A sequential quadratic Hamiltonian scheme for solving optimal control problems with non-smooth cost functionals

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Motivation

- Apply the Pontryagin maximum principle (PMP) to optimal control problems governed by ordinary (ODE) or partial differential equations (PDE) with different cost functionals (non-smooth, non-convex, discontinuous).
- Formulate a PMP consistent numerical method to calculate optimal controls.
- Investigate PMP necessary optimality conditions.
- Extend applicability of optimal control theory.

Examples of optimal control problems

$$\min J(y,u) := \int_Q \left(\frac{1}{2}(y - y_d)^2 + g(u) \right) dz$$
$$\text{s.t.} \quad \partial_t y - \Delta y = f(z, y, u), \qquad y(\cdot, 0) = y_0,\ y = 0 \text{ on } \partial\Omega$$
$$u \in U_{ad}$$

$$U_{ad} := \{ u \in L^q(Q) \,|\, u(z) \in K_U \text{ a.e.} \}, \quad K_U \subseteq \mathbb{R},\ \text{compact},$$

where $Q = \Omega \times (0, T)$ space-time domain, $q \geq 2$, $z := (x, t) \in Q$. We require g lower semi-continuous (l.s.c) (at least). In particular

$$g(u) = \gamma \begin{cases} 1 & \text{if } |\mathrm{u}| \neq 0 \\ 0 & \text{else} \end{cases}, \ \gamma > 0; \qquad g(u) = \frac{\alpha}{2} u^2 + \beta |u|,\ \alpha, \beta \geq 0,\ \alpha + \beta > 0.$$

Further, we consider

$$f(z, y, u) = u, \qquad f(z, y, u) = -u\, y.$$

About existence of optimal solutions

- Control to state map $S : U_{ad} \to L^2(Q)$, $u \mapsto y = S(u)$
- Reduced cost functional

$$\hat{J}(u) := J(S(u), u)$$

- Existence of a solution $\bar{u} \in U_{ad}$ with

$$\hat{J}(\bar{u}) = \inf_{u \in U_{ad}} \hat{J}(u)$$

  for g bounded from below, Lipschitz continuous and convex
  - $\hat{J}$ bounded from below
  - Minimizing sequence
  - U_{ad} is weakly sequentially compact
  - $\hat{J}$ weakly lower semi-continuous

- For g non-convex, non-differentiable or discontinuous:
  Weakly lower semi-continuity of $\hat{J}$ can be lost (e.g. "L^0-norm")

Alternative concepts for existence

Existence by minimizing sequences for the non-convex case:

- Compact set of $L^q(Q)$

In general, suboptimal ϵ - solutions on U_{ad}:

- Setting:
  - g l.s.c.
  - g bounded from below
  - $S : U_{ad} \to L^2(Q)$ continuous
- Consequences:
  - $\hat{J}(u)$ l.s.c, bounded from below
  - Existence of $\inf_{u \in U_{ad}} \hat{J}(u)$
  - Existence of a suboptimal solution $\bar{u} \in U_{ad}$ with

$$\hat{J}(\bar{u}) \leq \inf_{u \in U_{ad}} \hat{J}(u) + \epsilon, \quad \epsilon > 0.$$

Lagrange approach if g and f are differentiable

- Functional formulation: Lagrange functional

$$L(y,u,p) := \frac{1}{2}\|y-y_d\|^2_{L^2(Q)} + \int_Q g(u(z))\,dz + \int_Q p(z)\left(f(z,y,u) - y'(z) + \Delta y(z)\right)dz$$

- Necessary optimality conditions for optimal solution $\bar{u}$:
  - State equation
  - Adjoint equation

$$-\partial_t p - \Delta p = (y-y_d) + p\,\frac{\partial}{\partial y} f(z,y,u), \qquad p(\cdot,T) = 0.$$

  - Variational inequality

$$\left(\frac{\partial g(\bar{u})}{\partial \bar{u}} + p\,\frac{\partial f}{\partial \bar{u}}\right)(w-\bar{u}) \geq 0, \qquad w \in U_{ad}.$$

Pontryagin maximum principle[1]

- Pointwise formulation: Hamilton-Pontryagin (HP) function
  $H : \mathbb{R}^n \times \mathbb{R} \times K_U \times \mathbb{R} \to \mathbb{R}$:

$$H(z, y, u, p) := \frac{1}{2}(y - y_d)^2 + g(u) + p\, f(z, y, u)$$

- Adjoint equation:

$$-\partial_t p - \Delta p = (y - y_d) + p \frac{\partial}{\partial y} f(z, y, u), \qquad p(\cdot, T) = 0.$$

Theorem 1: A necessary condition for $\bar{u}$ to be an optimal control is given by

$$H(z, \bar{y}(z), \bar{u}(z), \bar{p}(z)) \leq H(z, \bar{y}(z), v, \bar{p}(z)) \text{ for all } v \in K_U$$

for almost all $z \in Q$, where $\bar{y}$ is the solution to the state equation for $u \leftarrow \bar{u}$, and $\bar{p}$ is the solution to the adjoint equation for $y \leftarrow \bar{y}$ and $u \leftarrow \bar{u}$.

[1] Pontryagin, Boltyanskii, Gamkrelidze, Mishchenko. The Mathematical Theory of Optimal Processes, Wiley & Sons, 1962

To prove the PMP: The needle variation[2,3]

Needle variation of $u^* \in U_{ad}$ at $z \in Q$ with $v \in K_U$, index $k \in \mathbb{N}$:

$$u_k(z) := \begin{cases} v & \text{if } z \in S_k(z) \cap Q \\ u^*(z) & \text{if } z \in Q \backslash S_k(z) \end{cases}$$

Lemma 2 Connection of J and H:

$$\lim_{k\to\infty} \frac{1}{|S_k(z)|} \left(J(y_k, u_k) - J(y^*, u^*) \right) = H(z, y^*, v, p^*) - H(z, y^*, u^*, p^*)$$

at almost every $z \in Q$, and
y_k solution to the state equation for $u \leftarrow u_k$
y^* solution to the state equation for $u \leftarrow u^*$
p^* solution to adjoint equation for $y \leftarrow y^*$ and $u \leftarrow u^*$

[2] X. Li, J. Yong. Optimal Control Theory for Infinity Dimensional Systems, Birkhäuser, 1995

[3] J.-P. Raymond, H. Zidani. Hamiltonian Pontryagin's principles for control problems governed by semilinear parabolic equations, Applied Mathematics and Optimization, 1999

Suboptimal solutions & PMP

For functions $u_1, u_2 \in U_{ad} \subseteq U$, define the distance $d(u_1, u_2) = |\{z \in Q | u_1(z) \neq u_2(z)\}|$: U complete metric space.

By Ekeland's variational principle[4]: For any $\epsilon > 0$ there exists $\bar{u} \in U_{ad}$:

$$\hat{J}(w) - \hat{J}(\bar{u}) > -\epsilon\, d(w, \bar{u})$$

for all $w \in U_{ad} \backslash \{\bar{u}\}$. In particular, with $w = u_k$ needle variation of $\bar{u}$:

$$\frac{1}{|S_k(z)|}\left(\hat{J}(u_k) - \hat{J}(\bar{u})\right) > -\epsilon$$

Theorem 3[5] Existence of a suboptimal solution $\bar{u}$ such that

$$H(z, \bar{y}(z), \bar{u}(z), \bar{p}(z)) \leq H(z, \bar{y}(z), v, \bar{p}(z)) + \epsilon$$

for almost all $z \in Q$ and all $v \in K_U$, where $\bar{y}$ is the solution to the state equation for $u \leftarrow \bar{u}$, and $\bar{p}$ is the solution to the adjoint equation for $y \leftarrow \bar{y}$ and $u \leftarrow \bar{u}$.

[4] I. Ekeland. On the variational principle, Journal of Mathematical Analysis and Applications, 1974

[5] A. Hamel. Suboptimality theorems in optimal control, Birkhäuser, 1998

Calculation of (sub-)optimal solutions

Minimizing H is associated to minimizing J:

$$\lim_{k\to\infty} \frac{1}{|S_k(z)|}\left(J(y_k,u_k) - J(y^*,u^*)\right) = H(z,y^*,v,p^*) - H(z,y^*,u^*,p^*)$$

Minimize the HP function: Successive approximation method[6]

- Control update $u^{k+1}(z) = \arg\min_{w\in K_U} H\left(z,y^k,w,p^k\right)$
- Update the state and adjoint after each control update
- Fast calculation, but not robust with respect to convergence

Penalize the control update[7], $\epsilon > 0$:

$$K_\epsilon\left(z,y^k,w,u^k,p^k\right) := H\left(z,y^k,w,p^k\right) + \epsilon\left(w-u^k\right)^2$$

- Control update $u^{k+1}(z) = \arg\min_{w\in K_U} K_\epsilon\left(z,y^k,w,u^k,p^k\right)$
- Requires strategies to update the state
- Robust with respect to convergence, convergence theory

[6] I.A. Krylov, F.L.Chernous'ko. On a method of successive approximations for the solution of problems of optimal control, USSR Computational mathematics and Mathematical Physics, 1963

[7] Y. Shindo, Y. Sakawa. On global convergence of an algorithm for optimal control, IEEE Transactions on Automatic Control, 1980

Combine the advantages of successive approximation and penalization

- Augmented Hamiltonian

$$K_\epsilon\left(z, y^k, w, u^k, p^k\right) := H\left(z, y^k, w, p^k\right) + \epsilon\left(w - u^k\right)^2$$

- Control update $u(z) = \arg\min_{w\in K_U} K_\epsilon\left(z, y^k, w, u^k, p^k\right)$
- Penalization term for efficient and robust convergence performance
- The state y^k valid for the entire updated control sweep
- Fast calculation
- Convergence theory[8]

[8] Shindo & Sakawa; J. F. Bonnans. On an algorithm for optimal control using Pontryagin's maximum principle, SIAM Journal on Control and Optimization, 24(3):579–588, 1986.

The SQH method

1. Choose $\epsilon > 0$, $\kappa \geq 0$, $\sigma > 1$, $\zeta \in (0,1)$, $\eta \in (0,\infty)$, $u^0 \in U_{ad}$, compute y^0 corresponding to $u = u^0$, and p^0 corresponding to $y = y^0$ and $u = u^0$; set $k \leftarrow 0$
2. Update the control
$$u(z) = \underset{w \in K_U}{\arg\min}\, K_\epsilon\left(z, y^k, w, u^k, p^k\right)$$
for all $z \in Q$ (sweep)
3. Compute y corresponding to u and $\tau := \|u - u^k\|^2_{L^2(Q)}$
4. If $J(y,u) - J\left(y^k, u^k\right) > -\eta\tau$: Choose $\epsilon \leftarrow \sigma\epsilon$
Else:
Choose $\epsilon \leftarrow \zeta\epsilon$, $y^{k+1} \leftarrow y$, $u^{k+1} \leftarrow u$, calculate p^{k+1} by the adjoint equation for $y \leftarrow y^{k+1}$ and $u \leftarrow u^{k+1}$, set $k \leftarrow k+1$
5. If $\tau < \kappa$: STOP and return u^k
Else go to 2.

Problem P0 - Non-smooth cost functional

$$\min J(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)} + \beta\|u\|_{L^1(\Omega)}$$
$$\text{s.t.} \quad -\Delta y = u, \qquad y = 0 \text{ on } \partial\Omega$$

We consider a two-dimensional domain $\Omega = (0,1) \times (0,1)$, we choose $K_U = [-100, 100]$, and $y_d(x) := \sin(2\pi x_1)\cos(2\pi x_2) + 1$. $\alpha = 10^{-10}$, $\beta = 10^{-3}$.

In the SQH scheme, we initialize with $\epsilon = 10^{-2}$ and $u^0 = 0$. We set $\kappa = 10^{-6}$, $\sigma = 50$, $\zeta = \frac{3}{20}$, $\eta = 10^{-9}$. $N_x = 200$.

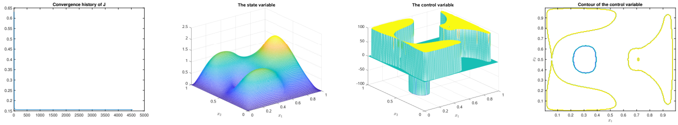


Figure: Convergence history, the state y, the optimal control u, and u as a contour plot.

Codes available: https://opus.bibliothek.uni-wuerzburg.de

Problem P1 - Elliptic, discontinuous cost functional

$$\min J(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} + G(u)$$
$$\text{s.t.} \quad -\Delta y = u, \qquad y = 0 \text{ on } \partial\Omega$$

$$G(u) = \gamma \int_\Omega g(u(x))\,dx, \quad g(u) = \begin{cases} |u| & \text{if } |u| > s \\ 0 & \text{else} \end{cases}$$

where $u \in U_{ad}$. We choose $K_U = [0, 100]$, and
$y_d(x) := \sin(2\pi x_1)\cos(2\pi x_2) + 1$; $\gamma = 10^{-3}$, $s = 20$.

In the SQH scheme, we initialize with $\epsilon = 10^{-2}$ and $u^0 = 0$. We set
$\kappa = 10^{-6}$, $\sigma = 50$, $\zeta = \frac{3}{20}$, $\eta = 10^{-9}$. $N_x = 200$.

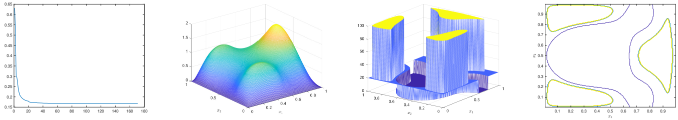


Figure: Convergence history, the state y, the optimal control u, and u as a contour plot.

Problem P2 - Parabolic, discontinuous cost functional

$$\min J(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2(Q)} + G(u)$$
$$\text{s.t.} \quad \partial_t y - \Delta y = u, \qquad y(\cdot,0) = y_0,\ y = 0 \text{ on } \partial\Omega$$
$$u \in U_{ad},$$

$$G(u) = \gamma \int_Q g(u(z))\,dz, \quad g(u) = \begin{cases} |u| & \text{if } |u| > s \\ 0 & \text{else} \end{cases}$$

- Adjoint equation :

$$-\partial_t p - \Delta p = y - y_d, \qquad p(\cdot,T) = 0,\ p = 0 \text{ on } \partial\Omega$$

- HP function:

$$H(x,t,y,u,p) = \frac{1}{2}(y - y_d)^2 + \frac{\alpha}{2}u^2 + \gamma g(u) + p\,u$$

- Augmented Hamiltonian:

$$K_\epsilon(x,t,y,u,v,p) = \frac{1}{2}(y - y_d)^2 + \frac{\alpha}{2}u^2 + \gamma g(u) + p\,u + \epsilon(u - v)^2$$

Numerical results with P2

We choose $\Omega = (0,1)$ and $T = 1$. We have $K_U = [0,10]$, and the desired trajectory

$$y_d(x,t) = \begin{cases} 5 & \text{if } \bar{x}(t) - c \le x \le \bar{x}(t) + c \\ 0 & \text{else,} \end{cases}$$

where $\bar{x}(t) := x_0 + \frac{2}{5}(b-a)\sin\left(2\pi \frac{t}{T}\right)$, $x_0 = \frac{b+a}{2}$, $a = 0$ $b = 1$, and $c = \frac{7}{100}(b-a)$. Further, we have $\alpha = 10^{-5}$, $\gamma = 10^{-1}$, $s = 1$.

In the SQH scheme, we initialize with $\epsilon = 10^{-1}$ and $u^0 = 0$. We set $\kappa = 10^{-6}$, $\sigma = 50$, $\zeta = \frac{3}{20}$, $\eta = 10^{-9}$. $N_x = 100$, $N_t = 200$.

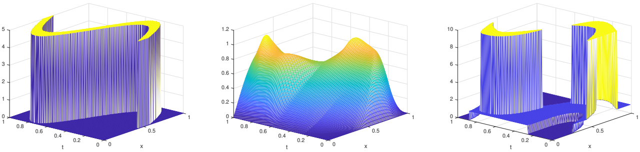


Figure: The target function y_d, the state y, and the optimal control u.

PMP test

- Return value from SQH method (y, u, p) :

$$\triangle H(z) := H(z, y, u, p) - \min_{w \in K_U} H(z, y, w, p)$$

- PMP test:

$$0 \leq \triangle H \lessapprox \text{eps}, \ \text{eps} = 2.2 \cdot 10^{-16}$$

- For problem P2:

$N_t \times N_x$ \ κ	10^{-1}	10^{-3}	10^{-6}	10^{-16}
100×200	0	0.9973	0.9988	0.9998
200×400	$6.28 \cdot 10^{-5}$	0.9966	0.9998	0.9998
400×800	$6.70 \cdot 10^{-4}$	0.9934	0.9981	0.9998
800×1600	$1.59 \cdot 10^{-3}$	0.9868	0.9998	0.9998

Table: PMP test: ratio of grid points where the PMP condition is satisfied to machine eps, κ stopping criterion in the SQH scheme.

About Step 2 in the SQH scheme: pointwise minimization

- The function $u \mapsto K_\epsilon(z, y, u, v, p)$ attains minimum for any $(z, y, v, p) \in \mathbb{R}^n \times \mathbb{R}_0^+ \times \mathbb{R} \times K_U \times \mathbb{R}$ and $\epsilon \in \mathbb{R}$
  - $u \mapsto K_\epsilon(z, y, u, v, p)$ l.s.c
  - K_U compact
  - Direct search (e.g., secant method) or exact computation
- Lebesgue measurability of $u(z) = \arg\min_{w \in K_U} K_\epsilon(z, w)$, where

$$K_\epsilon(z, w) := K_\epsilon(z, y(z), w, v(z), p(z)).$$

  This is the case if [9]

  - $z \mapsto K_\epsilon(z, w)$ Lebesgue measurable for any $w \in K_U$
  - $w \mapsto K_\epsilon(z, w)$ continuous for any $z \in Q$

  If K_ϵ is only lower semi-continuous in w for any $z \in Q$, then, in general, we cannot guarantee that u is Lebesgue measurable.

[9] R. T. Rockafellar and R. J.-B. Wets. *Variational Analysis*, Springer, 2009.

Analytical formula for pointwise minimization

Consider problem P2. We have $K_U = [0, 10]$ and

$$K_\epsilon(x,t,y,u,v,p) = \frac{1}{2}(y-y_d)^2 + \frac{\alpha}{2}u^2 + \gamma g(u) + pu + \epsilon(u-v)^2$$

- Minimum u:
  1. $0 \leq u \leq s$

     $$u_1 := \min\left(\max\left(0, \frac{2\epsilon v - p}{2\epsilon + \alpha}\right), s\right)$$

  2. $s < u \leq 10$

     $$u_2 := \min\left(\max\left(s, \frac{2\epsilon v - (p+\gamma)}{2\epsilon + \alpha}\right), 10\right)$$

- Function $u(z)$ measurable

$$u(z) := \begin{cases} u_1(z) & K_\epsilon(z, u_1(z)) \leq K_\epsilon(z, u_2(z)) \\ u_2(z) & K_\epsilon(z, u_1(z)) > K_\epsilon(z, u_2(z)) \end{cases}$$

Enables fast SQH control update

Minimization of the cost functional

In the SQH scheme, increasing ϵ allows to obtain decrease of the value of the cost functional in Step 4

$$J(y,u) - J\left(y^k, u^k\right) \le -\eta \left\| u - u^k \right\|_{L^2(Q)}^2$$

- Lemma 4 Existence of $\theta > 0$ (independent of ϵ) such that

$$J(y,u) - J\left(y^k, u^k\right) \le -(\epsilon - \theta) \left\| u - u^k \right\|_{L^2(Q)}^2$$

- $\epsilon > \theta$:

$$J(y,u) - J\left(y^k, u^k\right) < 0$$

- $\epsilon \ge \theta + \eta$:

$$J(y,u) - J\left(y^k, u^k\right) \le -\eta \| u - u^k \|_{L^2(Q)}^2$$

Updates ($\epsilon \leftarrow \sigma\epsilon$) for minimization in finitely many steps

Investigation of the SQH sequence of iterates

Lemma 5 If u^k is PMP optimal

$$H\left(z, y^k, u^k, p^k\right) = \min_{w \in K_U} H\left(z, y^k, w, p^k\right),$$

then the SQH method stops returning u^k

.

Investigation of the sequence of iterates $\left(u^k\right)_{k \in \mathbb{N}_0}$:

Theorem 6 $J\left(y^k, u^k\right)$ monotonically decreases with

$$\lim_{k \to \infty} \left(J\left(y^{k+1}, u^{k+1}\right) - J\left(y^k, u^k\right)\right) = 0$$

and $\lim_{k \to \infty} \|u^{k+1} - u^k\|_{L^2(Q)} = 0$.

Theorem 7 If g continuously differentiable, $\epsilon > \epsilon_0 > 0$, for each accumulation point $\bar{u}$ of $\left(u^k\right)$ with sub.seq. $\lim_{\tilde{k} \to \infty} \|u^{\tilde{k}} - \bar{u}\|_{L^q(Q)} = 0$: $\nabla \hat{J}\left(\bar{u}\right)\left(z\right)\left(w\left(z\right) - \bar{u}\left(z\right)\right) \geq 0$ a.e. for all $w \in U_{ad}$

PMP-consistent convergence

In general, not clear if $\lim_{k\to\infty} \hat{J}\left(u^k\right) = \inf_{u\in U_{ad}} \hat{J}\left(u\right)$

Instead of differentiability, require:
For any iterate u^k, $k \in \mathbb{N}_0$ and for any ϵ, existence of $r \geq \epsilon$ such that the sufficient decrease conditions

$$K_\epsilon\left(z, y^k, u^{k+1}, u^k, p^k\right) + r\left(v - u^{k+1}(z)\right)^2 \leq K_\epsilon\left(z, y^k, v, u^k, p^k\right)$$

holds for all $v \in K_U$ and for all $z \in Q$. Verifiable for L^1, L^2 and $L^1 - L^2$ cost functionals

Theorem 8 With sufficient decrease condition, for any accumulation point $\bar{u}$, $\lim_{\tilde{k}\to\infty} \|u^{\tilde{k}} - \bar{u}\|_{L^2(Q)} = 0$, there exists a subsequence $\left(u^{\bar{k}}\right)_{\bar{k}\in\bar{K}}$ such that

- $\lim_{\bar{k}\to\infty} u^{\bar{k}}(z) = \bar{u}(z)$ a.e.
- $H(z, \bar{y}, \bar{u}, \bar{p}) = \min_{v\in K_U} H(z, \bar{y}, v, \bar{p})$ a.e.
- For almost any $z \in Q$ and $\mu > 0$: Existence of $\hat{k}$ such that

$$H\left(z, y^{m+1}, u^{m+1}, p^{m+1}\right) \leq H\left(z, y^{m+1}, v, p^{m+1}\right) + \mu$$

for all $v \in K_U$ and all $m \geq \hat{k}$

Problem P3: An ODE quantum control problem

Consider the optimal control of two 1/2-spin particles in the NMR framework.

$$
\begin{aligned}
\min J(y,u) &:= \frac{1}{2}\sum_{i=1}^{n}\left(y_i(T)-(y_d)_i\right)^2+\int_0^T g_{\alpha,\beta,\gamma,\delta}(u(t))\,dt \\
\text{s.t.} \quad & y' = (A+u\,B)\,y,\ \ t\in(0,T) \\
& y(0)=y_0 \\
& u\in U_{ad}:=\left\{u\in L^2(0,T)\mid u(t)\in K_U \text{ a.e.}\right\}
\end{aligned}
$$

where

$$
g_{\alpha,\beta,\gamma,\delta}(u):=\frac{\alpha}{2}u^2+\beta\,|u|+\gamma\,|u|_0+\delta\,|u|_s,
$$

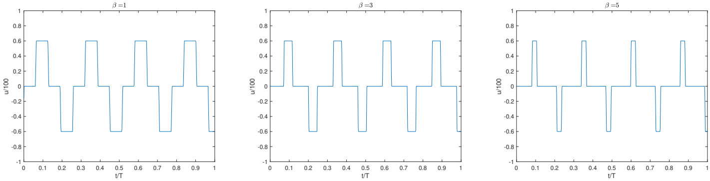
and

$$
|u|_0:=\begin{cases}0 & \text{if } u=0\\ 1 & \text{else}\end{cases},\qquad |u|_s:=\begin{cases}|u| & \text{if } |u|>s\\ 0 & \text{else}\end{cases},\quad s>0.
$$

$$
K_\epsilon(t,y,u,v,p):=\frac{1}{2}(y-y_d)^2+g_{\alpha,\beta,\gamma,\delta}(u)+p^T(A+uB)\,y+\epsilon\,(u-v)^2 .
$$

Numerical results with P3 - Experiment I

The case $\alpha = 10^{-3}$, $\beta > 0$, $\gamma = 0$, $\delta = 0$. $K_U = [-60, 60]$.
SQH scheme $\zeta = 0.8$, $\sigma = 2$, $\eta = 10^{-9}$, $\kappa = 10^{-15}$, $\epsilon = 0.005$, and $u^0 = 0$.



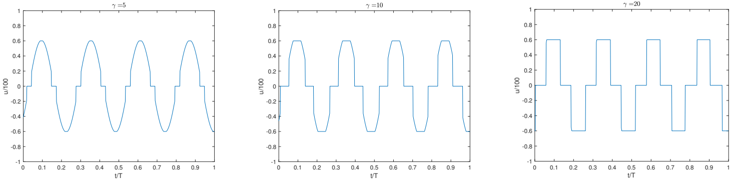
PMP test : $0 \leq \Delta H \leq 10^{-\ell}$

β	$\frac{N^4_\%}{\%}$	$\frac{N^5_\%}{\%}$	$\frac{N^8_\%}{\%}$	$\frac{N^{15}_\%}{\%}$	CPU time/s		# it	# up
					SQH	SSN		
1	96.01	95.88	95.88	90.14	0.77	94	51	24
3	100	100	98.00	82.65	0.78	21	50	25
5	100	100	98.13	84.27	0.66	28	42	23

The number of SQH iterations is denoted with # it, and the number of sweeps of updates of the control is denoted with # up.

Numerical results with P3 - Experiment II

The (L^0) case $\alpha = 10^{-2}$, $\beta = 0$, $\gamma > 0$, $\delta = 0$. $K_U = [-60, 60]$.

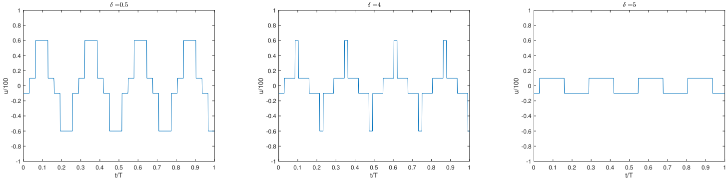


PMP test : $0 \leq \Delta H \leq 10^{-\ell}$

γ	$\frac{N^{4}_{\%}}{\%}$	$\frac{N^{5}_{\%}}{\%}$	$\frac{N^{8}_{\%}}{\%}$	$\frac{N^{15}_{\%}}{\%}$	CPU time/s	# it	# up
1	84.52	82.02	30.09	30.09	1.6	110	70
5	90.39	90.01	73.78	67.54	2.3	152	103
20	96.25	96.25	96.25	96.25	1.2	78	50

Numerical results with P3 - Experiment III

The (discontinuous L^1) case $\alpha = 10^{-2}$, $\beta = 0$, $\gamma = 0$, $\delta > 0$ and $s = 10$. $K_U = [-60, 60]$.



PMP test : $0 \leq \Delta H \leq 10^{-\ell}$

δ	$\frac{N^{4}_{\%}}{\%}$	$\frac{N^{5}_{\%}}{\%}$	$\frac{N^{8}_{\%}}{\%}$	$\frac{N^{15}_{\%}}{\%}$	CPU time/s	# it	# up
0.5	99.63	99.63	99.63	98.88	1.5	77	58
4	98.13	98.13	98.13	98.13	0.33	16	12
5	100	100	100	100	0.17	7	7

Problem P4: Parabolic, bilinear, discontinuous

Consider the following bilinear parabolic optimal control problem

$$\min J(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(Q)} + G(u)$$
$$\text{s.t.} \quad \partial_t y - \Delta y + u\,y = \tilde{f}, \qquad y(\cdot,0) = y_0,\; y = 0 \text{ on } \partial\Omega$$
$$u \in U_{ad},$$

$$G(u) = \gamma \int_Q g(u(z))\,dz, \quad g(u) = \begin{cases} |u| & \text{if } |u| > s \\ 0 & \text{else} \end{cases}$$

In this case the HP function is given by

$$H(x,t,y,u,p) = \frac{1}{2}(y - y_d)^2 + \gamma\, g(u) - u\,y\,p$$

Numerical results with P4

Consider $\Omega = (0,1)$, $T = 1$, and the target function

$$y_d(x,t) = \begin{cases} \frac{1}{2} & \text{if } \bar{x}(t) - \frac{7}{100} \leq x \leq \bar{x}(t) + \frac{7}{100} \\ 0 & \text{else} \end{cases}, \text{ where}$$

$\bar{x}(t) := \frac{1}{2} + \frac{2}{5}\sin(2\pi t)$; $\tilde{f} = 1$. We choose $\gamma = 10^{-4}$, $s = 10$, and $K_U = [0, 15]$.

In the SQH scheme, we initialize with $\epsilon = 10^{-1}$ and $u^0 = 0$. We set $\kappa = 10^{-12}$, $\sigma = 50$, $\zeta = \frac{3}{20}$, $\eta = 10^{-12}$. $N_x = 200$, $N_t = 400$.

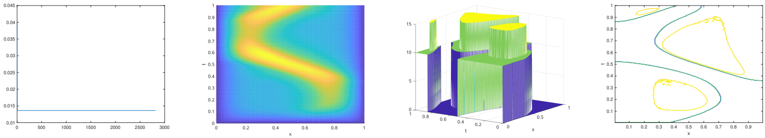


Figure: Convergence history, the state y, the optimal control u, and u as a contour plot.

Problem P5: A mixed-integer optimal control problem

$$\min J(y,u) = \|y - y_d\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2(Q)} + \gamma \int_Q |u|^{\frac{1}{2}}\, dz$$

$$\text{s.t. } \partial_t y - \Delta y = u \qquad y(\cdot,0) = y_0,\ y = 0 \text{ on } \partial\Omega$$

$$u \in U_{ad},$$

$$u \in U_{ad} := \left\{ u \in L^2(Q) \mid K_U = \{-30, -15, -5, 0, 5, 15, 30\} \right\}$$

We choose $\alpha = 10^{-2}$ and $\gamma = 10^{-3}$.

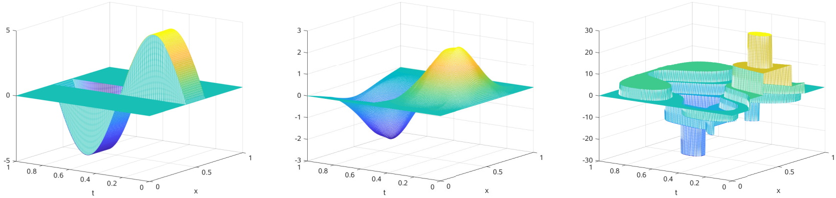


Figure: Desired trajectory y_d, the state y, and the optimal control u.

Problem P6: A state-constrained optimal control problem

$$\min J(y,u) = \frac{1}{2}\int_\Omega (y(x) - y_d(x))^2 \, dx + \int_\Omega g(u(x)) \, dx$$

$$\text{s.t.} \qquad -\Delta y = u, \qquad y = 0 \text{ on } \partial\Omega$$

$$y \le \xi, \qquad u \in U_{ad}$$

where $g(u) := \gamma \begin{cases} |u| & \text{if } |u| > s \\ 0 & \text{else} \end{cases}$, $\xi \in \mathbb{R}$. We assume that this problem admits a solution $(\bar{y}, \bar{u})$.

We consider a regularization of this problem [10] that removes the state constraint and augments the tracking term by

$$h_\xi(y;\rho) := \frac{1}{2}(y(x) - y_d(x))^2 + \rho\,(\max(0, y - \xi))^3$$

We consider a sequence of increasing values of $\rho > 0$, i.e. (ρ_k), $k = 1, 2, \ldots$, $\lim_{k\to\infty} \rho_k = \infty$, and denote with (y_k, u_k) the solutions to the corresponding optimal control problems.

[10] V. Karl, D. Wachsmuth. An augmented Lagrange method for elliptic state constrained optimal control problems, Computational Optimization and Applications, 2018

Approximation properties

Theorem 9 Let (y_k, u_k) be the solution to the optimal control problem with $\rho = \rho_k$. Define $M_k := \{x \in \Omega |\ y_k(x) > \xi\}$ and denote with $(\bar{y}, \bar{u})$ the solution to the original control problem with state constraint. Then $\lim_{k\to\infty} \int_{M_k} (y_k(x) - \xi)^3\, dx = 0$, and for all $k \in \mathbb{N}$ it holds

$$J(y_k, u_k) = \int_\Omega h_\xi(y_k(x), 0) + g(u_k(x))\, dx \leq J(\bar{y}, \bar{u}).$$

We choose $\Omega = (0,1) \times (0,1)$, $\gamma = 10^{-3}$, $s = 10$, $K_U := [-100, 100]$, $\xi = 0.6$.

ρ_k	$\max_{x\in\Omega} y(x)$	$\int_{M_k} \left(y_k(x) - \frac{3}{5}\right)^3 dz$	$\|M_k\|$
1	0.8218	$1.7843 \cdot 10^{-4}$	0.0461
100	0.6543	$1.3580 \cdot 10^{-6}$	0.0289
10000	0.6081	$2.9827 \cdot 10^{-9}$	0.0137

Numerical results for P6

In the SQH scheme, we choose $\epsilon = 10^{-2}$ and $u^0 = 0$, $\sigma = 50$, $\zeta = \frac{3}{20}$, $\eta = 10^{-9}$, $\xi = \frac{3}{5}$; $N_x = 100$, $\kappa = 10^{-10}$. The desired configuration is given by $y_d(x) := \sin(2\pi x_1)\cos(2\pi x_2)$.

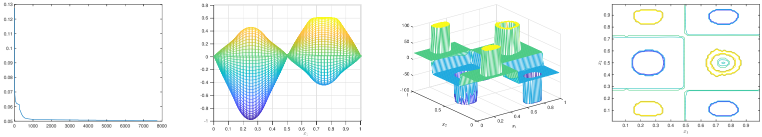


Figure: Convergence history, the state y (section view), the optimal control u, and u as a contour plot; $\rho = 100000$.

PMP test: $0 \leq \Delta H \leq \cdot 10^{-15}$ is fulfilled at 6.45% of points for $\kappa = 10^{-4}$, at 76.53% of points for $\kappa = 10^{-8}$ and at 81.16% of points for $\kappa = 10^{-12}$.

Problem P7: The case of a L^1 tracking term and non-smooth PDE

$$\min J(y,u) := \int_\Omega |y(x) - y_d(x)| + g(u(x))\, dx$$
$$\text{s.t.} \quad -\Delta y + \max(0,y) = u, \qquad y = 0 \text{ on } \partial\Omega$$

where

$$g(z) = \gamma \log(1 + |z|), \qquad \gamma > 0.$$

We have the HP function

$$H(x,y,u,p) = |y - y_d| + \gamma \log(1+|u|) + p\,u - p\,\max(0,y)$$

We define the adjoint equation

$$\int_\Omega \nabla p(x) \nabla v(x) + h_2(y(x))\, p(x)\, v(x)\, dx = \int_\Omega h_1(y(x))\, v(x)\, dx,$$

where $v \in H_0^1(\Omega)$ and

$$h_1(y(x)) := \begin{cases} 1 & \text{if } y(x) \geq y_d(x) \\ -1 & \text{else} \end{cases} \qquad h_2(y) := \begin{cases} 1 & \text{if } y \geq 0 \\ 0 & \text{else} \end{cases}$$

Numerical results with P7

We have $\Omega := (0,1) \times (0,1)$, $y_d(x) := \sin(2\pi x_1)\sin(2\pi x_2) + 1$, $K_U = [-100, 100]$ and $\gamma = 10^{-1}$.
In the SQH scheme, we initialize with $\epsilon = 10^{-2}$ and $u^0 = 0$. We set $\kappa = 10^{-8}$, $\sigma = 50$, $\zeta = \frac{3}{20}$, $\eta = 10^{-9}$. $N_x = 100$.

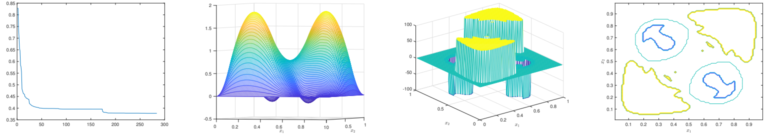


Figure: Convergence history, the state y, the optimal control u, and u as a contour plot.

PMP test: For $\kappa = 10^{-8}$, the $0 \leq \Delta H \leq \cdot 10^{-12}$ is fulfilled at 75.33% of the grid points.

Optimal control of stochastic models

In stochastic optimal control theory, given a stochastic process $X(t)$ subject to a control function u, one considers

$$J(X,u) = \mathbb{E}[\int_0^T G(X(t),u(X(t),t))\,dt + F(X(T))],$$

where $\mathbb{E}[\cdot]$ represents the expectation with respect to the probability measure induced by the process $X(t)$.
We consider the following n-dimensional controlled Itō stochastic process

$$\begin{cases} dX(t) & = b(X(t),u(X(t),t))dt + \sigma(X(t))\,dW(t), \qquad t \in (t_0,T] \\ X(t_0) & = X_0, \end{cases}$$

where the state variable $X(t) \in \Omega \subset \mathbb{R}^n$.
We assume that the state configuration of the stochastic process at t_0 is given by X_0, and we suppose that the control function $u \in \mathcal{U}$, where $\mathcal{U}$ represents the set of Markovian controls containing all jointly measurable functions u with $u(x,t) \in K_U \subset \mathbb{R}^n$, and K_U is a compact set in $\mathbb{R}^n$.

Value function and HJB equation

Corresponding to the SDE and a closed-loop control setting, we consider the following functional

$$C_{t_0,x_0}(u) = \mathbb{E}[\int_{t_0}^{T} G(X(s), u(X(s), s))ds + F(X(T)) \mid X(t_0) = x_0],$$

conditional expectation to $X(t)$ taking the value x_0 at time t_0.
The optimal control $\bar{u}$ that minimizes $C_{t_0,x_0}(u)$

$$\bar{u} = \text{argmin}_{u \in \mathcal{U}} C_{t_0,x_0}(u).$$

Correspondingly, one defines the following value function

$$q(x,t) := \min_{u \in \mathcal{U}} C_{t,x}(u) = C_{t,x}(\bar{u}).$$

A fundamental result: q is the solution to the HJB equation

$$\begin{cases} \partial_t q + \mathcal{H}(x,t,Dq,D^2q) = 0, \\ q(x,T) = F(x), \end{cases}$$

with the HJB Hamiltonian function

$$\mathcal{H}(x,t,Dq,D^2q) := \min_{v \in K_U} \Big[G(x,v) + \sum_{i=1}^{n} b_i(x,v)\, \partial_{x_i} q(x,t) + \sum_{i,j=1}^{n} a_{ij}(x)\, \partial^2_{x_i x_j} q(x,t)$$

The Fokker-Planck equation

$$\begin{aligned}\partial_t f(x,t) + \sum_{i=1}^{n} \partial_{x_i} \left(b_i(x,u)\, f(x,t)\right) - \sum_{i,j=1}^{n} \partial^2_{x_i x_j}(a_{ij}(x)\, f(x,t)) &= 0 \\ f(x,0) &= f_0(x)\end{aligned}$$

where f denotes the PDF of the stochastic process, f_0 represents the initial PDF distribution of the initial state of the process X_0, and hence we require $f_0(x) \geq 0$ with $\int_\Omega f_0(x)\, dx = 1$.
Assume absorbing barriers that correspond to homogeneous Dirichlet boundary conditions for f on $\partial\Omega$, $t \in [0, T]$.
Let us assume that $f_0(x) = \delta(x - x_0)$ at $t = t_0$ fixed; notice that the expectation can be explicitly written in terms of the PDF solving the FP problem

$$J(f(u), u) := \int_{t_0}^{T} \int_\Omega G(x, u(x,s))\, f(x,s)\, ds\, dx + \int_\Omega F(x) f(x,T)\, dx.$$

FP optimality system

In the Lagrange framework, we can derive the following first-order necessary optimality conditions

$$\begin{aligned}&\partial_t f(x,t) + \textstyle\sum_{i=1}^n \partial_{x_i}\left(b_i(x,u(x,t))\, f(x,t)\right) - \sum_{ij=1}^n \partial_{x_i x_j}(a_{ij}(x) f(x,t)) = 0,\\ &f(x,t_0) = f_0(x),\end{aligned}$$

$$\begin{aligned}&\partial_t p(x,t) + \textstyle\sum_{i=1}^n b_i(x,u(x,t))\, \partial_{x_i} p(x,t) + \sum_{ij=1}^n a_{ij}(x) \partial_{x_i x_j} p(x,t) + G(x,u(x,t)) = 0,\\ &p(x,T) = F(x),\end{aligned}$$

and

$$\int_{t_0}^T \int_\Omega \left(f(x,t) \left(\sum_{i=1}^n \partial_u b_i(x,u(x,t))\, \partial_{x_i} p(x,t) + \partial_u G(x,u(x,t)) \right) \right) (v(x,t) - u(x,t))\, dt\, dx \geq$$

for all $v \in \mathcal{U}$.

PMP optimality condition

In the PMP framework the optimality condition is given by

$$H\left(x,t,\bar{f}(x,t),\bar{u}(x,t),\nabla\bar{p}(x,t)\right)=\min_{v\in K_U} H\left(x,t,\bar{f}(x,t),v,\nabla\bar{p}(x,t)\right),$$

for almost all $(x,t)\in Q$, where the HP function is given by

$$H\left(x,t,f,v,\zeta\right):=\left(G\left(x,v\right)+b(x,v)\cdot\zeta\right)\,f$$

We see that, whenever $f(x,t)>0$, the minimizer $\bar{u}(x,t)$ of H at (x,t), coincides with that of the HJB equation, thus

$$\mathcal{H}(x,t,Dq,D^2q)=G(x,\bar{u})+\sum_{i=1}^{n} b_i(x,\bar{u})\,\partial_{x_i}q(x,t)+\sum_{i,j=1}^{n} a_{ij}(x)\,\partial^2_{x_ix_j}q(x,t).$$

Therefore at optimality, the adjoint equation can be written as $\partial_t p+\mathcal{H}(x,t,Dp,D^2p)=0$, which allows to identify p with the value function q.

Some results

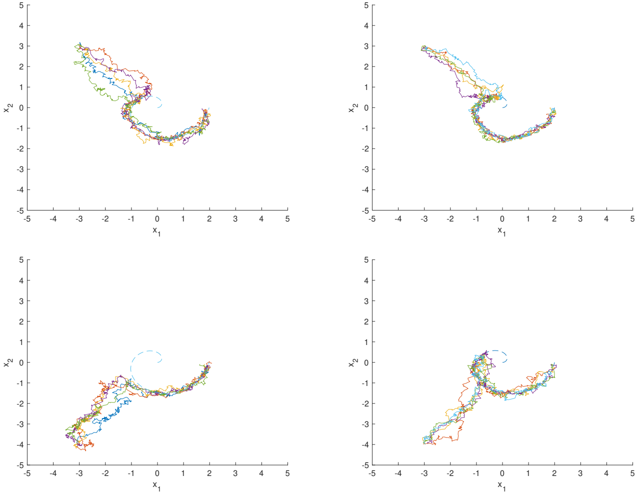


Figure: **Monte Carlo simulation with the controls obtained with the HJB equation (left) and with the SQH method (right).**

Thank you for your attention!

- T. Breitenbach and A. Borzì. A sequential quadratic Hamiltonian method for solving parabolic optimal control problems with discontinuous cost functionals, Journal of Dynamical and Control Systems, 25 (2019), 403–435.
- T. Breitenbach and A. Borzì. On the SQH scheme to solve non-smooth PDE optimal control problems, Journal of Numerical Functional Analysis and Optimization, 40 (2019), 1489–1531.
- T. Breitenbach and A. Borzì. A sequential quadratic Hamiltonian scheme for solving non-smooth quantum control problems with sparsity, submitted to JCAM, 2019.
- T. Breitenbach and A. Borzì. The Pontryagin maximum principle for solving Fokker-Planck optimal control problems, submitted to COAP, 2019.