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# Optimal control of a semilinear parabolic equation with singular arcs

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## Optimal control of a semilinear parabolic equation with singular arcs

J. Frédéric Bonnans\*

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**Abstract:** This paper develops a theory of singular arc, and the corresponding second order necessary and sufficient conditions, for the optimal control of a semilinear parabolic equation with scalar control applied on the r.h.s. We obtain in particular an extension of Kelley's condition, and the characterization of a quadratic growth property for a weak norm.

**Key-words:** Parabolic equation, optimal control, singular arc, second order optimality conditions, characterization of quadratic growth.

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## Commande optimale d'une équation parabolique avec arcs singuliers

**Résumé :** L'article développe une théorie des arcs singuliers, et les conditions d'optimalité correspondantes du premier et second ordre, pour un problème de minimisation d'un critère quadratique en l'état et linéaire en la commande, avec une équation d'état semilinéaire elliptique et une commande scalaire intervenant au second membre de l'équation. La commande est soumise à des bornes. Nous obtenons en particulier une extension de la condition de Kelley, et la caractérisation de la croissance optimale dans une norme faible.

**Mots-clés :** Equation parabolique, commande optimale, arc singulier, conditions d'optimalité du second ordre, caractérisation de la croissance quadratique.

## 1 Introduction

We consider in this paper an optimal control problem of a parabolic equation with a scalar control subject to bounds, in which the state equation and integrand of cost function are affine functions of the control. Such *affine control problems* have been extensively studied in the ODE setting. Concerning second order optimality conditions which are the subject of the paper, in the totally singular case (the control is out of bounds at any time), the key results are the extended Legendre condition due to Kelley [18], and the Goh transform [16] allowing to obtain second order necessary conditions involving the primitive of the control rather than the control itself. Dmitruk [13] derived sufficient conditions for weak optimality, and in [12, 14] obtained necessary or sufficient optimality conditions in the case of a non unique multiplier. In the singular-bang setting, Poggiolini and Stefani [22] obtained second-order sufficient conditions for the strong local optimality for the minimum time problem, and Aronna et al. [1] obtained second-order necessary conditions, and some sufficient conditions without uniqueness of the multiplier.

There are very few papers on the optimal control of PDEs for affine control systems. When the control is distributed, if the control is out of bounds on some open set, it is sometimes possible to give an explicit expression of the control: this is the theory of generalized bang-bang control, see Bergounioux and Tiba [2], Tröltzsch [23], Bonnans and Tiba [3].

In the elliptic case, Casas [8] considered the case of a distributed control and obtained second order sufficient conditions. While the technique is quite specific since time does not appear, these sufficient conditions are in the spirit of those obtained in Goh's theory, since they involve an Hilbert norm that is weaker than the  $L^2$  norm of the control. Casas, Herzog and Wachsmuth [9] consider the case of an  $L^1$  cost function, which may be viewed as an affine control problem if we take as new control the positive and negative parts of the original control. Casas, Clason and Kunisch [10] study related problems in the setting of a parabolic equation.

Therefore there exists presently no analogous of the Goh theory in the setting of control of parabolic equations; our goal is to set some first steps in this direction. The paper is organized as follows. We present the problem, and derive the second order necessary conditions in Goh's form in section 2. Then we derive the second order sufficient conditions, that characterize quadratic growth in a weak norm, in section 3. Some numerical experiments, that give an experimental argument in favor of the existence of singular arcs for optimal control problems of parabolic equations, are presented in section 4. We conclude in section 5 by discussing some open problems and possible extensions.

## 2 Setting and classical results

### 2.1 Setting

Let  $\Omega$  be a smooth open subset of  $\mathbb{R}^n$ , with  $n \leq 3$ . Set  $Q := \Omega \times (0, T)$ . We recall that, for  $\mu \in [1, \infty]$  and  $p \in \mathbb{N}$ ,  $p \geq 1$ ,  $W^{p,\mu}(\Omega)$  denotes the Sobolev space of functions in  $L^\mu(\Omega)$  with derivatives up to order  $p$  (taken in the distribution sense) in  $L^\mu(\Omega)$ . We denote the closure of  $\mathcal{D}(\Omega)$  (set of  $C^\infty$  functions over  $\Omega$  with compact support) in  $W^{p,\mu}(\Omega)$  by  $W_0^{p,\mu}(\Omega)$ , and set  $H^p(\Omega) := W^{p,2}(\Omega)$  and  $H_0^p(\Omega) := W_0^{p,2}(\Omega)$ . Similarly,  $W^{2,1,\mu}(Q)$  denotes the Sobolev space of function in  $L^\mu(Q)$  whose second derivative in space and first derivative in time belong to  $L^\mu(Q)$ , and  $H^{2,1}(Q) := W^{2,1,2}(Q)$ . Set also

$$W_\Sigma^{2,1,\mu}(Q) := \{y \in W^{2,1,\mu}(Q); \quad y = 0 \text{ on } \partial\Omega \times (0, T)\}. \quad (1)$$

The critical value

$$\mu_c := \frac{1}{2}(n + 2) \quad (2)$$

is such that, see [19, Rem. 2.5, p. 21]:

$$W^{2,1,\mu}(Q) \subset L^\infty(Q), \text{ for all } \mu > \mu_c. \quad (3)$$

Fix  $\gamma \geq 0$  and  $T > 0$ . We assume that

$$(i) \ y_0 \in W_0^{1,\infty}(\Omega); \quad (ii) \ B \in W_0^{2,\infty}(\Omega). \quad (4)$$

We consider the following semilinear parabolic controlled equation [19]:

$$\begin{cases} \dot{y}(x, t) - \Delta y(x, t) + \gamma y^3(x, t) = u(t)B(x) & \text{in } Q := \Omega \times [0, T], \\ y = 0 \text{ on } \partial\Omega \times [0, T]; \quad y(\cdot, 0) = y_0. \end{cases} \quad (5)$$

This is a prototype of a semilinear equation; taking the explicit nonlinearity  $y^3$  allows to simplify the analysis of the nonlinearity and to concentrate on the essential features. Indeed, in the case when  $\gamma = 0$ , although the problem is convex, our characterization of quadratic growth is still of interest.

Consider the cost function

$$J(u, y) = \frac{1}{2} \int_Q (y(x, t) - y_d(x, t))^2 dx dt + \alpha \int_0^T u(t) dt.$$

Here  $\alpha \in \mathbb{R}$ , the *desired state*  $y_d$  belongs to  $L^{\bar{\mu}}(Q)$ , for some  $\bar{\mu}$  such that

$$\bar{\mu} > 3\mu_c = \frac{3}{2}(n+2). \quad (6)$$

We have control bounds

$$a \leq u(t) \leq b, \quad \text{for all } t \in (0, T), \quad (7)$$

for some real numbers  $a < b$ . The optimal control problem is therefore (we will be more precise on the functional framework later):

$$(P) \quad \underset{u, y}{\text{Min}} J(u, y) \text{ s.t. } (5)-(7).$$

The well-posedness of the state equation can be deduced from the following result, in which we consider a more general r.h.s.:

$$\begin{cases} \dot{y}(x, t) - \Delta y(x, t) + \gamma y^3(x, t) = f(x, t) & \text{in } Q := \Omega \times [0, T] \\ y = 0 \text{ on } \partial\Omega \times [0, T]; \quad y(\cdot, 0) = y_0. \end{cases} \quad (8)$$

**Proposition 2.1.** *Let  $f \in L^\infty(Q)$  and  $y_0 \in W_0^{1,\infty}$ . Then (8) has a unique solution  $y[f]$  in  $W^{2,1,q}(Q)$  for all  $q \in (1, \infty)$ , and the mapping  $f \mapsto y[f]$  is of class  $C^\infty$  from  $L^\infty(Q)$  into  $W^{2,1,\mu}(Q)$ .*

*Proof.* We just give a sketch of the argument; see also e.g. [4, 19]. One classically obtains a priori estimate in  $L^\infty(0, T, L^2(\Omega) \cap L^2(0, T, H_0^1(\Omega)))$  by multiplying (8) by  $y(x, t)$  and integrating over  $Q$ . More generally, for  $q \in (2, \infty)$ , with conjugate number  $q'$  such that  $1/q + 1/q' = 1$ , combining Hölder inequality and Young's inequality  $ab \leq a^{q'}/q' + b^q/q$ , for any nonnegative  $a$  and  $b$ , we get

$$\int_\Omega |f||y|^{q-1} \leq \|f\|_q \| |y|^{q-1} \|_{q'} = \|f\|_q \| |y| \|_q^{q/q'} \leq \frac{1}{q} \|f(t)\|_q^q + \frac{1}{q'} \|y\|_q^q. \quad (9)$$

Multiplying (8) by  $|y(x, t)|^{q-2}y(x, t)$ , and integrating over  $Q$ , it follows that

$$\frac{1}{q} \frac{d}{dt} \|y\|_q^q + \gamma \int_{\Omega} |y|^{q+2} \leq \frac{1}{q} \|f(t)\|_q^q + \frac{1}{q'} \|y\|_q^q. \quad (10)$$

Since  $\|f(t)\|_q^q \in L^1(0, T)$ , with Gronwall's lemma, this gives an a priori estimate of  $y$  in  $L^\infty(0, T, L^q(\Omega))$ . Taking  $q = \bar{\mu}$ , it follows that for some  $\mu > \mu_c$ ,  $y^3 \in L^\mu(Q)$  and so  $\dot{y} - \Delta y \in L^\mu(Q)$  too. By the standard estimates for linear equations, we deduce that  $y[f]$  belongs to  $W^{2,1,\mu}(Q)$ , and so by (3),  $y[f] \in L^\infty(Q)$ .

The conclusion follows by applying the implicit function theorem to the mapping  $F : W_{\Sigma}^{2,1,q}(Q) \times L^\infty(Q) \rightarrow L^q(Q) \times W_0^{1,q}(\Omega)$ ,

$$F(y, f) := (\dot{y} - \Delta y + \gamma y^3 - f, y(\cdot, 0) - y_0). \quad (11)$$

This mapping is obviously of class  $C^\infty$ . That its partial derivative w.r.t.  $y$  is an isomorphism is equivalent to check that, for any  $(f, g) \in L^q(Q) \times W_0^{1,q}(\Omega)$ , the linearized state equation below has a unique solution  $z \in W_{\Sigma}^{2,1,q}(Q)$ :

$$\begin{cases} \dot{z} - \Delta z + 3\gamma \bar{y}^2 z = f & \text{in } Q, \\ z = 0 & \text{on } \partial\Omega \times [0, T]; \quad z(\cdot, 0) = g. \end{cases} \quad (12)$$

Since  $\bar{y} \in L^\infty(Q)$  this is easily checked.  $\square$

A composition of  $C^\infty$  mappings being of class  $C^\infty$ , we obtain that

**Corollary 2.2.** *With each  $u \in L^\infty(0, T)$  is associated a unique state  $y[u] \in W^{2,1,q}(Q)$ , for all  $q \in [2, \infty)$ , and the mapping  $u \mapsto y[u]$  is of class  $C^\infty$ .*

**Theorem 2.3.** *The problem (P) has a nonempty set of solutions. If  $\gamma = 0$ , then the solution is unique.*

*Proof.* The existence is obtained by standard arguments based on minimizing sequences, passing to the limit on the nonlinearity of the state equation, see e.g. [4, 19]. If  $\gamma = 0$  since the cost function is strictly convexity w.r.t. the state, the optimal state is unique, and then so is the optimal control.  $\square$

In the sequel we denote by  $(\bar{u}, \bar{y})$  a solution of (P).

## 2.2 First order optimality system

The costate equation is

$$\begin{cases} -\dot{\bar{p}} - \Delta \bar{p} + 3\gamma \bar{y}^2 \bar{p} = y - y_d & \text{in } Q \\ \bar{p} = 0 & \text{on } \partial\Omega \times [0, T]; \quad \bar{p}(\cdot, T) = 0. \end{cases} \quad (13)$$

Since  $y_d \in L^{\bar{\mu}}(Q)$ , this equation has a unique solution  $\bar{p} \in W^{2,1,\bar{\mu}}(Q) \subset L^\infty(Q)$ . We denote by  $F(u) := J(u, y[u])$  the cost viewed as function of the control only. This is a function of class  $C^\infty$  over  $L^\infty(0, T)$ . In the context of affine control problems, it is customary to call *switching function* the following amount

$$\Psi(t) := \alpha + \int_{\Omega} B(x) \bar{p}(x, t) dx. \quad (14)$$



The linearized state equation is

$$\begin{cases} \dot{z} - \Delta z + 3\gamma\bar{y}^2 z = v(t)B(x) & \text{in } Q, \\ z = 0 \text{ on } \partial\Omega \times [0, T]; \quad z(\cdot, 0) = 0. \end{cases} \quad (15)$$

For  $v \in L^2(Q)$ , it has a unique solution  $z[v] \in H^{2,1}(Q)$ . The following result is classical.

**Lemma 2.4.** *The switching function coincides with the derivative of  $F$ , in the sense that*

$$DF(\bar{u})v = \int_0^T \Psi(t)v(t)dt, \quad \text{for all } v \in L^\infty(0, T). \quad (16)$$

*Proof.* Let  $z = z[v]$  denote the solution of the linearized state equation (15). By the chain rule, we have that using the integration by parts formula

$$\begin{aligned} DF(u)v &= \int_Q (y - y_d)z dxdt + \alpha \int_0^T v(t)dt \\ &= \int_Q (-\dot{\bar{p}} - \Delta\bar{p} + 3\gamma\bar{y}^2\bar{p})z(x, t)dxdt + \alpha \int_0^T v(t)dt \\ &= \int_Q \bar{p}(\dot{z} - \Delta z + 3\gamma\bar{y}^2 z)dxdt + \alpha \int_0^T v(t)dt \\ &= \int_Q \bar{p}(x, t)B(x)v(t)dxdt + \alpha \int_0^T v(t)dt. \end{aligned} \quad (17)$$

The conclusion follows.  $\square$

The (again classical) *first order optimality conditions* follow, denoting the contact set by  $I(\bar{u}) = I_a(\bar{u}) \cup I_b(\bar{u})$ , where

$$I_a(\bar{u}) := \{t \in (0, T); u(t) = a\}; \quad I_b(\bar{u}) := \{t \in (0, T); u(t) = b\}. \quad (18)$$

Note that these sets are defined up to a null measure set.

**Proposition 2.5.** *We have that up to a null measure set:*

$$\{t; \Psi(t) > 0\} \subset I_a(\bar{u}); \quad \{t; \Psi(t) < 0\} \subset I_b(\bar{u}). \quad (19)$$

We next need to analyze the first and second derivative of the switching function. The switching function has a derivative in  $L^2(0, T)$ , and since  $B \in W_0^{2,\infty}(\Omega)$ , we have that

$$\begin{cases} \dot{\Psi}(t) &:= - \int_\Omega B(x)\Delta\bar{p}(x, t)dx + \int_\Omega B(x)(3\bar{y}^2(x, t)\bar{p}(x, t) - \bar{y}(x, t) + y_d(x, t))dx \\ &= - \int_\Omega \bar{p}(x, t)\Delta B(x)dx + \int_\Omega B(x)(3\bar{y}^2(x, t)\bar{p}(x, t) - \bar{y}(x, t) + y_d(x, t))dx. \end{cases} \quad (20)$$

As expected from the theory of affine control problems in the case of ODEs, the derivative of the switching function does not depend on the control. Set

$$\begin{cases} \kappa(x, t) &:= 1 - 6\gamma\bar{p}(x, t)\bar{y}(x, t), \quad (x, t) \in Q; \\ R(t) &:= \int_\Omega \kappa(x, t)B(x)^2 dx. \end{cases} \quad (21)$$

It is easily checked that  $\kappa(x, t)$  and  $R(t)$  are essentially bounded. By (20), if  $y_d$  is smooth enough,  $\Psi$  has a second derivative in  $L^2(0, T)$ . The latter is necessarily an affine function of the control, and it is easily checked that the following holds:

$$R(t) := -\frac{\partial \ddot{\Psi}(t)}{\partial u}. \quad (22)$$

In view of Kelley's result in [18], and of its extension to the case of control constraints in [1], we may expect that  $R(t) \geq 0$  if the control constraints are not active near time  $t$ . We will indeed prove this result.

### 2.3 Classical second order necessary conditions

We will state second order necessary conditions based on the polyhedricity concept [17, 21]; see e.g., in an elliptic framework, [6, Section 6.3]. We first need to define boundary and singular arcs.

*Definition 2.6.* Let  $t_1, t_2$  belong to  $[0, T]$  with  $t_1 < t_2$ . We say that  $(t_1, t_2)$  is a *singular arc* if there exists  $\varepsilon > 0$  such that  $\bar{u}(t) \in [a + \varepsilon, b - \varepsilon]$  for a.a.  $t \in (t_1, t_2)$ , a *lower bound arc* if  $\bar{u}(t) = a$  for a.a.  $t \in (t_1, t_2)$ , and an *upper bound arc* if  $\bar{u}(t) = b$  for a.a.  $t \in (t_1, t_2)$ . Lower and upper bound arcs are called boundary arcs.

We will consider only maximal arcs (that are not strictly included in another arc) and assume that

$$\text{There are finitely many maximal arcs, whose union is } [0, T], \quad (23)$$

and the *strict complementarity hypothesis*, in the sense that

$$\Psi \text{ has nonzero values over each boundary arc.} \quad (24)$$

Note that,  $\Psi$  being a continuous function, the above definition makes sense. We may then redefine "punctually" the contact sets  $I_a(\bar{u})$  and  $I_b(\bar{u})$  as

$$I_a(\bar{u}) = \{t \in [0, T]; \Psi(t) > 0\}; \quad I_b(\bar{u}) = \{t \in [0, T]; \Psi(t) < 0\}. \quad (25)$$

Assuming strict complementarity, we have that the critical cone  $C(\bar{u})$  and its extension  $C_2(\bar{u})$  to  $L^2(0, T)$  have the following expressions:

$$\begin{cases} C_2(\bar{u}) = \{v \in L^2(0, T); v(t) = 0, t \in I(\bar{u})\}; \\ C(\bar{u}) := C_2(\bar{u}) \cap L^\infty(0, T). \end{cases} \quad (26)$$

We recall that the linearized state equation and its solution denoted by  $z[v]$  were defined in (15). The following quadratic form (where  $\kappa \in L^\infty(Q)$  has been defined in (21)) is obviously well-defined and continuous over  $L^2(\Omega)$ :

$$Q(v) := \int_Q \kappa(x, t) z(x, t)^2 dt. \quad (27)$$

**Theorem 2.7.** *We have that*

$$Q(v) \geq 0 \quad \text{for all } v \in C_2(\bar{u}). \quad (28)$$

*Proof.* The technique being classical and similar to the one in [6, Section 6.3], we may leave details to the reader. □

## 2.4 Goh transform

We next extend the Goh transform theory [16] to the present setting as follows. Define the “new control”  $w(t) = \int_0^t v(t)dt$ , and the “new linearized state”  $\xi = z - w(t)B(x)$ . The latter satisfies  $\dot{\xi} = \dot{z} - uB = \Delta z - 3\bar{y}^2 z$ , and so is solution of

$$\begin{cases} \dot{\xi}(x, t) - \Delta \xi(x, t) + 3\bar{y}(x, t)^2 \xi(x, t) = w(t)\Delta B(x) - 3w(t)\bar{y}(x, t)^2 B(x) & \text{in } \Omega. \\ \xi = 0 \text{ on } \partial\Omega \times [0, T]; \quad \xi(\cdot, 0) = 0. \end{cases} \quad (29)$$

Since  $\bar{y} \in L^\infty(Q)$ , (4) implies that (29) has a unique solution  $\xi[w] \in W^{2,1,s}(Q)$  whenever  $w \in L^s(0, T)$ , with  $s \in [2, \infty)$ .

In view of (23) the set of *primitives of critical directions* in with value 0 at time 0 is therefore

$$PC(\bar{u}) = \{w \in W^{1,\infty}(0, T); \quad \dot{w}(t) = 0, \quad t \in I(\bar{u})\}. \quad (30)$$

Set

$$\hat{Q}(w) = \int_Q \kappa(x, t)(\xi[w](x, t) + w(t)B(x))^2 dt. \quad (31)$$

Again this quadratic form is well defined and continuous over  $H^1(0, T)$ , and obviously  $Q(v) = \hat{Q}(w)$ . By (28) and the previous discussion we get

**Lemma 2.8.** *We have that  $\hat{Q}(w) \geq 0$ , for all  $w \in PC(\bar{u})$ .*

Next, observe that the closure in  $L^2$  of primitives of critical directions is

$$PC_2(\bar{u}) = \{w \in L^2(0, T); \quad \dot{w}(t) = 0, \quad t \in I(\bar{u})\}, \quad (32)$$

where we take the time derivative of  $w$  in the distribution sense, on the relative interior of the set of times where the constraint is active. Then  $\hat{Q}$  has a continuous extension over  $L^2(0, T)$ . With lemma 2.8 we deduce that

**Lemma 2.9.** *We have that  $\hat{Q}(w) \geq 0$ , for all  $w \in PC_2(\bar{u})$ .*

**Corollary 2.10.** *We have that*

$$R(t) \geq 0, \quad \text{for } t \notin I(\bar{u}). \quad (33)$$

*Proof.* Consider the problem of minimizing the quadratic form  $\hat{Q}$  over the set

$$PC'_2(\bar{u}) = \{w \in L^2(0, T); \quad w = 0 \text{ on } I(\bar{u})\}. \quad (34)$$

Since  $PC'_2(\bar{u}) \subset PC_2(\bar{u})$ , we have that  $\bar{w} = 0$  is solution of this problem. By the Legendre condition for this problem (itself a consequence of Pontryagin’s principle [7]), we deduce that the conclusion holds.  $\square$

*Remark 2.11.* As in the finite dimensional setting we have recovered the Kelley condition [18]: when the control constraint is not active, (22) is nonnegative.

### 3 Second order sufficient conditions

We first state the main result of this section. Consider the following condition:

$$\text{There exists } \rho > 0 \text{ such that } \Omega(w) \geq \rho \|w\|_2^2, \text{ for all } w \in C_2(\bar{u}). \quad (35)$$

**Theorem 3.1.** *Let (35) hold. Then there exists  $\rho' > 0$  such that, if  $u \in F(P)$ , then setting  $v := u - \bar{u}$  and  $w(t) = \int_0^t v(s)ds$ , we have that*

$$J(\bar{u} + v) \geq J(\bar{u}) + \rho' \|w\|_2^2, \quad \text{if } \|v\|_2 \text{ is small enough.} \quad (36)$$

We first need to prove the following statement.

**Proposition 3.2.** *Let  $\bar{u} + v$  be feasible, and set  $w(t) = \int_0^t v(s)ds$ . Then we have that:*

$$J(\bar{u} + v) = J(\bar{u}) + \int_Q \Psi v + \frac{1}{2} \hat{Q}(w) + O(\|y - \bar{y}\|_\infty \|w\|_2^2). \quad (37)$$

*Remark 3.3.* This is to be compared to the classical expansion, consequence of the Implicit Function Theorem, taking  $L^\infty(0, T)$  as control space, i.e.

$$J(\bar{u} + v) = J(\bar{u}) + \int_Q \Psi v + \frac{1}{2} \hat{Q}(w) + O(\|v\|_\infty^3). \quad (38)$$

In the sequel we denote

$$\varphi(y) = \gamma y^3. \quad (39)$$

*Proof.* a) Let us consider the quadratic form corresponding to the Hessian of the Lagrangian (where  $\kappa$  was defined in (21)):

$$\tilde{Q}(z) := \int_Q \kappa(x, t) z(x, t)^2 dt. \quad (40)$$

This is a continuous quadratic form over  $L^2(Q)$ . Let  $y = \bar{y} + \delta y$  be the state associated with the control  $\bar{u} + v$ . Skipping arguments of functions when no confusions may occur, we claim that

$$F(\bar{u} + v) = F(\bar{u}) + \int_0^T \Psi v + \tilde{Q}(\delta y) + O(\|\delta y\|_3^3). \quad (41)$$

Indeed, we have that

$$J(\bar{u} + v, \bar{y} + \delta y) = J(\bar{u}, \bar{y}) + \int_O (\alpha v + (\bar{y} - y_d) \delta y + (\delta y)^2), \quad (42)$$

and since  $\bar{u} + v \in F(P)$ , the state  $y$  remains in a compact set, so that

$$\varphi(\bar{y} + \delta y) = \varphi(\bar{y}) + \varphi'(\bar{y}) \delta y + \frac{1}{2} \varphi''(\bar{y}) (\delta y)^2 + O(|\delta y|^3). \quad (43)$$

Multiplying the costate by the difference of state equations with the pairs  $(u, y)$  and  $(\bar{u}, \bar{y})$ , we get

$$\left\{ \begin{array}{l} 0 = \int_Q \bar{p} (\Delta \delta y - \varphi(y) + \varphi(\bar{y}) + vB - \dot{\delta y}) \\ = \int_Q (\dot{\bar{p}} + \Delta \bar{p} - \varphi'(\bar{y}) \bar{p}) \delta y + \int_Q (\bar{p} v B - \frac{1}{2} \bar{p} \varphi''(\bar{y}) (\delta y)^2) + O(\|\bar{p} \delta y\|_\infty^3) \\ = - \int_Q (\bar{y} - y_d) \delta y + \int_Q (\bar{p} v B - \frac{1}{2} \bar{p} \varphi''(\bar{y}) (\delta y)^2) + O(\|\bar{p} \delta y\|_\infty^3) \end{array} \right. \quad (44)$$

Adding with (42), and using  $\bar{p} \in L^\infty(Q)$  and (21), we prove our claim (41).

b) Reminding that  $z$  is the solution of the linearized equation (12), we claim that

$$\left| \tilde{Q}(\delta y) - \tilde{Q}(z) \right| \leq O(\|\delta y\|_\infty \|w\|_2^2). \quad (45)$$

We have that

$$\tilde{Q}(\delta y) - \tilde{Q}(z) = \int_Q \kappa((\delta y)^2 - z^2) = \int_Q \kappa(\delta y + z)(\delta y - z), \quad (46)$$

and so, since  $\kappa \in l^\infty(Q)$ :

$$\left| \tilde{Q}(\delta y) - \tilde{Q}(z) \right| \leq \|\kappa\|_\infty (\|\delta y\|_2 + \|z\|_2) \|\delta y - z\|_2. \quad (47)$$

We next obtain estimates for  $\|\delta y\|_2 + \|z\|_2$  and  $\|\delta y - z\|_2$ . For this we apply a variant of the Goh transform to the state equation. Set  $\hat{w}(t) := \int_0^t (\bar{u}(s) + v(s)) ds$ . Then  $\eta := y - \hat{w}b$  is solution of  $\dot{\eta} = \dot{y} - \hat{w}B = \Delta y - \varphi(y)$ , and so

$$\begin{cases} \dot{\eta} - \Delta \eta + \varphi(\eta + \hat{w}b) = \hat{w} \Delta B & \text{in } Q, \\ \eta = 0 & \text{on } \partial\Omega \times [0, T]; \quad \eta(\cdot, 0) = y_0. \end{cases} \quad (48)$$

Set  $\bar{w}(t) := \int_0^t \bar{u}(s) ds$ ,  $\bar{\eta} = \bar{y} - \bar{w}b$ , and  $\delta \eta = \eta - \bar{\eta}$ . We get

$$\begin{cases} \dot{\delta \eta} - \Delta \delta \eta + \varphi(\eta + \hat{w}b) - \varphi(\bar{\eta} + \bar{w}b) = w \Delta B & \text{in } Q, \\ \delta \eta = 0 & \text{on } \partial\Omega \times [0, T]; \quad \delta \eta(\cdot, 0) = y_0. \end{cases} \quad (49)$$

Since  $\bar{u} + v \in F(P)$  a.e., the arguments of  $\varphi$  (equal to  $y$  and  $\bar{y}$ ) are uniformly bounded, and so there exists  $\theta[v]$  in a uniformly bounded subset of  $L^\infty(Q)$  such that

$$\varphi(\eta + \hat{w}b) - \varphi(\bar{\eta} + \bar{w}b) = \theta[v](\delta \eta + wB). \quad (50)$$

Substituting this expression in (49), we get that  $\|\delta \eta\|_{H^{2,1}(Q)} = O(\|w\|_2)$ , and so

$$\|\delta y\|_2 = \|\delta \eta + wB\|_2 \leq \|\delta \eta\|_2 + \|B\|_\infty \|w\|_2 = O(\|w\|_2). \quad (51)$$

By similar arguments we get that

$$\|z\|_2 = \|\xi + wB\|_2 \leq \|\xi\|_2 + \|B\|_\infty \|w\|_2 = O(\|w\|_2). \quad (52)$$

Next, by (29) and (49), we have that  $\chi := \delta \eta - \xi$  is solution of

$$\dot{\chi} - \Delta \chi + \varphi'(\bar{y})\chi = \varphi(\bar{y}) - \varphi(y) + \varphi'(\bar{y})\delta y = c(x, t)(\delta y)^2, \quad (53)$$

for some bounded function  $c$ . If  $\delta y = 0$ , the conclusion obviously holds. Otherwise,  $\hat{\chi} = \chi / \|\delta y\|_\infty$  is solution of

$$\dot{\hat{\chi}} - \Delta \hat{\chi} + \varphi'(\bar{y})\hat{\chi} = c(x, t)(\delta y)^2 / \|\delta y\|_\infty. \quad (54)$$

The  $L^2$  norm of the r.h.s. is by (51) of order  $\|\delta y\|_2 = O(\|w\|_2)$ , and so

$$\|\delta y - z\|_{H^{2,1}} = \|\delta \eta - \xi\|_{H^{2,1}} = \|\chi\|_{H^{2,1}} = \|\delta y\|_\infty \|\hat{\chi}\|_{H^{2,1}} = O(\|\delta y\|_\infty \|w\|_2). \quad (55)$$

Combining with (47) and (51)-(52), we deduce that the claim (45) holds.

c) We also have with (51) that

$$\|\delta y\|_3^3 \leq \|\delta y\|_\infty \|\delta y\|_2^2 = O(\|\delta y\|_\infty \|w\|_2^2). \quad (56)$$

We conclude by combining this inequality with the claims (41) and (45).  $\square$

*Proof of theorem 3.1.* a) Let the sequence  $(v_k, w_k)$  contradict the conclusion, i.e.,  $\bar{u} + v_k \in F(P)$ ,  $v_k \neq 0$ ,  $\|v_k\|_2 \rightarrow 0$ ,  $w_k$  is the primitive of  $v_k$  with zero initial value, and

$$J(\bar{u} + v_k) \leq J(\bar{u}) + o(\|w_k\|_2^2). \quad (57)$$

Set  $\hat{w}_k := w_k/\|w_k\|_2$ . Extracting if necessary a subsequence, we may assume that  $v_k \rightarrow 0$  a.e., and that the unit sequence  $\hat{w}_k$  has a weak limit say  $\hat{w}$  in  $L^2(0, T)$ . By the dominated convergence theorem,  $v_k \rightarrow 0$  in  $L^s(0, T)$  for all  $s \in [1, \infty)$ , and so  $y_k \rightarrow 0$  uniformly.

b) We claim that  $\hat{w} \in PC_2(\bar{u})$ . By proposition 3.2, we have that

$$J(\bar{u} + v_k) - J(\bar{u}) = \int_0^T \Psi(t)v_k(t)dt + O(\|w_k\|_2^2). \quad (58)$$

By the first order optimality conditions, the above integral is nonnegative. Majorizing it using (57), we get that

$$\frac{1}{\|w_k\|_2} \int_0^T \Psi(t)v_k(t)dt \rightarrow 0. \quad (59)$$

Let  $(c, d) \subset (0, T)$  be a boundary arc, and let  $\varphi \in \mathcal{D}_+(c, d)$ , i.e.,  $\varphi$  is of nonnegative, and of class  $C^\infty$  with compact support in  $(c, d)$ . The integrand in (59) being nonnegative, we deduce that

$$\int_c^d \varphi(t)\Psi(t)dw_k(t) = \frac{1}{\|w_k\|_2} \int_c^d \varphi(t)\Psi(t)v_k(t)dt \rightarrow 0. \quad (60)$$

Since  $\varphi\Psi \in H^1(0, T)$ , we may integrate by parts and we deduce that

$$0 = \lim_k \int_c^d \frac{d}{dt} (\varphi(t)\Psi(t)) \hat{w}_k(t)dt = \int_c^d \frac{d}{dt} (\varphi(t)\Psi(t)) \hat{w}(t)dt. \quad (61)$$

Assume for instance that  $\bar{u} = a$  on  $(c, d)$ . For some  $\varepsilon > 0$  the support of  $\varphi$  is contained in  $(c + \varepsilon, d - \varepsilon)$ . On  $(c, d)$  we have that  $v_k \geq 0$  and so  $w_k$  and  $\hat{w}$  are nondecreasing. In particular,  $\hat{w}$  has bounded variation on  $(c + \varepsilon, d - \varepsilon)$ . By the integration by parts formula with one of the function having only bounded variation, see [15, Vol. I, ch. 3, Theorem 22, p. 154], we get with (61) that

$$\int_{c+\varepsilon}^{d-\varepsilon} \varphi(t)\Psi(t)d\hat{w}(t) = 0. \quad (62)$$

Over  $[c + \varepsilon, d - \varepsilon]$ , since  $\Psi(t) > 0$  by the strict complementarity assumption (24),  $d\hat{w}(t) \geq 0$ , and  $\varphi$  is an arbitrary element of  $\mathcal{D}_+(c, d)$  with support in  $(c + \varepsilon, d - \varepsilon)$ , we deduce that  $\hat{w}$  is constant over  $(c + \varepsilon, d - \varepsilon)$ . Since  $\varepsilon > 0$  may be taken arbitrarily small, the claim follows.

c) By (57) and proposition 3.2,  $\int_0^T \Psi(t)v_k(t)dt \geq 0$ , and  $\|y_k - \bar{y}\|_\infty \rightarrow 0$ , we have that

$$\limsup_k \hat{Q}(\hat{w}_k) \leq o(1). \quad (63)$$

Next let  $I_+ := [0, T] \setminus I$  denote the set of times when the control constraint is not active. For  $\varepsilon > 0$ , let

$$I_+^\varepsilon := \{t \in [0, T]; \text{dist}(t, I_+) \leq \varepsilon\}; \quad I_0^\varepsilon := [0, T] \setminus I_+^\varepsilon. \quad (64)$$

Set, for  $w \in PC_2(\bar{u})$ ,  $\hat{Q}_\rho(w) := \hat{Q}(w) - \rho \int_0^T w(t)^2 dt$ . Applying corollary 2.10 to this nonnegative quadratic form, we deduce that  $R(t) \geq \rho$  over  $I_+$ . Since  $R(t)$  is a continuous function, we deduce that there exists  $\varepsilon > 0$  such that

$$R(t) \geq \frac{1}{2}\rho \text{ over } I_+^\varepsilon. \quad (65)$$

Now write, in view of (31),

$$\hat{Q}(\hat{w}_k) = \hat{Q}_1(\hat{w}_k) + \hat{Q}_2(\hat{w}_k) + \hat{Q}_3(\hat{w}_k), \quad (66)$$

with

$$\begin{cases} \hat{Q}_1(\hat{w}_k) & := \int_Q \kappa(x, t) (\xi[w](x, t)^2 + 2\xi[w](x, t)w(t)B(x)) dx dt, \\ \hat{Q}_2(\hat{w}_k) & := \int_{I_+^\varepsilon} R(t)w(t)^2 dt, \quad \hat{Q}_3(\hat{w}_k) := \int_{I_0^\varepsilon} R(t)w(t)^2 dt. \end{cases} \quad (67)$$

Since the mapping  $w \rightarrow \xi[w]$  is compact  $L^2(0, T) \rightarrow L^2(Q)$  we have that  $\hat{Q}_1$  is weakly continuous. By (65),  $\hat{Q}_2$  restricted to  $L^2(I_+^\varepsilon)$  is a Legendre form, in the sense that, it is weakly l.s.c. and satisfies

$$w_k \rightharpoonup w \text{ and } \hat{Q}(w_k) \rightarrow \hat{Q}(w) \text{ implies } w \rightarrow w \text{ in } L^2(I_+^\varepsilon). \quad (68)$$

Now, let  $(c, d)$  be a connected component of  $I_0^\varepsilon$  and  $\varphi \in \mathcal{D}(c, d)$ , uniformly positive over  $[c+\varepsilon, d-\varepsilon]$  for  $\varepsilon > 0$  small enough. By (60), since  $\Psi$  is uniformly positive in  $[c+\varepsilon, d-\varepsilon]$  for any  $\varepsilon > 0$  small enough, it follows that for some  $\beta > 0$ ,  $\varphi(t)\Psi(t) \geq \beta > 0$  for all  $t \in [c+\varepsilon, d-\varepsilon]$ , and so

$$0 = \lim_k \int_c^d \varphi(t)\Psi(t) dw_k(t) \geq \lim_k \int_{c+\varepsilon}^{d-\varepsilon} \varphi(t)\Psi(t) dw_k(t) \geq \beta \int_{c+\varepsilon}^{d-\varepsilon} dw_k(t) \quad (69)$$

and since  $w_k$  is nondecreasing it follows that  $w_k(d-\varepsilon) - w_k(c+\varepsilon) \rightarrow 0$ , proving that  $w_k$  strongly converges over  $I_0^\varepsilon$ , to a function that is constant over each maximal boundary arc. So we have that

$$\hat{Q}_1(\hat{w}) = \lim_k \hat{Q}_1(\hat{w}_k); \quad \hat{Q}_2(\hat{w}) \leq \lim_k \hat{Q}_2(\hat{w}_k); \quad \hat{Q}_3(\hat{w}) = \lim_k \hat{Q}_3(\hat{w}_k) = 0. \quad (70)$$

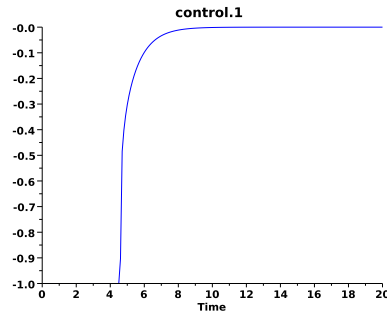
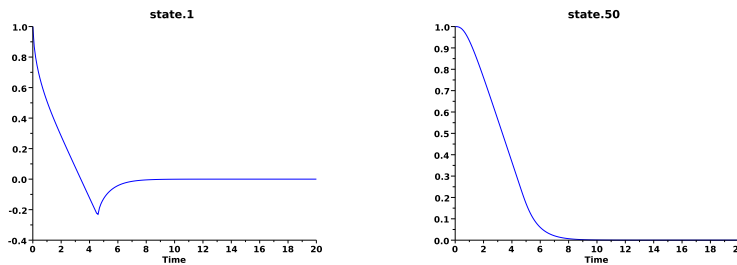
With (63) this implies that  $\hat{Q}(\hat{w}) \leq 0$ . Since  $\hat{w} \in PC_2(\bar{u})$ , by (35),  $\hat{w} = 0$ . By (70),  $\hat{Q}_2(\hat{w}_k) \rightarrow \hat{Q}_2(\hat{w})$ . We deduce that  $\hat{w}_k \rightarrow \hat{w}$  in  $L^2(0, T)$ , in contradiction with the fact that  $\hat{w}_k$  is a unit sequence and  $\hat{w} = 0$ .  $\square$

## 4 Numerical experiments

An open question is the existence of singular arcs. We could consider the convex case when  $\gamma = 0$  and try to solve explicitly the optimality system; this however seems very difficult. We refer to Dhamo and Tröltzsch [11] for an example of an almost analytic resolution of an optimality system, in the context of parabolic equations.

On the other hand we can try numerical experiments and see if a singular arc seems to occur and is stable with respect to the discretization. We discretize the problem by standard finite differences, and solve the resulting optimal control problem with finitely many states using the optimal control toolbox BOCOP [5], which itself uses the nonlinear programming solver IPOPT [24].

The problem consists in controlling the one dimensional heat equation by the Neumann condition at one end. More precisely,  $\Omega = (0, 1)$ , the control is the Neumann condition at  $x = 0$ , and the Neumann condition at  $x = 1$  is zero. We present the results obtained with 50 space steps, 200 time steps, the implicit Euler scheme, and taking  $y_0 = 1$ ,  $y_d = 0$ ,  $\alpha = 0$ . We display next the optimal control, and the states function of time. The control constraint is  $u(t) \in [-1, 1]$ , and we see that it is not active for  $t \geq 5$ . The same behavior is observed if we perturb the data and stepsize. So we may conjecture that this problem really has a singular arc.

Figure 1: Optimal control:  $u \in [-1, 1]$ .Figure 2: State at boundary  $x = 0$ .

## 5 Conclusion

We have established second order necessary and sufficient conditions for the local optimality of an optimal control problem of a parabolic equation, the Hamiltonian being affine w.r.t. the control, in the case when the optimal control has a singular arc. The main result is a characterization of a weak form of quadratic growth, that extends to the setting of control of parabolic equations the recent results and techniques in [1] (see in particular the proof of our key theorem 3.1).

It is not easy to prove if such singular arcs occur. However, we give strong numerical arguments supporting such an existence, actually in the case of a boundary control.

The present study deals with a simple case. It seems possible and of interest to extend our results in several directions: (i) the case of finitely many control variables, (ii) the case when the coefficients of the control, in the cost function and state equation, also depend on the state, (iii) the case when finitely many constraints on the terminal state are present.

Note also that, in real engineering devices, the action on the state equation is not the control itself, but rather the result of some integrations of the real control. To be specific, we might consider the case when  $\dot{u} = v$  where  $v$  is now the control, and  $u$  becomes a state variable, which is of course subject to bounds. This raises the question of extending the present framework to the case of state constraints. Let us observe that little is known, even in the ODE setting (see the analysis of optimality conditions in [20]).



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