

AN A POSTERIORI ERROR ESTIMATE FOR SYMPLECTIC EULER APPROXIMATION OF OPTIMAL CONTROL PROBLEMS*

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Abstract. This work focuses on numerical solutions of optimal control problems. A time discretization error representation is derived for the approximation of the associated value function. It concerns Symplectic Euler solutions of the Hamiltonian system connected with the optimal control problem. The error representation has a leading order term consisting of an error density that is computable from Symplectic Euler solutions. Under an assumption of the pathwise convergence of the approximate dual function as the maximum time step goes to zero, we prove that the remainder is of higher order than the leading error density part in the error representation. With the error representation, it is possible to perform adaptive time stepping. We apply an adaptive algorithm originally developed for ordinary differential equations. The performance is illustrated by numerical tests.

Key words. Optimal Control, Error Estimates, Adaptivity, Error Control

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1. Introduction. In this work, we will present an asymptotic a posteriori error estimate for optimal control problems. The estimate consists of a term that is a posteriori computable from the solution, plus a remainder that is of higher order. It is the main tool for construction of adaptive algorithms. We present and test numerically one such algorithm.

The optimal control problem is to minimize the functional

$$\int_0^T h(X(t), \alpha(t)) dt + g(X(T)), \quad (1.1)$$

with given functions $h : \mathbb{R}^d \times \mathcal{B} \rightarrow \mathbb{R}$ and $g : \mathbb{R}^d \rightarrow \mathbb{R}$, with respect to the state variable $X : [0, T] \rightarrow \mathbb{R}^d$ and the control $\alpha : [0, T] \rightarrow \mathcal{B}$, with control set, \mathcal{B} , a subset of some Euclidean space, $\mathbb{R}^{d'}$, such that the ODE constraint,

$$\begin{aligned} X'(t) &= f(X(t), \alpha(t)), & 0 < t \leq T, \\ X(0) &= x_0, \end{aligned} \quad (1.2)$$

is fulfilled. This optimal control problem can be solved (globally) using the Hamilton-Jacobi-Bellman (HJB) equation

$$\begin{aligned} u_t + H(x, u_x) &= 0, & x \in \mathbb{R}^d, & 0 \leq t < T, \\ u(\cdot, T) &= g(\cdot), & x \in \mathbb{R}^d, \end{aligned} \quad (1.3)$$

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with u_t and u_x denoting the time derivative and spatial gradient of u , respectively, and the Hamiltonian, $H : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$, defined by

$$H(x, \lambda) := \min_{\alpha \in \mathcal{B}} \left\{ \lambda \cdot f(x, \alpha) + h(x, \alpha) \right\}, \quad (1.4)$$

and value function

$$u(x, t) := \inf_{X: [t, T] \rightarrow \mathbb{R}^d, \alpha: [t, T] \rightarrow \mathcal{B}} \left\{ \int_t^T h(X(s), \alpha(s)) \, ds + g(X(T)) \right\}, \quad (1.5)$$

where

$$\begin{aligned} X'(s) &= f(X(s), \alpha(s)), \quad t < s \leq T, \\ X(t) &= x. \end{aligned}$$

The global minimum to the optimal control problem (1.1)-(1.2) is thus given by $u(x_0, 0)$.

If the Hamiltonian is sufficiently smooth, the bi-characteristics to the HJB equation (1.3) are given by the following Hamiltonian system:

$$\begin{aligned} X'(t) &= H_\lambda(X(t), \lambda(t)), \quad 0 < t \leq T, \\ X(0) &= x_0, \\ -\lambda'(t) &= H_x(X(t), \lambda(t)), \quad 0 \leq t < T, \\ \lambda(T) &= g_x(X(T)), \end{aligned} \quad (1.6)$$

where H_λ , H_x , and g_x denote gradients with respect to λ and x , respectively, and the dual variable, $\lambda : [0, T] \rightarrow \mathbb{R}^d$, satisfies $\lambda(t) = u_x(X(t), t)$ along the characteristic.

In Section 2, we present an error representation for the following discretization of (1.6), which is used as a cornerstone for an adaptive algorithm. It is the Symplectic (forward) Euler method:

$$\begin{aligned} X_{n+1} - X_n &= \Delta t_n H_\lambda(X_n, \lambda_{n+1}), \quad n = 0, \dots, N-1, \\ X_0 &= x_0, \\ \lambda_n - \lambda_{n+1} &= \Delta t_n H_x(X_n, \lambda_{n+1}), \quad n = 0, \dots, N-1, \\ \lambda_N &= g_x(X_N), \end{aligned} \quad (1.7)$$

with $0 = t_0 < t_1 < \dots < t_N = T$, $\Delta t_n := t_{n+1} - t_n$, and $X_n, \lambda_n \in \mathbb{R}^d$. An alternative approach uses the dual weighted residual method, see [4, 1], to adaptively refine finite element solutions of the Euler-Lagrange equation associated with the optimal control problem, see [6, 8, 7].

The adaptive algorithm in Section 2 uses a Hamiltonian that is of C^2 regularity. In [14, 13] first-order convergence of the so-called Symplectic Pontryagin method, a Symplectic Euler scheme (1.7) with a regularized Hamiltonian H^δ replacing H , is shown. The Symplectic Pontryagin scheme works in the more general optimal control setting where the Hamiltonian is non-smooth. It uses the fact that if u and u^δ are the solutions to the Hamilton-Jacobi equation (1.3) with the original (possibly non-smooth) Hamiltonian H , and the regularized Hamiltonian, H^δ , then

$$\|u - u^\delta\|_{L^\infty([0, T] \times \mathbb{R}^d)} \leq T \|H - H^\delta\|_{L^\infty(\mathbb{R}^d \times \mathbb{R}^d)} = \mathcal{O}(\delta), \quad (1.8)$$

if $\|H - H^\delta\|_{L^\infty(\mathbb{R}^d \times \mathbb{R}^d)} = \mathcal{O}(\delta)$. Equation (1.8) is a direct consequence of the maximum principle for viscosity solutions to Hamilton-Jacobi equations, see e.g., [2, 5, 3]. For the error representation result in Theorem 2.4, we need C^2 regularity of H . A possibility to use this error representation to find a solution adaptively in the case where the Hamiltonian is non-differentiable, is to add the error from the time discretization (the TOL in Theorem 2.8) when the adaptive algorithm 2.6 is used with a regularized Hamiltonian, H^δ , to the error $\mathcal{O}(\delta)$, in (1.8). We show in Section 3 that this method works well for a test case in which the Hamiltonian is non-differentiable. Even though it works well in the cases we have studied, it is difficult to justify this method theoretically. This is because the size of the remainder term in Theorem 2.4 depends on the size of the second-order derivatives of the Hamiltonian, H , which typically are of order δ^{-1} when a regularized H^δ is used.

REMARK 1.1 (Time-dependent Hamiltonian). *The analysis in this paper is presented for the optimal control problem (1.1), (1.2), i.e., the case where the running cost, h , and the flux, f , have no explicit time dependence. The more general situation with explicit time dependence, to minimize*

$$\int_0^T h(t, X(t), \alpha(t)) dt + g(X(T)),$$

for $\alpha \in \mathcal{B}$ such that the constraint

$$\begin{aligned} X'(t) &= f(t, X(t), \alpha(t)), & 0 < t \leq T, \\ X(0) &= x_0, \end{aligned}$$

is fulfilled, can be put in the form (1.1), (1.2) by introducing a state variable, $s(t) = t$, for the time dependence, i.e., to minimize

$$\int_0^T h(s(t), X(t), \alpha(t)) dt + g(X(T)),$$

such that the constraint

$$\begin{aligned} X'(t) &= f(s(t), X(t), \alpha(t)), & 0 < t \leq T, \\ s'(t) &= 1, & 0 < t \leq T, \\ X(0) &= X_0, \\ s(0) &= 0, \end{aligned}$$

is fulfilled. The Hamiltonian then becomes

$$H(x, s, \lambda_1, \lambda_2) := \min_{\alpha \in \mathcal{B}} \left\{ \lambda_1 \cdot f(x, \alpha, s) + \lambda_2 + h(x, \alpha, s) \right\},$$

where λ_1 is the dual variable corresponding to X , while λ_2 corresponds to s .

2. Error estimation and adaptivity. In this section, we present an error representation for the Symplectic Euler scheme in Theorem 2.4. With this error representation, it is possible to build an adaptive algorithm (alg. 2.6). The error representation in Theorem 2.4 concerns approximation of the value function, u , defined in (1.5). To define an approximate value function, \bar{u} , we need the following definition of a running cost, a Legendre-type transform of the Hamiltonian:

$$L(x, \beta) = \sup_{\lambda \in \mathbb{R}^d} \left(-\beta \cdot \lambda + H(x, \lambda) \right), \quad (2.1)$$

for all x and β in \mathbb{R}^d . The running cost function is convex in its second argument and extended valued, i.e., its values belong to $\mathbb{R} \cup \{+\infty\}$. If the Hamiltonian is real-valued and concave in its second variable, it is possible to retrieve it from L :

$$H(x, \lambda) = \inf_{\beta \in \mathbb{R}^d} (\lambda \cdot \beta + L(x, \beta)). \quad (2.2)$$

This is a consequence of the bijectivity of the Legendre-Fenchel transform, see [11, 13].

We now define a discrete value function:

$$\bar{u}(y, t_m) := \inf \{ J_{(y, t_m)}(\beta_m, \dots, \beta_{N-1}) \mid \beta_m, \dots, \beta_{N-1} \in \mathbb{R}^d \}, \quad (2.3)$$

where

$$J_{(y, t_m)}(\beta_m, \dots, \beta_{N-1}) := \sum_{n=m}^{N-1} \Delta t_n L(X_n, \beta_n) + g(X_N), \quad (2.4)$$

and

$$\begin{aligned} X_{n+1} &= X_n + \Delta t_n \beta_n, \quad \text{for } m \leq n \leq N-1, \\ X_m &= y. \end{aligned} \quad (2.5)$$

The appearance of a discrete path denoted $\{X_n\}$ in both the Symplectic Euler scheme (1.7) and in the definition of \bar{u} in (2.5) is not just a coincidence. The following theorem, taken from [13], shows that to the minimizing path $\{X_n\}$ in the definition of \bar{u} corresponds a discrete dual path $\{\lambda_n\}$, such that $\{X_n, \lambda_n\}$ solves the Symplectic Euler scheme (1.7). For the statement and proof of Theorem 2.3 we need the following definitions.

DEFINITION 2.1. *Let S be a subset of \mathbb{R}^d . We say that a function $f : S \rightarrow \mathbb{R}$ is semiconcave if there exists a nondecreasing upper semicontinuous function $\omega : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that $\lim_{\rho \rightarrow 0^+} \omega(\rho) = 0$ and*

$$wf(x) + (1-w)f(y) - f(wx + (1-w)y) \leq w(1-w)|x-y|\omega(|x-y|)$$

for any pair $x, y \in S$, such that the segment $[x, y]$ is contained in S and for any $w \in [0, 1]$. We say that f is locally semiconcave on S if it is semiconcave on every compact subset of S . There exist alternative definitions of semiconcavity, see [5], but this is the one used in this paper.

DEFINITION 2.2. *An element $p \in \mathbb{R}^d$ belongs to the superdifferential of the function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ at x , denoted $D^+f(x)$, if*

$$\limsup_{y \rightarrow x} \frac{f(y) - f(x) - p \cdot (y-x)}{|y-x|} \leq 0.$$

THEOREM 2.3. *Let y be any element in \mathbb{R}^d , and $g : \mathbb{R}^d \rightarrow \mathbb{R}$ a locally semiconcave function such that $g(x) \geq -k(1+|x|)$, for some constant k , and all $x \in \mathbb{R}^d$. Let the Hamiltonian $H : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ satisfy the following conditions:*

- H is differentiable everywhere in $\mathbb{R}^d \times \mathbb{R}^d$.
- $H_\lambda(\cdot, \lambda)$ is locally Lipschitz continuous for every $\lambda \in \mathbb{R}^d$.
- H_x is continuous everywhere in $\mathbb{R}^d \times \mathbb{R}^d$.
- There exists a convex, nondecreasing function $\mu : [0, \infty) \rightarrow \mathbb{R}$ and positive constants A and B such that

$$-H(x, \lambda) \leq \mu(|\lambda|) + |x|(A + B|\lambda|) \quad \text{for all } (x, \lambda) \in \mathbb{R}^d \times \mathbb{R}^d. \quad (2.6)$$

• $H(x, \cdot)$ is concave for every $x \in \mathbb{R}^d$.
Let L be defined by (2.1). Then, there exists a minimizer $(\beta_m, \dots, \beta_{N-1})$ of the function $J_{(y, t_m)}$ in (2.4). Let (X_m, \dots, X_N) be the corresponding solution to (2.5). Then, for each $\lambda_N \in D^+g(X_N)$, there exists a discrete dual path $(\lambda_m, \dots, \lambda_{N-1})$, that satisfies

$$\begin{aligned} X_{n+1} &= X_n + \Delta t_n H_\lambda(X_n, \lambda_{n+1}), \quad \text{for all } m \leq n \leq N-1, \\ X_m &= y \\ \lambda_n &= \lambda_{n+1} + \Delta t_n H_x(X_n, \lambda_{n+1}), \quad \text{for all } m \leq n \leq N-1. \end{aligned} \tag{2.7}$$

Hence,

$$\beta_n = H_\lambda(X_n, \lambda_{n+1}) \tag{2.8}$$

for all $m \leq n \leq N-1$.

The proof of Theorem 2.3 from [13] is reproduced in the appendix.

With the correspondence between the Symplectic Euler scheme and discrete minimization in Theorem 2.3, we are now ready to formulate the error representation result. We will use the terminology that a function is bounded in C^k if it belongs to C^k and has bounded derivatives of order less than or equal to k .

THEOREM 2.4. *Assume that all conditions in Theorem 2.3 are satisfied, that the Hamiltonian, H , is bounded in $C^2(\mathbb{R}^d \times \mathbb{R}^d)$, and that there exists a constant, C , such that for every discretization $\{t_n\}$ the difference between the discrete dual and the gradient of the value function is bounded as*

$$|\lambda_n - u_x(X_n, t_n)| \leq C \Delta t_{\max},$$

where $\Delta t_{\max} := \max_n \Delta t_n$. Assume further that either of the following two conditions holds:

1. The value function, u , is bounded in $C^3([0, T] \times \mathbb{R}^d)$.
2. There exists a neighborhood in $C([0, T], \mathbb{R}^d)$ around the minimizer $X : [0, T] \rightarrow \mathbb{R}^d$ of $u(x_0, 0)$ in (1.5) in which the value function, u , is bounded in C^3 . Moreover, the discrete solutions $\{X_n\}$ converge to the continuous solution $X(t)$ in the sense that

$$\max_n |X_n - X(t_n)| \rightarrow 0, \quad \text{as } \Delta t_{\max} \rightarrow 0.$$

If Condition 1 holds, then for every discretization $\{t_n\}$, the error $\bar{u}(x_0, 0) - u(x_0, 0)$ is given as

$$\bar{u}(x_0, 0) - u(x_0, 0) = \sum_{n=0}^{N-1} \Delta t_n^2 \rho_n + R, \tag{2.9}$$

with density

$$\rho_n := -\frac{H_\lambda(X_n, \lambda_{n+1}) \cdot H_x(X_n, \lambda_{n+1})}{2} \tag{2.10}$$

and the remainder term, $|R| \leq C' \Delta t_{\max}^2$, for some constant C' .

If Condition 2 holds, then there exists a threshold time step, Δt_{thres} , such that for every discretization with $\Delta t_{\max} \leq \Delta t_{\text{thres}}$ the error representation (2.9) holds.

REMARK 2.5. In the proof of the theorem, we show that equation (2.9) is satisfied with the error density

$$\begin{aligned} \tilde{\rho}_n := & \frac{H(X_n, \lambda_{n+1})}{\Delta t_n} - \frac{H(X_n, \lambda_n) + H(X_{n+1}, \lambda_{n+1})}{2\Delta t_n} \\ & + \frac{\lambda_n - \lambda_{n+1}}{2} \cdot \frac{H_\lambda(X_n, \lambda_{n+1})}{\Delta t_n} \end{aligned} \quad (2.11)$$

replacing ρ_n . Under the assumption that the Hamiltonian, H , is bounded in C^2 , we have that $|\rho_n - \tilde{\rho}_n| = \mathcal{O}(\Delta t_n)$. This follows by Taylor expansion and by using that $\{X_n, \lambda_n\}$ solves the Symplectic Euler scheme (1.7). Hence, the theorem holds also with the error density ρ_n . An advantage of ρ_n is that it is given by a simple expression. The error density $\tilde{\rho}_n$ has the advantage that it is the one that is obtained in the proof, and then ρ_n is derived from it. One could therefore expect that $\tilde{\rho}_n$ would give a slightly more accurate error representation. Moreover, $\tilde{\rho}_n$ is directly computable (as is ρ_n) once a solution $\{X_n, \lambda_n\}$ has been computed.

Proof. By Theorem 2.3, the error can be expressed as

$$(\bar{u} - u)(x_0, 0) = \sum_{n=0}^{N-1} \Delta t_n L(X_n, \beta_n) + g(X_N) - u(x_0, 0), \quad (2.12)$$

where

$$g(X_N) = u(X_N, T), \quad \beta_n = H_\lambda(X_n, \lambda_{n+1}).$$

Define the piecewise linear function $\bar{X}(t)$ to be

$$\bar{X}(t) = X_n + (t - t_n)H_\lambda(X_n, \lambda_{n+1}), \quad t \in (t_n, t_{n+1}), \quad n = 0, \dots, N-1.$$

If Condition 2 in the theorem holds, we now assume that Δt_{\max} is small enough, such that the path $\bar{X}(t)$ belongs to the neighborhood of $X(t)$ in $C([0, T], \mathbb{R}^d)$ where the value function belongs to C^3 . If Condition 1 holds, the following analysis is also valid, without restriction on Δt_{\max} . From (2.12) and the Hamilton-Jacobi-Bellman equation, we have

$$\begin{aligned} (\bar{u} - u)(x_0, 0) &= \sum_{n=0}^{N-1} \Delta t_n L(X_n, \beta_n) + u(X_N, T) - u(x_0, 0) \\ &= \sum_{n=0}^{N-1} \Delta t_n L(X_n, \beta_n) + \int_0^T \frac{d}{dt} u(\bar{X}(t), t) dt \\ &= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} L(X_n, \beta_n) dt \\ &\quad + \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} u_t(\bar{X}(t), t) + u_x(\bar{X}(t), t) \cdot H_\lambda(X_n, \lambda_{n+1}) dt. \end{aligned} \quad (2.13)$$

By (2.1) and (2.8) we have

$$H(X_n, \lambda_{n+1}) = \lambda_{n+1} \cdot H_\lambda(X_n, \lambda_{n+1}) + L(X_n, \beta_n),$$

which together with the Hamilton-Jacobi equation

$$u_t(\bar{X}(t), t) = -H(\bar{X}(t), u_x(\bar{X}(t), t))$$

implies that the error can be written as

$$\begin{aligned} (\bar{u} - u)(x_0, 0) &= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} H(X_n, \lambda_{n+1}) - H(\bar{X}(t), u_x(\bar{X}(t), t)) dt \\ &\quad + \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} (u_x(\bar{X}(t), t) - \lambda_{n+1}) \cdot H_\lambda(X_n, \lambda_{n+1}) dt \\ &=: \sum_{n=0}^{N-1} E_n. \end{aligned} \quad (2.14)$$

By the boundedness of the Hamiltonian, H , in C^2 and the value function, u , in C^3 , it follows that the trapezoidal rule can be applied to the integrals in (2.14) with an error of order Δt_n^3 . Hence, we obtain that

$$\begin{aligned} E_n &= \Delta t_n \left(H(X_n, \lambda_{n+1}) - \frac{H(X_n, u_x(X_n, t_n)) + H(X_{n+1}, u_x(X_{n+1}, t_{n+1}))}{2} \right) \\ &\quad + \Delta t_n \left(\frac{u_x(X_n, t_n) + u_x(X_{n+1}, t_{n+1})}{2} - \lambda_{n+1} \right) \cdot H_\lambda(X_n, \lambda_{n+1}) + \bar{R}_n \end{aligned} \quad (2.15)$$

with remainder $\bar{R}_n = \mathcal{O}(\Delta t_n^3)$.

What remains for us to show is that we can exchange the gradient of the continuous value function, u , in (2.15) with the discrete dual, λ_n , with an error bounded by Δt_{\max}^2 . We write this difference using the error density, $\tilde{\rho}_n$, from (2.11):

$$\begin{aligned} \Delta t_n^2 \tilde{\rho}_n - E_n &= -\frac{\Delta t_n}{2} \left(H(X_n, \lambda_n) - H(X_n, u_x(X_n, t_n)) \right) \\ &\quad - \frac{\Delta t_n}{2} \left(H(X_{n+1}, \lambda_{n+1}) - H(X_{n+1}, u_x(X_{n+1}, t_{n+1})) \right) \\ &\quad + \frac{\Delta t_n}{2} \left(\lambda_n - u_x(X_n, t_n) + \lambda_{n+1} - u_x(X_{n+1}, t_{n+1}) \right) \cdot H_\lambda(X_n, \lambda_{n+1}) - \bar{R}_n \\ &= \frac{\Delta t_n}{2} \left(-E_n^I - E_{n+1}^I + (\xi_n + \xi_{n+1}) \cdot H_\lambda(X_n, \lambda_{n+1}) \right) - \bar{R}_n, \end{aligned}$$

where

$$\begin{aligned} E_n^I &:= H(X_n, \lambda_n) - H(X_n, u_x(X_n, t_n)) = H_\lambda(X_n, \lambda_n) \cdot \xi_n + \mathcal{O}(|\xi_n|^2), \\ \xi_n &:= \lambda_n - u_x(X_n, t_n). \end{aligned}$$

Further Taylor expansion gives the difference

$$\begin{aligned} E_n^I - \xi_n \cdot H_\lambda(X_n, \lambda_{n+1}) &= \left(H_\lambda(X_n, \lambda_n) - H_\lambda(X_n, \lambda_{n+1}) \right) \cdot \xi_n + \mathcal{O}(|\xi_n|^2) \\ &= \mathcal{O}(\Delta t_n |\xi_n| + |\xi_n|^2) = \mathcal{O}(\Delta t_{\max}^2), \end{aligned}$$

and similarly

$$E_{n+1}^I - \xi_{n+1} \cdot H_\lambda(X_n, \lambda_{n+1}) = \mathcal{O}(\Delta t_{\max}^2).$$

Finally, summing the difference $\Delta t_n^2 \bar{\rho}_n - E_n$ over $n = 0, \dots, N-1$ gives, together with the above Taylor expansions, the bound $|R| \leq C \Delta t_{\max}^2$ in the theorem.

□

In what follows, we formulate an adaptive algorithm (2.6) and three theorems (2.7–2.9) on its performance. These are all taken from [10] more or less directly. Since the proofs are practically unchanged, they are not repeated here.

ALGORITHM 2.6 (Adaptivity). *Choose the error tolerance TOL, the initial grid $\{t_n\}_{n=0}^N$, the parameters s and M , and repeat the following points:*

1. Calculate $\{(X_n, \lambda_n)\}_{n=0}^N$ with the symplectic Euler scheme (1.7).
2. Calculate error densities $\{\rho_n\}_{n=0}^{N-1}$ and the corresponding approximate error densities

$$\bar{\rho}_n := \text{sgn}(\rho_n) \max(|\rho_n|, K \sqrt{\Delta t_{\max}}).$$

3. Break if

$$\max_n \bar{r}_n < \frac{\text{TOL}}{N}$$

where the error indicators are defined by $\bar{r}_n := |\bar{\rho}_n| \Delta t_n^2$.

4. Traverse through the mesh and subdivide an interval (t_n, t_{n+1}) into M parts if

$$\bar{r}_n > s \frac{\text{TOL}}{N}.$$

5. Update N and $\{t_n\}_{n=0}^N$ to reflect the new mesh.

The goal of the algorithm is to construct a partition of the time interval $[0, T]$ such that

$$\bar{r}_n \approx \frac{\text{TOL}}{N},$$

for all n . The constant $s < 1$ is present in order to achieve a substantial reduction of the error, described further in Theorem 2.7. The constant K in the algorithm should be chosen small (relative to the size of the solution). In the numerical experiments presented in Section 3, we use $K = 10^{-6}$.

Let $\Delta t(t)[k]$ be defined as the piecewise constant function that equals the local time step

$$\Delta t(t) = \Delta t_n, \quad \text{if } t \in [t_n, t_{n+1}),$$

on mesh refinement level k . As in [10], we have that

$$\lim_{\text{TOL} \rightarrow 0^+} \max_t \Delta t(t)[J] = 0,$$

where mesh J is the finest mesh where the algorithm stops. By the assumptions on the convergence of the approximate paths $\{X_n, \lambda_n\}$, it follows that there exists a limit

$$|\bar{\rho}| \rightarrow |\bar{\rho}|, \quad \text{as } \max \Delta t \rightarrow 0.$$

We introduce a constant, $c = c(t)$, such that

$$\begin{aligned} c &\leq \left| \frac{\bar{\rho}(t)[\text{parent}(n, k)]}{\bar{\rho}(t)[k]} \right| \leq c^{-1}, \\ c &\leq \left| \frac{\bar{\rho}(t)[k-1]}{\bar{\rho}(t)[k]} \right| \leq c^{-1}, \end{aligned} \tag{2.16}$$

holds for all time steps, $t \in \Delta t_n[k]$, and all refinement levels, k . Here, $\text{parent}(n, k)$ means the refinement level where a coarser interval was split into a number of finer subintervals of which $\Delta t_n[k]$ is one. Since $|\bar{\rho}|$ converges as $\text{TOL} \rightarrow 0$ and is bounded away from zero, c will be close to 1 for sufficiently fine meshes.

THEOREM 2.7. *[Stopping] Assume that c satisfies (2.16) for the time steps corresponding to the maximal error indicator on each refinement level, and that*

$$M^2 > c^{-1}, \quad s \leq \frac{c}{M}. \quad (2.17)$$

Then, each refinement level either decreases the maximal error indicator with the factor

$$\max_n \bar{r}_n[k+1] \leq \frac{c^{-1}}{M^2} \max_n \bar{r}_n[k],$$

or stops the algorithm.

The inequalities in (2.17) give (at least in principle) an idea how to determine the parameters M and s . When the constant, $c = c(t)$, has been determined approximately, say after one or a few refinements, M can be chosen using the first inequality and then s can be chosen using the other.

THEOREM 2.8. *[Accuracy] The adaptive Algorithm 2.6 satisfies*

$$\limsup_{\text{TOL} \rightarrow 0^+} (\text{TOL}^{-1} |u(x_0, 0) - \bar{u}(x_0, 0)|) \leq 1.$$

THEOREM 2.9. *[Efficiency] Assume that $c = c(t)$ satisfies (2.16) for all time steps at the final refinement level, and that all initial time steps have been divided when the algorithm stops. Then, there exists a constant, $C > 0$, bounded by $M^2 s^{-1}$, such that the final number of adaptive steps, N , of the Algorithm 2.6, satisfies*

$$\text{TOL } N \leq C \left\| \frac{\bar{\rho}}{c} \right\|_{L^{\frac{1}{2}}} \leq \|\bar{\rho}\|_{L^{\frac{1}{2}}} \max_{0 \leq t \leq T} c(t)^{-1},$$

and $\|\bar{\rho}\|_{L^{\frac{1}{2}}} \rightarrow \|\tilde{\rho}\|_{L^{\frac{1}{2}}}$ asymptotically as $\text{TOL} \rightarrow 0^+$.

REMARK 2.10. *Note that the optimal number N_a of non-constant (i.e., adaptive) time steps to have the error $\sum_n \Delta t_n^2 \bar{\rho}_n$ smaller than TOL satisfies $\text{TOL} N_a \approx \|\bar{\rho}\|_{L^{1/2}}$, see [10], while the number of uniform time steps N_u required satisfies $\text{TOL} N_u \approx \|\bar{\rho}\|_{L^1}$.*

REMARK 2.11. *It is natural to use adaptivity when optimal control problems are solved using the Hamiltonian system (1.6). Since it is a coupled ODE system with a terminal condition linking the primal and dual functions, it is necessary to solve using some iterative method. When an initial guess is to be provided to the iterative method, it is natural to interpolate a solution obtained on a coarser mesh. Solutions on several meshes therefore need be computed, as is the case when adaptivity is used.*

3. Numerical examples. In this section, we consider three numerical examples. The first is an optimal control problem that satisfies the assumption of a C^2 Hamiltonian in Theorem 2.4. The second is a problem in which the Hamiltonian is non-differentiable, and hence does not fulfill the smoothness assumption of Theorem 2.4. We investigate the influence of a regularization of the Hamiltonian. The third example is a problem in which the controlled ODE has an explicit time dependence with a singularity.

We will compare the work and error for the adaptive mesh refinement in Algorithm 2.6 with that of uniform mesh refinement. The work is represented by the cumulative number of time steps on all refinement levels, and the error is represented by either an estimation of the true error, using the value function from the finest uniform mesh as our true solution, or estimating the error by

$$E := \left| \sum_{n=1}^{N-1} \bar{\rho}_n \Delta t_n^2 \right|, \quad (3.1)$$

using the approximate error densities,

$$\bar{\rho}_n := \text{sgn}(\rho_n) \max(|\rho_n|, 10^{-6} \sqrt{\Delta t_{\max}}).$$

In all examples, we let $s = 0.25$ and $M = 2$ (since $c \approx 1$). On each mesh, the discretized Hamiltonian system (1.7) is solved with MATLAB's FSOLVE routine, with default parameters and a user-supplied Jacobian, and using the solution from the previous mesh as a starting guess.

EXAMPLE 3.1 (Hyper-sensitive optimal control). *This is a version of Example 6.1 in [7] and Example 51 in [12]. Minimize*

$$\int_0^{25} (X(t)^2 + \alpha(t)^2) dt + \gamma(X(25) - 1)^2,$$

subject to

$$\begin{aligned} X'(t) &= -X(t)^3 + \alpha(t), & 0 < t \leq 25, \\ X(0) &= 1, \end{aligned}$$

for some large $\gamma > 0$. The Hamiltonian is then given by

$$H(x, \lambda) := \min_{\alpha} \left\{ -\lambda x^3 + \lambda \alpha + x^2 + \alpha^2 \right\} = -\lambda x^3 - \lambda^2/4 + x^2.$$

First, we run the adaptive algorithm with tolerance, TOL, leading to the estimated error, E_{adap} . Finally, the problem is rerun using uniform refinement with stopping criteria, $E_{\text{unif}} \leq E_{\text{adap}}$.

Figure 3.1 shows the solution and final mesh when computed with the adaptive Algorithm 2.6. Figure 3.2 shows the error density and error indicator, while Figure 3.3 gives a comparison between the error estimate from equation (3.1) with an estimate of the error using a uniform mesh solution with a small step size as a reference. Figure 3.4 shows error estimates versus computational work as the cumulative number of time steps.

The error representation in Theorem 2.4 concerns approximation of the value function when the Symplectic Euler scheme is used with a C^2 Hamiltonian. In general, the minimizing α in the definition of the Hamiltonian (1.4) depends discontinuously on x and λ , which most probably leads to a non-differentiable Hamiltonian. In Example 3.2 we consider a simple optimal control problem with an associated Hamiltonian that is non-differentiable. We denote by H^δ a C^2 regularization of the Hamiltonian, H , such that

$$\|H - H^\delta\|_{L^\infty(\mathbb{R}^d \times \mathbb{R}^d)} = \mathcal{O}(\delta).$$

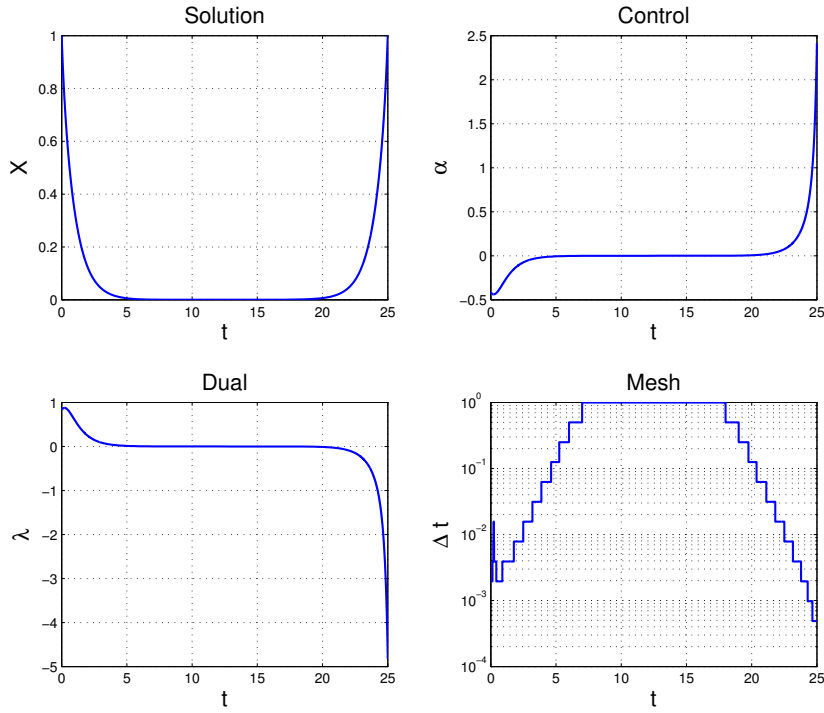


FIG. 3.1. The solution, X , control, α , dual, λ , and mesh, Δt , for the hyper-sensitive optimal control problem in Example 3.1, with $\gamma = 10^6$ and $\text{TOL} = 10^{-2}$.

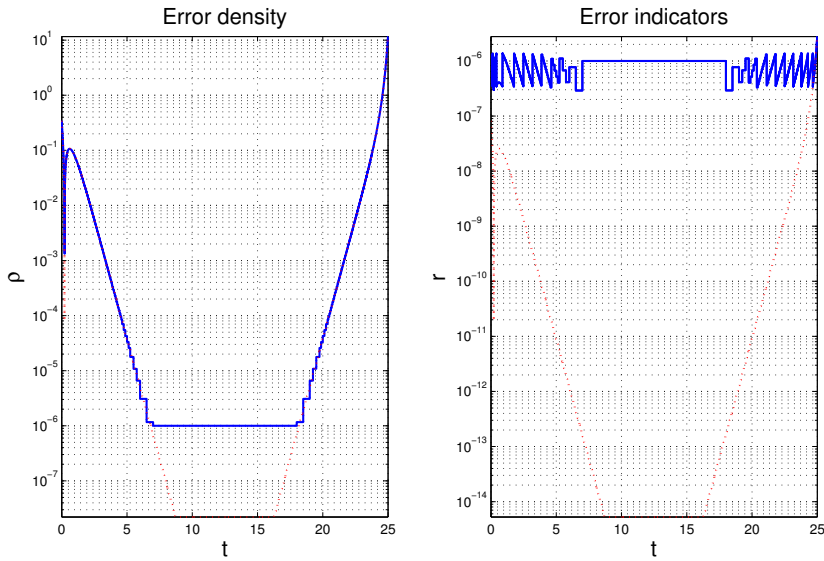


FIG. 3.2. Error densities, $|\bar{\rho}_n|$, and error indicators, \bar{r}_n , for the hyper-sensitive optimal control problem in Example 3.1. The solid and dotted lines correspond to solutions with adaptive and uniform time stepping, respectively.

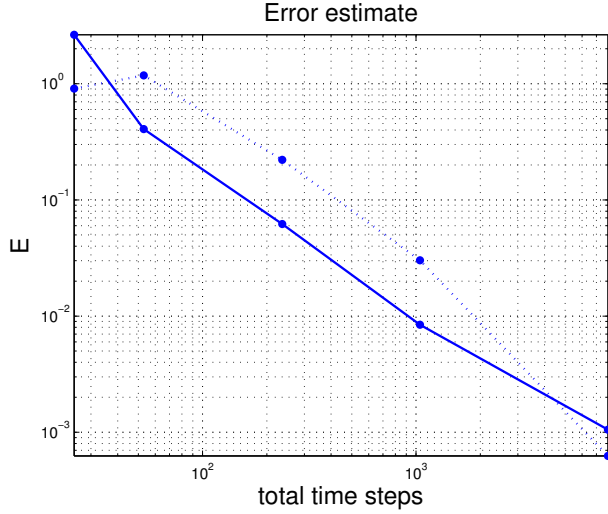


FIG. 3.3. Error estimates for the hyper-sensitive optimal control problem in Example 3.1. The solid line indicates the error estimate in (3.1), and the dotted line indicates the difference between the value function and the value function using a fine uniform mesh with 51200 time steps. The error estimate from (3.1) for the uniform mesh is approximately as large as the estimate for the finest adaptive level. Hence, the dotted line is only an approximation of the true error.

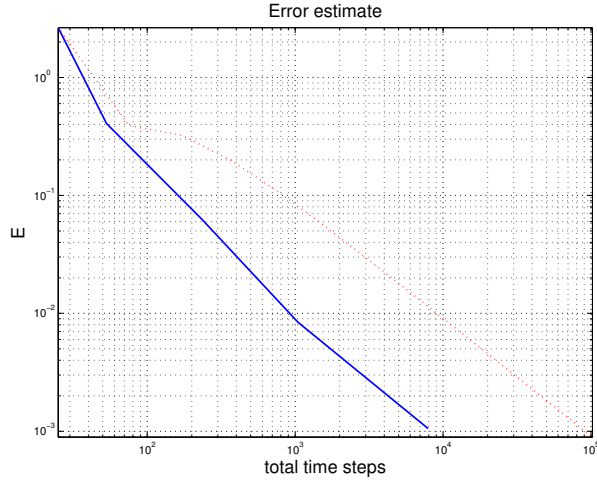


FIG. 3.4. Error estimates for the hyper-sensitive optimal control problem in Example 3.1 using (3.1), versus the cumulative number of time steps on all refinement levels for the adaptive algorithm (solid) and uniform meshes (dotted). The number of time steps in the uniform meshes is doubled in each refinement.

Since the remainder term in Theorem 2.4 contains second-order derivatives of the Hamiltonian, which are of order δ^{-1} if a regularization H^δ is used, it could be expected that an estimate of the error using the error density term

$$\sum_{n=0}^{N-1} \Delta t_n^2 \rho_n \quad (3.2)$$

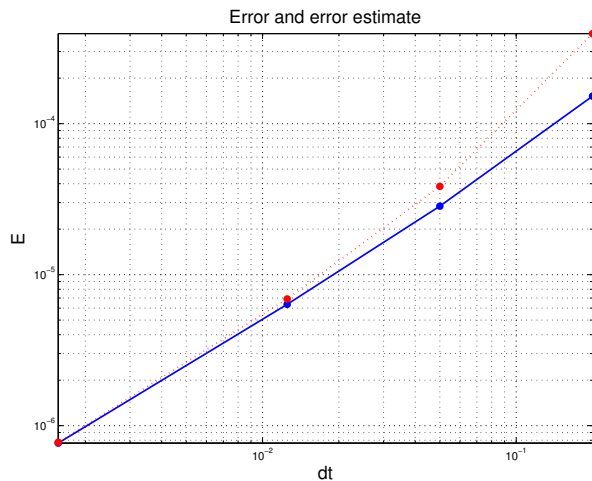


FIG. 3.5. The true error (solid) and error estimation using (3.2) (dotted) for the simple optimal control problem in Example 3.2 with regularization parameter $\delta = 10^{-10}$.

in (2.9) would be imprecise. However, the solution of Example 3.2 suggests that the approximation of the error in (3.2) might be accurate even in cases where regularization is needed and the regularization parameter, δ , is chosen to be small.

EXAMPLE 3.2 (A simple optimal control problem). *Minimize*

$$\int_0^1 X(t)^{10} dt, \quad (3.3)$$

subject to

$$\begin{aligned} X'(t) &= \alpha(t) \in [-1, 1], \quad 0 < t \leq T, \\ X(0) &= 0.5. \end{aligned}$$

The Hamiltonian is then non-smooth:

$$H(x, \lambda) := \min_{\alpha \in [-1, 1]} \{ \lambda \alpha + x^{10} \} = -|\lambda| + x^{10},$$

but can be regularized by

$$H_\delta(x, \lambda) := -\sqrt{\lambda^2 + \delta^2} + x^{10},$$

for some small $\delta > 0$.

The exact solution, without regularization, is $X(t) = (0.5 - t)$ for $t \in [0, 0.5]$ and $X(t) = 0$ elsewhere, with control $\alpha(t) = -1$ for $t \in [0, 0.5]$ and $\alpha(t) = 0$ elsewhere. This gives the optimal value of the cost functional (3.3) (the value function) to be $0.5^{11}/11$.

In Figure 3.5, a comparison is made between the error estimate, $\sum_{n=0}^{N-1} \Delta t_n^2 \rho_n$, and the true error. It seems clear that the error estimate converges to the true error as $\Delta t \rightarrow 0$. In this numerical test, the regularization parameter, $\delta = 10^{-10}$, and hence the part of the error from the regularization is negligible.

EXAMPLE 3.3 (A singular optimal control problem). *This example is based on the singular ODE example in [10], suitable for adaptive refinement. Consider the optimal control problem to minimize*

$$\int_0^4 (\alpha(t) - X(t))^2 dt + (X(4) - X_{\text{ref}}(4))^2 \quad (3.4)$$

under the constraint

$$\begin{aligned} X'(t) &= \frac{\alpha(t)}{((t - t_0)^2 + \varepsilon^2)^{\beta/2}}, \\ X(0) &= X_{\text{ref}}(0), \end{aligned}$$

where $t_0 = 5/3$. The reference $X_{\text{ref}}(t)$ solves

$$X'_{\text{ref}}(t) = \frac{X_{\text{ref}}(t)}{((t - 5/3)^2 + \varepsilon^2)^{\beta/2}}$$

and is given explicitly by

$$X_{\text{ref}}(t) = \exp\left(\frac{t - t_0}{\varepsilon^\beta} {}_2F_1\left(\frac{1}{2}, \frac{\beta}{2}, \frac{3}{2}; -\frac{(t - t_0)^2}{\varepsilon^2}\right)\right),$$

where ${}_2F_1$ is the hypergeometric function.

The unique minimizer to (3.4) is therefore given by $X(t) = \alpha(t) = X_{\text{ref}}(t)$ for all $t \in [0, 4]$. Since Example (3.3) has running cost h and flux f with explicit time dependence, we introduce an extra state dimension, $s(t) = t$, as in Remark 1.1. The Hamiltonian is then given by

$$H(x, s; \lambda_1, \lambda_2) = \frac{\lambda_1 x}{((s - t_0)^2 + \varepsilon^2)^{\beta/2}} - \frac{\lambda_1^2}{4((s - t_0)^2 + \varepsilon^2)^\beta} + \lambda_2,$$

where λ_2 is the dual corresponding to s .

Although the Hamiltonian is a smooth function, the problem is a regularization of a controlled ODE with a singularity,

$$X'(t) = \frac{\alpha(t)}{|t - t_0|^\beta},$$

and if the regularization parameter, ε , is small, the remainder term in Theorem 2.4 will be large unless the time steps are very small. As the minimum value of the functional in (3.4) is zero (attained for $\alpha = X = X_{\text{ref}}$), it is immediately clear what the error in this functional is for a numerical simulation. Figure 3.6 shows errors for adaptive and uniform time stepping versus the total number of time steps, and Figure 3.7 shows the dependence of the mesh size on the time parameter.

4. Conclusions. We have presented an a posteriori error representation for optimal control problems with a bound for the remainder term. With the error representation, it is possible to construct adaptive algorithms, and we have presented and tested one such algorithm here. The error representation theorem assumes that the Hamiltonian associated with the optimal control problem belongs to C^2 . As many optimal control problems have Hamiltonians that are only Lipschitz continuous, this is a

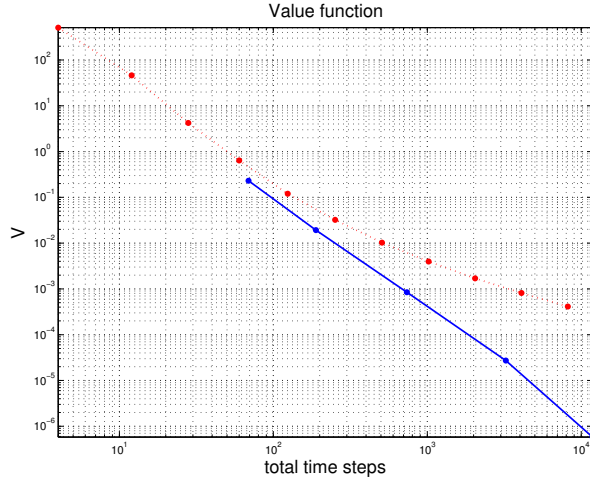


FIG. 3.6. The minimum value of the functional in (3.4) for the singular optimal control problem in Example 3.3, versus the cumulative number of time steps on all refinement levels for the adaptive algorithm (solid) and uniform time steps (dotted). Since the true value of (3.4) is zero the graphs also indicate the respective errors. The regularization parameters are $\varepsilon = 10^{-10}$ and $\beta = 3/4$.

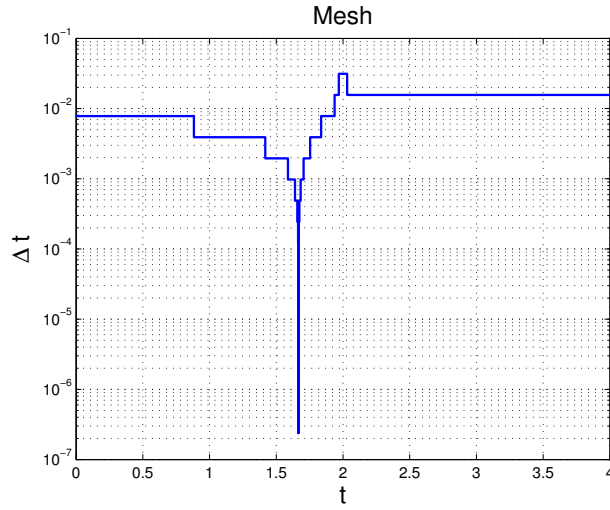


FIG. 3.7. Mesh size versus time for the singular optimal control problem in Example 3.3. The regularization parameters are $\varepsilon = 10^{-10}$ and $\beta = 3/4$.

serious restriction. We have illustrated with a simple test example that C^2 smoothness may not be necessary. To justify this rigorously remains an open problem.

Appendix. Proof of Theorem 2.3. *Step 1.* We show here that there exist a constant K , and a continuous function $S : [0, \infty) \rightarrow \mathbb{R}$, such that $\lim_{s \rightarrow \infty} S(s) = \infty$, and

$$L(x, \beta) \geq (|\beta| - B|x|)_+ S((|\beta| - B|x|)_+) - K(1 + |x|), \quad (\text{A.1})$$

where $y_+ = \max\{y, 0\}$. We will show (A.1) with $K = \max\{\mu(0), A\}$ and S defined by

$$S(\xi) = \int_0^\xi |\{\chi : \mu'(\chi) \leq t, \chi \geq 0\}| dt/\xi.$$

We start by noting that the absolutely continuous (since it is convex) function μ can be modified so that $\mu' > 1$ almost everywhere while (2.6) still holds. We will henceforth assume that μ satisfies this condition.

By the bound on the Hamiltonian, H , and the definition of the running cost, L , in (2.1), we have

$$L(x, \beta) \geq \sup_{\lambda \in \mathbb{R}^d} \{-\beta \cdot \lambda - \mu(|\lambda|) - |x|(A + B|\lambda|)\}.$$

By choosing $\lambda = -\chi\beta/|\beta|$, for $\chi \geq 0$, we have

$$L(x, \beta) \geq \chi|\beta| - \mu(\chi) - |x|(A + B\chi) =: G_{x,\beta}(\chi).$$

Since $G_{x,\beta}(\cdot)$ is concave on $[0, \infty)$, at least one of the following alternatives must hold:

- I. $L(x, \beta) = \infty$.
- II. $G_{x,\beta}$ is maximized at $\chi = 0$.
- III. $G_{x,\beta}$ is maximized at some $\chi^* \in (0, \infty)$.
- IV. $\sup_{0 \leq \chi < \infty} G_{x,\beta}(\chi) = \lim_{\chi \rightarrow \infty} G_{x,\beta}(\chi)$.

If alternative I holds, (A.1) is clearly satisfied with any S and K . If alternative II holds, then

$$L(x, \beta) \geq -\mu(0) - A|x|.$$

Since $\chi = 0$ maximizes $G_{x,\beta}$ and μ is convex it follows that $S((|\beta| - B|x|)_+) = 0$. Hence (A.1) holds.

If alternative III holds, we have

$$L(x, \beta) \geq (|\beta| - B|x|)\chi^* - \mu(\chi^*) - A|x|.$$

Since μ is convex, it is absolutely continuous, and we have

$$\mu(\chi^*) = \mu(0) + \int_0^{\chi^*} \mu'(\chi) d\chi.$$

Using a layer cake representation (see [9]) of this integral we get,

$$\begin{aligned} \int_0^{\chi^*} \mu'(\chi) d\chi &= \int_0^\infty |\{\chi : \mu'(\chi) > t, \chi \in [0, \chi^*]\}| dt \\ &= \int_0^{|\beta| - B|x|} |\{\chi : \mu'(\chi) > t, \chi \in [0, \chi^*]\}| dt, \end{aligned}$$

where the absolute sign in the integrals denotes the Lebesgue measure, and the last equality follows by the fact that $\mu'(\chi) \leq |\beta| - B|x|$ for $\chi \in [0, \chi^*]$ since χ^* maximizes $G_{x,\beta}(\chi)$. Since

$$(|\beta| - B|x|)\chi^* = \int_0^{|\beta| - B|x|} |[0, \chi^*]| dt,$$

we have

$$\begin{aligned} (|\beta| - B|x|)\chi^* - \mu(\chi^*) &= -\mu(0) + \int_0^{|\beta| - B|x|} |\{\chi : \mu'(\chi) \leq t, \chi \in [0, \chi^*]\}| dt \\ &= -\mu(0) + \int_0^{|\beta| - B|x|} |\{\chi : \mu'(\chi) \leq t, \chi \geq 0\}| dt, \end{aligned}$$

where the last inequality follows from the fact that $\mu'(\chi) \geq |\beta| - B|x|$, when $\chi \geq \chi^*$. Since μ' is finite-valued almost everywhere we have

$$\lim_{t \rightarrow \infty} |\{\chi : \mu'(\chi) \leq t, \chi \geq 0\}| = \infty,$$

and therefore $\lim_{s \rightarrow \infty} S(s) = \infty$. Since $\mu' \geq 1$, the function S is continuous. With $K = \max\{\mu(0), A\}$, (A.1) is satisfied.

If alternative IV holds we can use that

$$L(x, \beta) \geq (|\beta| - B|x| - \varepsilon)\chi - \mu(\chi) - A|x| =: G_{x, \beta}^\varepsilon(\chi)$$

for all $0 \leq \chi < \infty$ and $\varepsilon > 0$. For every $\varepsilon > 0$ the function $G_{x, \beta}$ is maximized at a $\chi_\varepsilon^* \in [0, \infty)$. This gives, as the analysis for alternatives II and III shows, that

$$L(x, \beta) \geq (|\beta| - B|x| - \varepsilon)_+ S((|\beta| - B|x| - \varepsilon)_+) - K(1 + |x|).$$

Since ε could be chosen arbitrarily small and positive (A.1) follows.

Step 2. We now show that for each time step t_n , there exists a constant K , such that

$$\bar{u}(x, t_n) \geq -K(1 + |x|). \quad (\text{A.2})$$

(The constant K is allowed to depend on the time step n and the step length Δt_n .) Assume (A.2) is satisfied at the time step t_{n+1} . We will show that this implies that it is satisfied at t_n as well.

The lower bound on $\bar{u}(\cdot, t_{n+1})$ and the lower bound on L in (A.1), together with dynamic programming gives

$$\begin{aligned} \bar{u}(x, t_n) &= \inf_{\beta \in \mathbb{R}^d} (\Delta t_n L(x, \beta) + \bar{u}(x + \Delta t_n \beta, t_{n+1})) \\ &\geq \inf_{\beta \in \mathbb{R}^d} (\Delta t_n (|\beta| - B|x|)_+ S((|\beta| - B|x|)_+) - \tilde{K} - \tilde{K}|x| - \tilde{K}|\beta|) =: \inf_{\beta \in \mathbb{R}^d} J(x, \beta), \end{aligned}$$

with a \tilde{K} depending on Δt_n . Since the function S grows to infinity, there exists a $C \geq 0$, such that $\xi \geq C$ implies $S(\xi) \geq \tilde{K}/\Delta t_n$. For such β that satisfy $|\beta| - B|x| \geq C$ it therefore holds that

$$J(x, \beta) \geq \tilde{K}(|\beta| - B|x|) - \tilde{K} - \tilde{K}|x| - \tilde{K}|\beta| = -\tilde{K} - (\tilde{K} + \tilde{K}B)|x|.$$

Since S is continuous the function

$$\xi \mapsto \xi_+ S(\xi_+)$$

attains a smallest value D on the set $\{\xi \in \mathbb{R}^d : |\xi| \leq C\}$. For every β satisfying $|\beta| - B|x| \leq C$ we therefore have

$$J(x, \beta) \geq D\Delta t_n - \tilde{K} - \tilde{K}|x| - \tilde{K}|\beta| \geq D\Delta t_n - \tilde{K} - \tilde{K}C - (\tilde{K} + \tilde{K}B)|x|.$$

With $\bar{K} = \max\{\tilde{K} + \tilde{K}B, \tilde{K} + \tilde{K}C - D\Delta t_n\}$, and hence independent of x , we have

$$\bar{u}(x, t_n) \geq -\bar{K}(1 + |x|).$$

Since $\bar{u}(\cdot, t_N)$ satisfies (A.2) with $K = k$, by the lower bound on g , induction backwards in time shows that (A.2) holds for all $n \leq N$, with different constants K .

Step 3. Assume that $\bar{u}(\cdot, t_{n+1})$ is locally semiconcave. It is then also continuous (even locally Lipschitz continuous, see e.g. [5]). Since the Hamiltonian, H , is finite-valued everywhere, $L(x, \cdot)$ is lower semicontinuous, for every $x \in \mathbb{R}^d$, see [11]. Let $\{\beta_i\}_{i=1}^\infty$ be a sequence of controls such that

$$\lim_{i \rightarrow \infty} \Delta t_n L(X_n, \beta_i) + \bar{u}(X_n + \Delta t_n \beta_i, t_{n+1}) \rightarrow \bar{u}(X_n, t_n).$$

By the lower bounds (A.1) and (A.2) for the functions L and $\bar{u}(\cdot, t_{n+1})$, proved in steps 1 and 2, it follows that the sequence $\{\beta_i\}_{i=1}^\infty$ is contained in a compact set in \mathbb{R}^d . It therefore contains a convergent subsequence

$$\beta_{i_j} \rightarrow \beta_n.$$

Since $\bar{u}(\cdot, t_{n+1})$ is continuous, and $L(X_n, \cdot)$ is lower semicontinuous, we have that

$$\bar{u}(X_n, t_n) = \Delta t_n L(X_n, \beta_n) + \bar{u}(X_n + \Delta t_n \beta_n, t_{n+1}).$$

Step 4. Assume that $\bar{u}(\cdot, t_{n+1})$ is locally semiconcave, and that λ_{n+1} is an element in $D^+ \bar{u}(X_{n+1}, t_{n+1})$, where $X_{n+1} = X_n + \Delta t_n \beta_n$, and β_n is the minimizer from the previous step. We will show that this implies that

$$\lambda_{n+1} \cdot \beta_n + L(X_n, \beta_n) = H(X_n, \lambda_{n+1}). \quad (\text{A.3})$$

Consider a closed unit ball B centered at β_n . By the local semiconcavity of $\bar{u}(\cdot, t_{n+1})$ we have that there exists an $\omega : \mathbb{R}^+ \rightarrow \mathbb{R}^+$, such that $\lim_{\rho \rightarrow 0^+} \omega(\rho) = 0$, and

$$\bar{u}(X_n + \Delta t_n \beta, t_{n+1}) \leq \bar{u}(X_{n+1}, t_{n+1}) + \Delta t_n \lambda_{n+1} \cdot (\beta - \beta_n) + |\beta - \beta_n| \omega(|\beta - \beta_n|), \quad (\text{A.4})$$

for all β in B , see [5]. Since we know that the function

$$\beta \mapsto \bar{u}(X_n + \Delta t_n \beta, t_{n+1}) + \Delta t_n L(X_n, \beta)$$

is minimized for $\beta = \beta_n$, the semiconcavity of \bar{u} in (A.4) implies that the function

$$\beta \mapsto \Delta t_n \lambda_{n+1} \cdot \beta + |\beta - \beta_n| \omega(|\beta - \beta_n|) + \Delta t_n L(X_n, \beta) \quad (\text{A.5})$$

is also minimized on B for $\beta = \beta_n$ (and therefore by the convexity of $L(X_n, \cdot)$ also minimized on \mathbb{R}^d). We will prove that the function

$$\beta \mapsto \lambda_{n+1} \cdot \beta + L(X_n, \beta) \quad (\text{A.6})$$

is minimized for $\beta = \beta_n$. Let us assume that this is false, so that there exists an $\beta^* \in \mathbb{R}^d$, and an $\varepsilon > 0$, such that

$$\lambda_{n+1} \cdot \beta_n + L(X_n, \beta_n) - \lambda_{n+1} \cdot \beta^* - L(X_n, \beta^*) \geq \varepsilon. \quad (\text{A.7})$$

Let $\xi \in [0, 1]$, and $\hat{\beta} = \xi\beta^* + (1 - \xi)\beta_n$. Insert $\hat{\beta}$ into the function in (A.5):

$$\begin{aligned}
& \Delta t \lambda_{n+1} \cdot \hat{\beta} + |\hat{\beta} - \beta_n| \omega(|\hat{\beta} - \beta_n|) + \Delta t_n L(X_n, \hat{\beta}) \\
&= \Delta t (\xi \lambda_{n+1} \cdot \beta^* + (1 - \xi) \lambda_{n+1} \cdot \beta_n) + \xi |\beta^* - \beta_n| \omega(\xi |\beta^* - \beta_n|) \\
&\quad + \Delta t_n L(X_n, \xi \beta^* + (1 - \xi) \beta_n) \\
&\leq \Delta t (\xi \lambda_{n+1} \cdot \beta^* + (1 - \xi) \lambda_{n+1} \cdot \beta_n) + \xi |\beta^* - \beta_n| \omega(\xi |\beta^* - \beta_n|) \\
&\quad + \Delta t_n \xi L(X_n, \beta^*) + \Delta t_n (1 - \xi) L(X_n, \beta_n) \\
&\leq \Delta t_n (\lambda_{n+1} \cdot \beta_n + L(X_n, \beta_n)) + \xi |\beta^* - \beta_n| \omega(\xi |\beta^* - \beta_n|) - \Delta t_n \xi \varepsilon \\
&\quad < \Delta t_n (\lambda_{n+1} \cdot \beta_n + L(X_n, \beta_n)),
\end{aligned}$$

for some small positive number ξ . This contradicts the fact that β_n is a minimizer to the function in (A.5). Hence we have shown that the function in (A.6) is minimized at β_n . By the relation between L and H in (2.2) our claim (A.3) follows.

Step 5. From the result in step 4, equation (A.3), and the definition of the running cost L in (2.1) it follows that $\beta_n = H_\lambda(X_n, \lambda_{n+1})$, for if this equation did not hold, then λ_{n+1} could not be the maximizer of $-\beta_n \cdot \lambda + H(X_n, \lambda)$.

Step 6 We now show that under the assumption that $\bar{u}(\cdot, t_{n+1})$ is locally semiconcave, then for each $F > 0$ there exists a $G > 0$, such that

$$|x| \leq F \implies |\beta_x| \leq G, \quad (\text{A.8})$$

where β_x is any optimal control at position (x, t_n) , i.e. $\bar{u}(x, t_n) = \bar{u}(x + \Delta t_n \beta_x, t_{n+1}) + \Delta t_n L(x, \beta_x)$. Step 5 proved that an optimal control is given by $\beta_n = H_\lambda(X_n, \lambda_{n+1})$, so that

$$\bar{u}(0, t_n) = \bar{u}(\Delta t_n H_\lambda(0, p), t_{n+1}) + \Delta t L(0, H_\lambda(0, p)),$$

where p is an element in $D^+ \bar{u}(\Delta t_n \beta_0, t_{n+1})$. Let us now consider the control $H_\lambda(x, p)$. Since this control is not necessarily optimal except at $(0, t_n)$, we have

$$\bar{u}(x, t_n) \leq \bar{u}(x + \Delta t_n H_\lambda(x, p), t_{n+1}) + \Delta t_n L(x, H_\lambda(x, p)).$$

Since $\bar{u}(\cdot, t_{n+1})$ is locally semiconcave it is also locally Lipschitz continuous (see [5]). By the definition of L in (2.1) it follows that

$$L(x, H_\lambda(x, p)) = -H_\lambda(x, p) \cdot p + H(x, p).$$

Since both $H(\cdot, p)$ and $H_\lambda(\cdot, p)$ are locally Lipschitz continuous by assumption it follows that there exists a constant $E > 0$ such that

$$\bar{u}(x, t_n) - \bar{u}(0, t_n) \leq E, \quad (\text{A.9})$$

for all $|x| \leq F$.

The inequalities (A.1) from step 1 and (A.2) from step 2, together with (A.9) give (A.8).

Step 7. In this step, we show that if $\bar{u}(\cdot, t_{n+1})$ is locally semiconcave, then so is $\bar{u}(\cdot, t_n)$. Furthermore, if β_x is an optimal control at (x, t_n) , and p is an element in $D^+ \bar{u}(x + \Delta t_n \beta_x, t_n)$, then

$$p + \Delta t_n H_x(x, p) \in D^+ \bar{u}(x, t_n).$$

We denote by B_r the closed ball centered at the origin with radius r . In order to prove that $\bar{u}(\cdot, t_n)$ is locally semiconcave it is enough to show that it is semiconcave on B_r , where r is any positive radius. To accomplish this we will use the result from step 6. We therefore take the radius $r = F$, which according to step 6 can be taken arbitrarily large.

In step 3 we showed that an optimal control β_x exists at every point $x \in \mathbb{R}^d$ at time t_n , under the assumption that $\bar{u}(\cdot, t_{n+1})$ is locally semiconcave. In step 6 we showed that given any radius F and $|x| \leq F$, there exists a constant G such that all optimal controls must satisfy $|\beta_x| \leq G$.

A locally semiconcave function from \mathbb{R}^d to \mathbb{R} is locally Lipschitz continuous (see [5]). Hence, for every $x \in B_{F+G\Delta t_n}$, and every $p \in D^+\bar{u}(x, t_{n+1})$, we have $|p| \leq E$, for some constant E . By continuity, there exists some constant J such that $|H_\lambda| \leq J$ on $B_F \times B_E$.

Let $R := \max\{F + G\Delta t_n, F + J\Delta t_n\}$. By the assumed local semiconcavity of $\bar{u}(\cdot, t_{n+1})$ we have that there exists an $\omega : \mathbb{R}^+ \rightarrow \mathbb{R}^+$, such that $\lim_{\rho \rightarrow 0} \omega(\rho) = 0$, and

$$\bar{u}(x, t_{n+1}) \leq \bar{u}(z, t_{n+1}) + p \cdot (x - z) + |x - z|\omega(|x - z|),$$

for all x and z in B_R , and p in $D^+\bar{u}(z, t_{n+1})$, see [5]. We take ω to be non-decreasing, which is clearly possible. Let us now consider the control $H_\lambda(x, p)$, where $p \in D^+\bar{u}(y + \Delta t_n \beta_y, t_{n+1})$, and β_y is an optimal control at the point $y \in B_F$ ($\beta_y = H_\lambda(y, p)$ according to step 5). Since this control is not necessarily optimal except at (y, t_n) , we have

$$\begin{aligned} \bar{u}(x, t_n) &\leq \bar{u}(x + \Delta t_n H_\lambda(x, p), t_{n+1}) + \Delta t_n L(x, H_\lambda(x, p)) \\ &\leq \bar{u}(y + \Delta t_n \beta_y, t_{n+1}) + p \cdot (x + \Delta t_n H_\lambda(x, p) - (y + \Delta t_n \beta_y)) + \Delta t_n L(x, H_\lambda(x, p)) \\ &\quad + |x + \Delta t_n H_\lambda(x, p) - (y + \Delta t_n \beta_y)|\omega(|x + \Delta t_n H_\lambda(x, p) - (y + \Delta t_n \beta_y)|). \end{aligned} \quad (\text{A.10})$$

By the bound on $|H_\lambda|$, this inequality holds for every x and y in B_F . By the definition of L in (2.1) it follows that

$$L(x, H_\lambda(x, p)) = -H_\lambda(x, p) \cdot p + H(x, p). \quad (\text{A.11})$$

With this fact in (A.10), and using that $\beta_y = H_\lambda(y, p)$, we have

$$\begin{aligned} \bar{u}(x, t_n) &\leq \bar{u}(y + \Delta t_n H_\lambda(y, p), t_{n+1}) + p \cdot (x - (y + \Delta t_n H_\lambda(y, p))) + \Delta t_n H(x, p) \\ &\quad + |x + \Delta t_n H_\lambda(x, p) - (y + \Delta t_n H_\lambda(y, p))|\omega(|x + \Delta t_n H_\lambda(x, p) - (y + \Delta t_n H_\lambda(y, p))|). \end{aligned} \quad (\text{A.12})$$

By the fact that $H_\lambda(\cdot, p)$ is locally Lipschitz continuous,

$$|x - y + \Delta t (H_\lambda(x, p) - H_\lambda(y, p))| \leq K|x - y|, \quad (\text{A.13})$$

for all x and y in B_F , and some constant K . We also need the fact that

$$\bar{u}(y, t_n) = \bar{u}(y + \Delta t_n H_\lambda(y, p), t_{n+1}) + \Delta t_n L(y, H_\lambda(y, p)). \quad (\text{A.14})$$

We insert the results (A.11), (A.13), and (A.14), into (A.12) to get

$$\begin{aligned} \bar{u}(x, t_n) &\leq \bar{u}(y, t_n) + p \cdot (x - y) + \Delta t_n (H(x, p) - H(y, p)) + K|x - y|\omega(K|x - y|) \\ &\leq \bar{u}(y, t_n) + (p + \Delta t_n H_x(y, p)) \cdot (x - y) + |x - y|\tilde{\omega}(|x - y|) \end{aligned} \quad (\text{A.15})$$

where

$$\tilde{\omega}(\rho) = K\omega(K\rho) + \max\{|H_x(z, q) - H_x(y, q)| : |z - y| \leq \rho, (z, y) \in B_F \times B_F\},$$

and $\lim_{\rho \rightarrow 0^+} \tilde{\omega}(\rho) = 0$, since H_x is assumed to be continuous.

We will now use equation (A.15) to show that $\bar{u}(\cdot, t_n)$ is semiconcave on B_F . Let x and z be any elements in B_F , and let $y = wx + (1 - w)z$, where $w \in [0, 1]$. As before, p is an element in $D^+\bar{u}(y + \Delta t_n \beta_y, t_{n+1})$. The inequality in (A.15) with this choice of y gives

$$\begin{aligned} \bar{u}(x, t_n) &\leq \bar{u}(wx + (1 - w)z, t_n) \\ &+ (1 - w)(p + \Delta t_n H_x(wx + (1 - w)z, p)) \cdot (x - z) + (1 - w)|x - z| \tilde{\omega}((1 - w)|x - z|), \end{aligned} \quad (\text{A.16})$$

and with x exchanged by z ,

$$\begin{aligned} \bar{u}(z, t_n) &\leq \bar{u}(wx + (1 - w)z, t_n) \\ &+ w(p + \Delta t_n H_x(wx + (1 - w)z, p)) \cdot (z - x) + w|x - z| \tilde{\omega}(w|x - z|). \end{aligned} \quad (\text{A.17})$$

We multiply (A.16) by w , and (A.17) by $1 - w$, and add the resulting equations, to get

$$\begin{aligned} &w\bar{u}(x, t_n) + (1 - w)\bar{u}(z, t_n) \\ &\leq \bar{u}(wx + (1 - w)z, t_n) + w(1 - w)|x - z| (\tilde{\omega}((1 - w)|x - z|) + \tilde{\omega}(w|x - z|)) \\ &\leq \bar{u}(wx + (1 - w)z, t_n) + w(1 - w)|x - z| \hat{\omega}(|x - z|), \end{aligned}$$

if we let

$$\hat{\omega}(\rho) := 2\tilde{\omega}(\rho).$$

Since x and z can be any points in B_F , this shows that $\bar{u}(\cdot, t_n)$ is locally semiconcave.

By (A.15) it also follows that

$$p + \Delta t_n H_x(y, p) \in D^+\bar{u}(y, t_n).$$

Step 8. Since $\bar{u}(x, T) = g(x)$, which is locally semiconcave, step 7 and induction backwards in time shows that $\bar{u}(\cdot, t_n)$ is locally semiconcave for all n . In step 3 we showed that optimal controls exist at every position in \mathbb{R}^d at time t_n , provided $\bar{u}(\cdot, t_{n+1})$ is locally semiconcave. Hence there exists a minimizer $(\beta_m, \dots, \beta_{N-1})$ to the discrete minimization functional $J_{(y, t_m)}$ in (2.4), for every $y \in \mathbb{R}^d$ and $0 \leq m \leq N$. Let (X_m, \dots, X_N) be a corresponding solution to (2.5), and λ_N an element in $D^+g(X_N)$. From steps 5 and 7, we have that $\beta_{N-1} = H_\lambda(X_{N-1}, \lambda_N)$, and $\lambda_{N-1} := \lambda_N + \Delta t_{N-1} H_x(X_{N-1}, \lambda_N) \in D^+\bar{u}(X_{N-1}, t_{N-1})$. Induction backwards in time shows that there exists a dual path λ_n , $n = m, \dots, N - 1$, such that it together with X_n , $n = m, \dots, N$, satisfies the discretized Hamiltonian system (2.7).

REFERENCES

- [1] W. BANGERTH AND R. RANNACHER, *Adaptive Finite Element Methods for Differential Equations*, Lectures in Mathematics ETH Zürich, Birkhäuser Verlag, Basel, 2003.

- [2] M. BARDI AND I. CAPUZZO-DOLCETTA, *Optimal Control and Viscosity Solutions of Hamilton-Jacobi-Bellman equations*, Systems & Control: Foundations & Applications, Birkhäuser Boston Inc., Boston, MA, 1997. With appendices by Maurizio Falcone and Pierpaolo Soravia.
- [3] G. BARLES, *Solutions de Viscosité des Équations de Hamilton-Jacobi*, vol. 17 of Mathématiques & Applications (Berlin) [Mathematics & Applications], Springer-Verlag, Paris, 1994.
- [4] R. BECKER AND R. RANNACHER, *An optimal control approach to a posteriori error estimation in finite element methods*, Acta Numer., 10 (2001), pp. 1–102.
- [5] P. CANNARSA AND C. SINISTRARI, *Semiconcave Functions, Hamilton-Jacobi Equations, and Optimal Control*, Progress in Nonlinear Differential Equations and their Applications, 58, Birkhäuser Boston Inc., Boston, MA, 2004.
- [6] K. KRAFT AND S. LARSSON, *The dual weighted residuals approach to optimal control of ordinary differential equations*, BIT, 50 (2010), pp. 587–607.
- [7] ———, *An adaptive finite element method for nonlinear optimal control problems*. <http://www.math.chalmers.se/Math/Research/Preprints/2011/1.pdf>, 2011.
- [8] ———, *Finite element approximation of variational inequalities in optimal control*. <http://www.math.chalmers.se/Math/Research/Preprints/2011/2.pdf>, 2011.
- [9] E. H. LIEB AND M. LOSS, *Analysis*, vol. 14 of Graduate Studies in Mathematics, American Mathematical Society, Providence, RI, 1997.
- [10] K.-S. MOON, A. SZEPESSY, R. TEMPONE, AND G. E. ZOURARIS, *A variational principle for adaptive approximation of ordinary differential equations*, Numer. Math., 96 (2003), pp. 131–152.
- [11] R. T. ROCKAFELLAR, *Monotone Processes of Convex and Concave Type*, Memoirs of the American Mathematical Society, No. 77, American Mathematical Society, Providence, R.I., 1967.
- [12] P. RUTQUIST AND M. EDVALL, *PROPT Manual*, Tomlab Optimization Inc. http://tomopt.com/docs/TOMLAB_PROPT.pdf.
- [13] M. SANDBERG, *Extended applicability of the symplectic Pontryagin method*, arXiv:0901.4805, (2009).
- [14] M. SANDBERG AND A. SZEPESSY, *Convergence rates of symplectic Pontryagin approximations in optimal control theory*, M2AN Math. Model. Numer. Anal., 40 (2006), pp. 149–173.