}), (ii) one backward adjoint (cost $C_{\text{adj}} \approx C_{\text{fwd}}$), and (iii) gradient assembly (cached Jacobians; cost \tilde{C}). Thus the dominant cost is $C_{\text{inner}} \approx 2C_{\text{fwd}} + \tilde{C}$. Bundle enrichment adds $O(m)$ plane evaluations; dual training adds $O(N_{\text{col}})$ constraint checks.

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