An a posteriori error estimate for Symplectic Euler approximation of optimal control problems

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Outline

- Optimal Control as ill-posed and well-posed problems
- Error representation
- Adaptive algorithm
- Numerical tests

Optimal Control

Minimize

$$\int_0^T h\big(X(s), \alpha(s)\big)\,ds + g\big(X(T)\big)$$

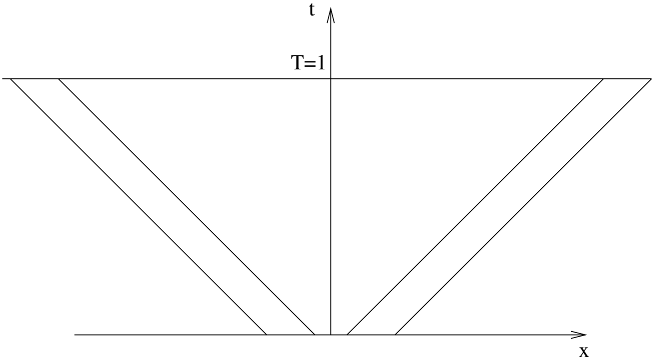
when X solves

$$X'(s) = f\big(X(s), \alpha(s)\big), \quad 0 < s < T$$
$$X(0) = x_0.$$

and $X(s) \in \mathbb{R}^d$, $\alpha(s) \in B$.

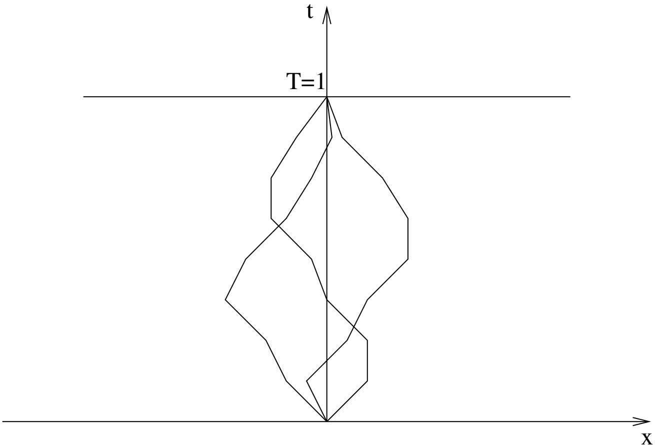
Optimal Control Ill-posed

Ex. Minimize $-|X(1)|$ over solutions $X' = \alpha \in [-1, 1]$.



Optimal Control Ill-posed

Ex. Minimize $|X(1)|$ over solutions $X' = \alpha \in [-1, 1]$.



Optimal Control Well-posed

$$u(x,t) = \inf_{\substack{\alpha \\ X_t = x}} \Big(\int_t^T h(X(s), \alpha(s))ds + g(X(T)) \Big)$$

Hamilton-Jacobi equation:

$$\begin{aligned} u_t + H(u_x, x) &= 0, \\ u(x,T) &= g(x), \end{aligned} \tag{1}$$

where

$$H(\lambda, x) = \min_a \big(\lambda \cdot f(x,a) + h(x,a) \big)$$

(See e.g. L. Evans "Partial Differential Equations".)

Optimal controls are characteristics

Theorem

Assume $H \in C^{1,1}_{loc}(\mathbb{R}^d \times \mathbb{R}^d)$, f, g, h smooth etc., and (α, X) optimal control and state variables for the starting position $(x,t) \in \mathbb{R}^d \times [0,T]$. Then $\exists$ dual path $\lambda : [t,T] \to \mathbb{R}^d$:

$$\begin{aligned} X'(s) &= H_\lambda\big(\lambda(s), X(s)\big), \\ -\lambda'(s) &= H_x\big(\lambda(s), X(s)\big), \\ \lambda(T) &= g'\big(X(T)\big). \end{aligned}$$

(See e.g. P. Cannarsa, C. Sinestrari, "Semiconcave Functions, Hamilton-Jacobi Equations, and Optimal Control.")
This is the Pontryagin principle for the case when the Hamiltonian is differentiable.

Hamilton-Jacobi vs. Pontryagin

	Hamilton-Jacobi	Pontryagin
Global min	+	-
High dimension	-	+

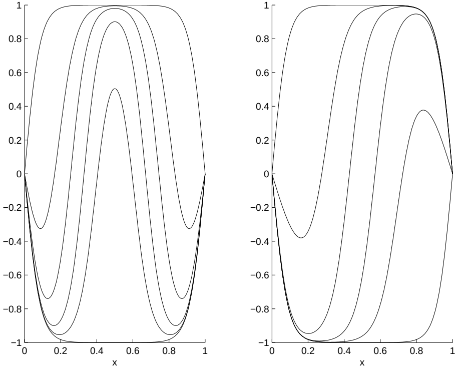
Idea: Use Pontryagin for numerical methods, and Hamilton-Jacobi for theoretical evaluation.

Allen-Cahn Ex.

$$\min_\alpha \int_0^T h\big(\alpha(t)\big)dt + g\big(\varphi(T)\big),$$
$$h(\alpha) = ||\alpha||^2_{L^2(0,1)}/2, \quad g(\varphi_T) = K||\varphi_T - \varphi_-||^2_{L^2(0,1)}$$

and φ solves

$$\varphi_t = \varepsilon\varphi_{xx} - \varepsilon^{-1}V'(\varphi) + \alpha, \quad \varphi(0,t) = \varphi(1,t) = 0,$$
$$\varphi(x,0) = \varphi_0(x).$$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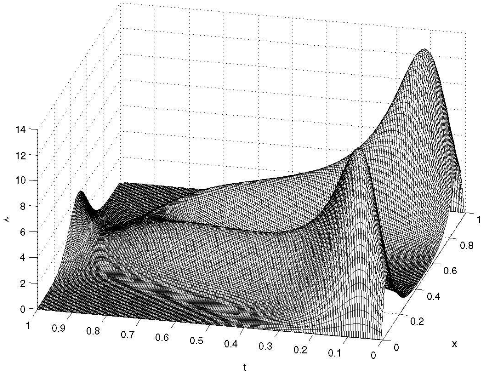
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0.2
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t
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0.2
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0.8
1
x

Variational representation of Hamilton-Jacobi

If $u : \mathbb{R}^d \times [0, T] \to \mathbb{R}$ viscosity solution of Hamilton-Jacobi-Bellman equation (1):

$$u(x,t) = \inf_{\beta} \Big\{ \int_t^T L(\beta, X) dt + g\big(X(T)\big) \big| X'(t) = \beta(t), X(t) = x \Big\},$$

where

$$L(x,\beta) = \sup_{\lambda} \big\{ -\beta \cdot \lambda + H(\lambda, x) \big\}, \text{ and } H(\lambda, x) = \inf_{\beta} \big\{ \lambda \cdot \beta + L(x, \beta) \big\}.$$

(Legendre-type transform)

Representation as discrete minimization

Symplectic Euler

$$
\begin{aligned}
X_{n+1} &= X_n + \Delta t_n H_\lambda(X_n, \lambda_{n+1}),\\
\lambda_n &= \lambda_{n+1} + \Delta t_n H_x(X_n, \lambda_{n+1}),
\end{aligned}
$$

corresponds to minimization of

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

where $X_{n+1} = X_n + \Delta t_n \beta_n$.

Proof

Assume $\bar{u}(\cdot, t_{n+1})$ semiconcave and $\lambda_{n+1} \in D^+\bar{u}(X_{n+1}, t_{n+1})$. Since

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

minimized for $\beta = \beta_n$, we have

$$\beta \mapsto \lambda_{n+1} \cdot \beta + L(X_n, \beta)$$

minimized for $\beta = \beta_n$. Hence $\beta_n = H_\lambda(X_n, \lambda_{n+1})$.

Need also show that semiconcavity of $\bar{u}(\cdot, t_{n+1})$ implies semiconcavity of $\bar{u}(\cdot, t_n)$, and $\lambda_n := \lambda_{n+1} + \Delta t H_x(X_n, \lambda_{n+1})$. Use control $H_\lambda(x, \lambda_{n+1})$.

Aim: Bound error $|\bar{u}(x_0,0) - u(x_0,0)|$

Introduce piecewise linear $\bar{X}(t)$ as

$$\bar{X}(t) = X_n + (t-t_n)\beta_n = X_n + (t-t_n)H_\lambda(X_n, \lambda_{n+1}), \qquad t \in (t_n, t_{n+1})$$

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

If we write

$$\begin{aligned}(\bar{u}-u)(x_0,0) &= \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}} L(X_n,\beta_n)+u_t(\bar{X}(t),t)+u_x(\bar{X}(t),t)\cdot\beta_n \mathrm{d}t\\ &= \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}} \big(u_t(\bar{X}(t),t)+u_x(\bar{X}(t),t)\cdot\beta_n+L(\bar{X}(t),\beta_n)\\ &\qquad\qquad + L(X_n,\beta_n)-L(\bar{X}(t),\beta_n)\big)\mathrm{d}t\end{aligned}$$

and use

$$H(x,\lambda)=\min_{\beta\in\mathbb{R}^d}\big(\lambda\cdot\beta+L(x,\beta)\big)$$

together with the fact that u solves a Hamilton-Jacobi equation we get

$$\bar{u}(x_0,0)-u(x_0,0)\geq\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\big(L(X_n,\beta_n)-L(\bar{X}(t),\beta_n)\big)dt.$$

Hence lower bound for the error.

Convergence of Symplectic Pontryagin

Theorem

Assume that the Hamiltonian satisfies

$$\begin{cases} |H(x,\lambda_1) - H(x,\lambda_2)| \le C|\lambda_1 - \lambda_2|, \\ |H(x_1,\lambda) - H(x_2,\lambda)| \le C|x_1 - x_2|(1+|\lambda|), \\ H(x,\cdot) \text{ is concave.} \end{cases}$$

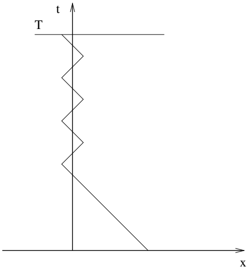
Assume that the terminal cost g is continuously differentiable, and $g(x) \ge -k(1+|x|)$.
Then there exists a solution $\{\bar{X}_n, \bar{\lambda}_n\}$ with associated value $\bar{u}$, such that

$$|u - \bar{u}| = \mathcal{O}(\delta + \Delta t).$$

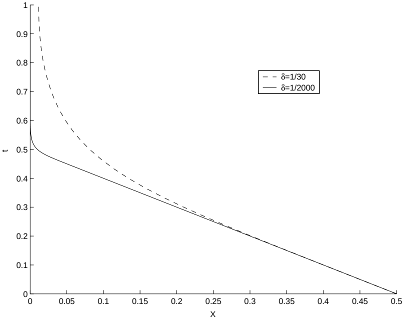
Example of a nondifferentiable Hamiltonian

$$f = \alpha \in \{-1, 1\}, \quad \inf \int_0^1 X^2 dt$$

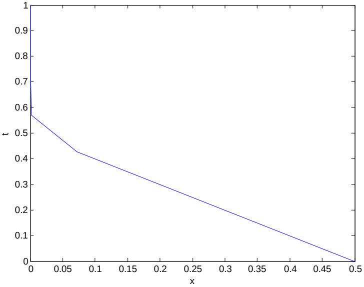
$$H(\lambda, x) = \min_a \big(\lambda \cdot f(x, a) + h(x, a)\big) = -|\lambda| + x^2$$



Nondifferentiable Hamiltonian example contd.



Nondifferentiable Hamiltonian example contd.



Back to $\bar{u} - u$ error

Using

$$\begin{aligned} u_t &= -H(x, u_x), \\ L(X_n, \beta_n) + \lambda_{n+1} \cdot \beta_n &= H(x_n, \lambda_{n+1}), \\ \beta_n &= H_\lambda(x_n, \lambda_{n+1}), \end{aligned}$$

we have

$$\begin{aligned} (\bar{u} - u)(x_0, 0) &= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} L(X_n, \beta_n) + u_t(\bar{X}(t), t) + u_x(\bar{X}(t), t) \cdot \beta_n \mathrm{d}t \\ &= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} H(X_n, \lambda_{n+1}) - H(\bar{X}(t), u_x(\bar{X}(t), t)) \, \mathrm{d}t + \\ &\quad \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \left(u_x(\bar{X}(t), t) - \lambda_{n+1} \right) \cdot H_\lambda(X_n, \lambda_{n+1}) \, \mathrm{d}t \end{aligned}$$

Error in approximate value function

The trapezoidal rule and an assumption on closeness between λ_n and $u_x(x_n, t_n)$ gives

Theorem

Assume $H \in C^2(\mathbb{R}^d \times \mathbb{R}^d)$ and $|\lambda_n - u_x(X_n, \lambda_n)| \leq C\Delta t_{max}$ and the value function u is bounded in $C^3((0,T) \times \mathbb{R}^d)$ (either globally or locally with an extra assumption on X_n convergence). Then

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

with density

$$\rho_n := -\frac{H_\lambda(X_n, \lambda_{n+1}) \cdot H_x(X_n, \lambda_{n+1})}{2} \tag{3}$$

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

Algorithm (Adaptivity (Numer. Math. 03 M. S. T. Z.))

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* $\{(X_n, \lambda_n)\}_{n=0}^N$.
2. *Calculate error densities* $\{\rho_n\}_{n=0}^N$ *and the corresponding approximate error densities*
$$\bar{\rho}_n := \operatorname{sgn}(\rho_n)\max(|\rho_n|, \sqrt{\Delta t_{max}}).$$
3. *Break if*
$$\max_n \bar{r}_n < \frac{TOL}{N}.$$
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*
$$\bar{r}_n > s\frac{TOL}{N}.$$
5. *Update N and* $\{t_n\}_{n=0}^N$ *to reflect the new mesh.*

Introduce a constant $c = c(t)$, such that

$$c \le \left|\frac{\bar\rho(t)[\text{parent}(n,k)]}{\bar\rho(t)[k]}\right| \le c^{-1},$$
$$c \le \left|\frac{\bar\rho(t)[k-1]}{\bar\rho(t)[k]}\right| \le c^{-1}, \tag{4}$$

holds for all time steps $t \in \Delta t_n[k]$ and all refinement levels k.

Theorem

[Stopping] Assume that c satisfies (4) for the time steps corresponding to the maximal error indicator on each refinement level, and that

$$M^2 > c^{-1},\ s \le \frac{c}{M}. \tag{5}$$

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

$$\max_n \bar r_n[k+1] \le \frac{c^{-1}}{M^2} \max_n \bar r_n[k],$$

or stops the algorithm.

Theorem

[Accuracy] The adaptive algorithm satisfies

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

Theorem

[Efficiency] Assume that $c = c(t)$ satisfies (4) 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 0.4, satisfies

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

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

Numerical Tests

Ex. (From PROPT Manual, by Rutquist, Edvall). Minimize

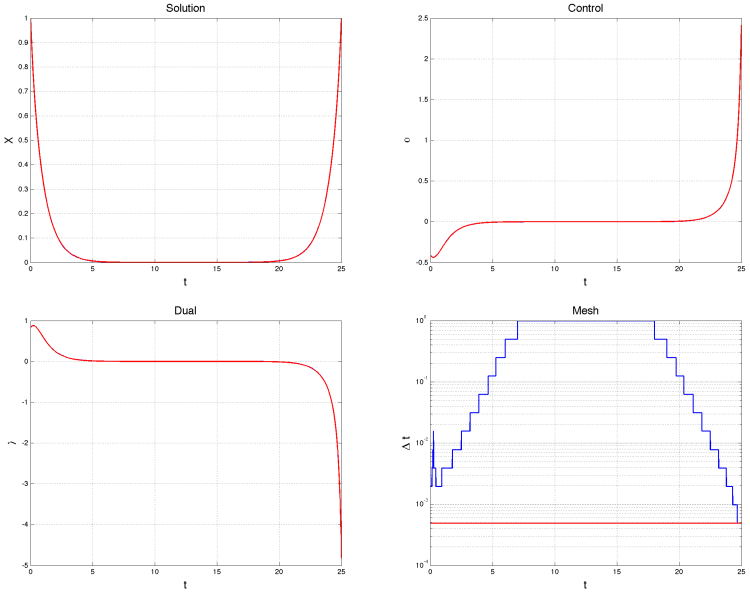
$$\int_0^{25} X(t)^2 + \alpha(t)^2 \mathrm{d}t + \gamma(X(25) - 1)^2,$$

subject to

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

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

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


Solution
X
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Dual
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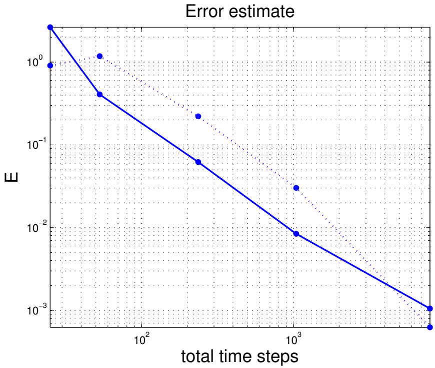
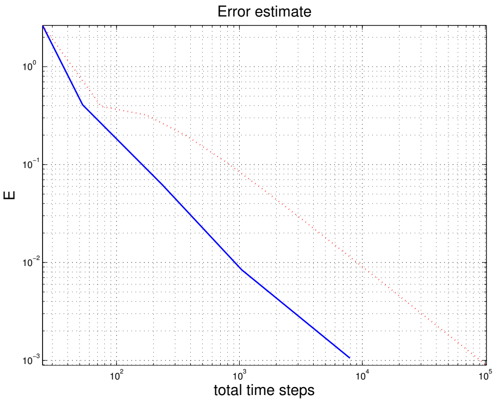


Error estimates for the hyper-sensitive optimal control problem. The solid line indicates the error estimate, and the dotted line indicates the difference between the value function and the value function using a fine uniform mesh with 51200 time steps. The error estimate for the uniform mesh is approximately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



Error estimates for the hyper-sensitive optimal control problem 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.

Example with non-smooth Hamiltonian

Ex. Minimize

$$\int_0^1 X(t)^{10}\mathrm{d}t,$$

subject to

$$X'(t) = \alpha(t) \in [-1, 1], \quad 0 < t \leq T,$$
$$X(0) = 0.5.$$

The Hamiltonian is then non-smooth

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

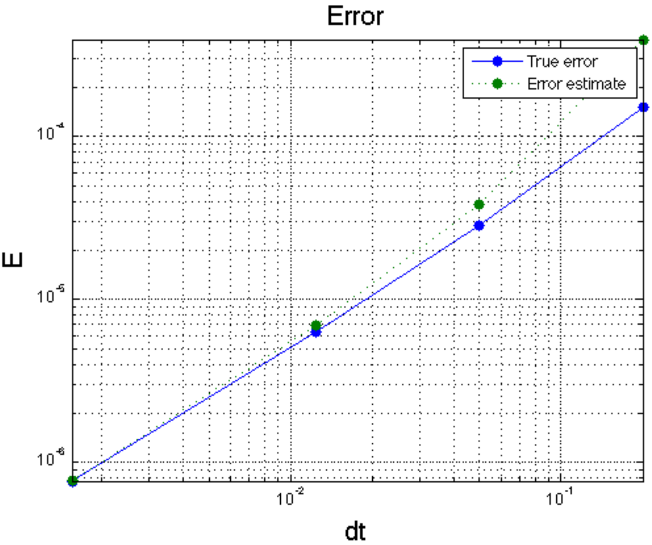
but can be regularized by

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

for some small $\delta > 0$.

Changing the Hamiltonian H to H^δ, with $|H - H^\delta| = \mathcal{O}(\delta)$ introduces an error of order δ in the value function u. However, the remainder term R in the error representation contains second derivatives of H, and $\partial_{\lambda\lambda} H^\delta = \mathcal{O}(\delta^{-1})$.

The a priori error result however gives bound $\mathcal{O}(\delta + \Delta t)$...


Error
True error
Error estimate
E
10^-4
10^-5
10^-6
10^-2
10^-1
dt

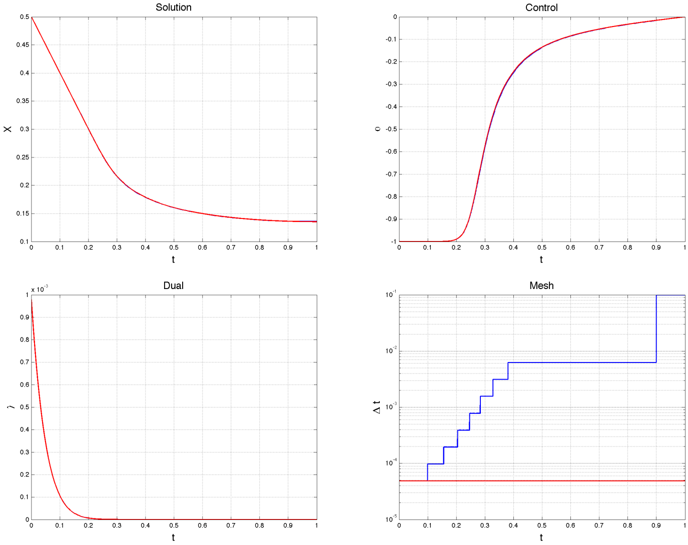


Figure : $\delta = 10^{-6}$ and $TOL = 10^{-6}$. The blue and red lines indicate solutions from adaptive and uniform meshes, respectively, corresponding to the lower right plot.

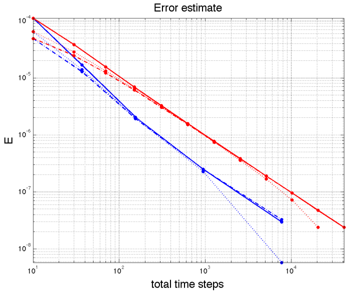


Figure : The solid lines indicate the error estimate while the dotted lines indicate the difference between the value function and the value function using the finest mesh for the uniform refinement.

Ex. (Fuller's problem)

(From PROPT Manual, by Rutquist, Edvall). Minimize

$$\int_0^1 X_1(t)^2 \mathrm{d}t + \gamma(X_1(1) - 0.01)^2 + \gamma X_2(1)^2,$$

subject to

$$\begin{aligned} X_1'(t) &= X_2(t), \\ X_2'(t) &= -\alpha(t), \end{aligned} \qquad 0 < t \le T, \qquad \begin{aligned} X_1(0) &= 0.01, \\ X_2(0) &= 0, \end{aligned}$$

and

$$|\alpha(t)| \le 1,$$

for some large $\gamma > 0$. The Hamiltonian is then non-smooth

$$H(x_1, x_2, \lambda_1, \lambda_2) := \min_{\alpha \in [-1,1]} \left\{ \lambda_1 x_2 - \lambda_2 \alpha + x_1^2 \right\} = \lambda_1 x_2 - |\lambda_2| + x_1^2,$$

but can be regularized by

$$H_\delta(x_1, x_2, \lambda_1, \lambda_2) := \lambda_1 x_2 - \sqrt{\lambda_2^2 + \delta^2} + x_1^2,$$

for some small $\delta > 0$.

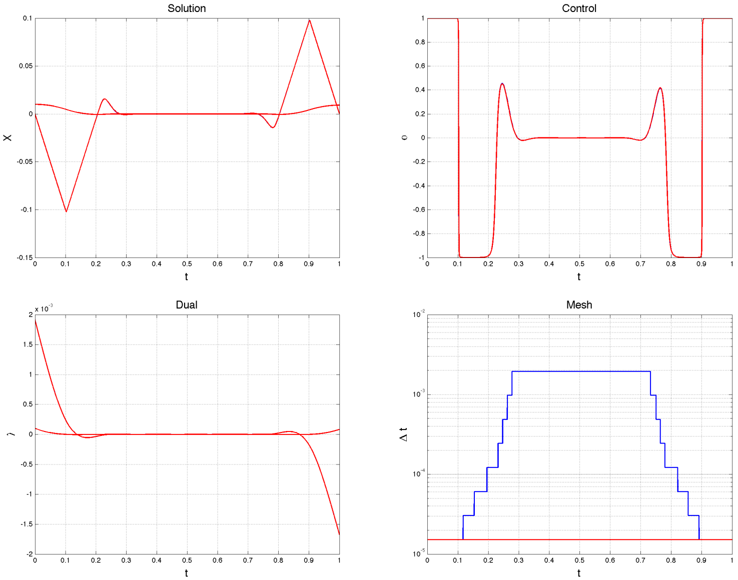


Figure : $\gamma = 1$, $\delta = 10^{-7}$ and $TOL = 10^{-6}$. The blue and red lines here indicate solutions from adaptive and uniform meshes, respectively.

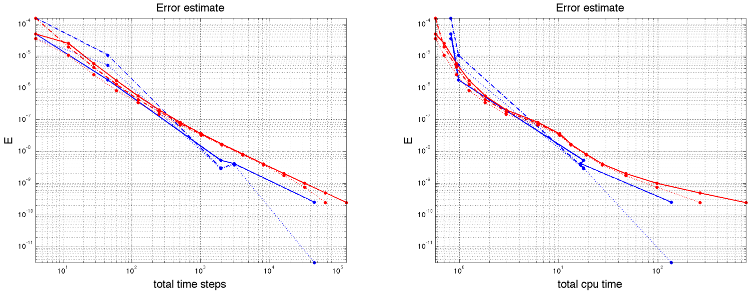


Figure : The solid lines indicate the error estimate and the dotted lines indicate the difference between the value function and the value function using the finest mesh for the uniform refinement.

Ex: Singular problem

Minimize

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

subject to

$$X'(t) = \frac{\alpha(t)}{\left((t-5/3)^2+\varepsilon^2\right)^{\beta/2}} \approx \frac{\alpha(t)}{|t-5/3|^{\beta}},$$
$$X(0) = X_{\text{ref}}(0).$$

Reference solves

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

and

$$X_{\text{ref}}(t) = \exp\left(\frac{t-5/3}{\varepsilon^{\beta}}\, {}_2F_1\Big(\frac{1}{2},\frac{\beta}{2},\frac{3}{2};-\frac{(t-5/3)^2}{\varepsilon^2}\Big)\right).$$

OC problem with explicit time dep. May be reformulated with time independent Hamiltonian by extending the state space:

$$s'(t) = 1, \quad s(0) = 0.$$

Then

$$H(x, s; \lambda_1, \lambda_2) = \frac{\lambda_1 x}{\left((s - 5/3)^2 + \varepsilon^2\right)^{\beta/2}} - \frac{\lambda_1^2}{4\left((s - 5/3)^2 + \varepsilon^2\right)^{\beta}} + \lambda_2.$$

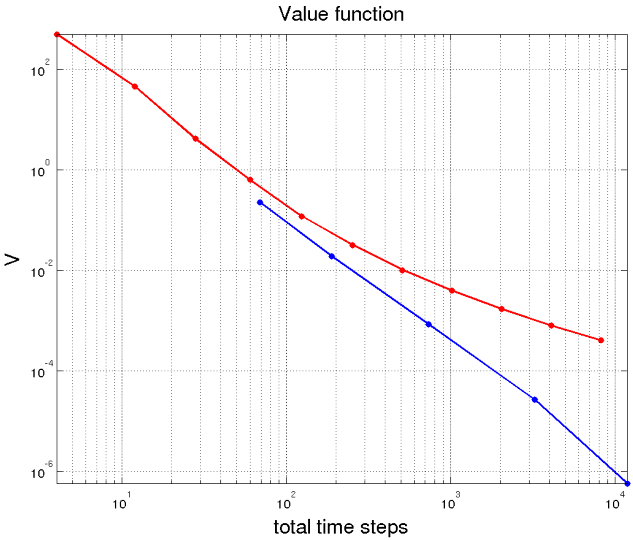


Figure : Red: Uniform. Blue: Adaptive. $\varepsilon = 10^{-10}$, $\beta = 3/4$.

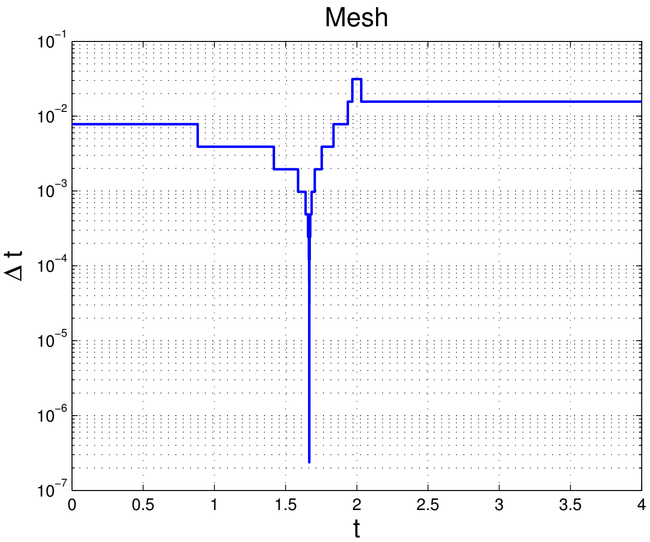
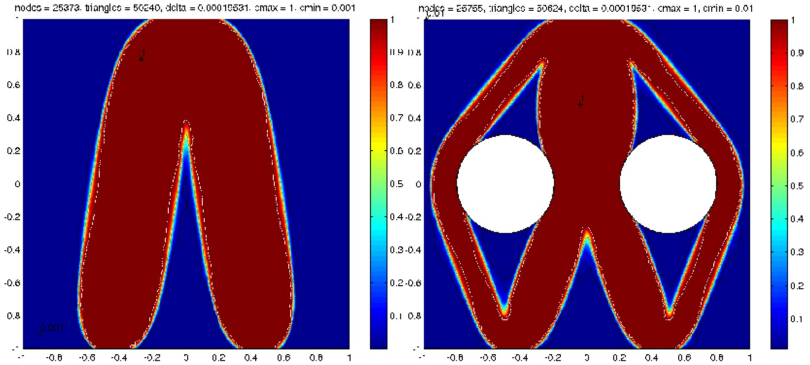


Figure : Mesh size versus time

Ex: Computation of optimal designs. Find $\sigma : \Omega \to \{\sigma_-, \sigma_+\}$

$$\mathrm{div}(\sigma \partial_x \varphi(x)) = 0 \quad x \in \Omega, \qquad \sigma \frac{\partial \varphi}{\partial n}\Big|_{\partial\Omega} = I$$

$$\min_{\sigma}\Big(\int_{\partial\Omega} I\varphi ds + \eta \int_{\Omega} \sigma dx\Big).$$



Regularized Hamiltonian H^{δ}, with $\delta \to 0$ possible.

- A priori error est.: Sandberg, Szepessy, "Convergence rates of symplectic Pontryagin approximations in optimal control theory", M2AN 40 (2006), no. 1, 149–173.
- A priori error est.: Sandberg, "Extended applicability of the Symplectic Pontryagin method", submitted.
- A posteriori error est.: Karlsson, Larsson, Sandberg, Szepessy, Tempone, "An a posteriori error estimate for Symplectic Euler approximations of optimal control problems", submitted.
- Application: Karlsson, Sandberg, Szepessy: "Symplectic Pontryagin approximations for optimal design", M2AN 43 (2009), no. 1 , 3–32.
- Application: Kiessling: "Calibration of a jump-diffusion process using optimal control", Num. anal. mult. comp., 259-277, Lect. Notes Comp. Sci. Eng. 82.
- Application: Karlsson: "Symplectic reconstruction of data for heat and wave equations" and "Pontryagin Approximations for Optimal Design of Elastic Structures", in J. K. PhD thesis: http://kth.diva-portal.org/smash/get/diva2:54461

Conclusions

- Error representation for value function associated with optimal control problems using discretization of Hamiltonian system.
- May be used for adaptive algorithms.
- Adaptivity natural since some iterative method must be used to solve the initial-terminal time boundary value problem. A solution on a grid level may be used as initial guess for the solution on the next level.
- Seems adaptivity is not essential for problems with discontinuous controls.
- Seems that the computable leading order term in the error representation is dominant even in cases where the Hamiltonian has large second order derivatives. Open problem to show this theoretically.