Generalized Solutions of Hamilton – Jacobi Equation to a Molecular Genetic Model

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Abstract. A boundary value problem with state constraints is under consideration for a nonlinear noncoercive Hamilton-Jacobi equation. The problem arises in molecular biology for the Crow – Kimura model of genetic evolution. A new notion of continuous generalized solution to the problem is suggested. Connections with viscosity and minimax generalized solutions are discussed. In this paper the problem is studied for the case of additional requirements to structure of solutions. Constructions of the solutions with prescribed properties are provided and justified via dynamic programming and calculus of variations. Results of simulations are exposed.

Keywords: Hamilton – Jacobi equation, method of characteristics, generalized solutions, viscosity solutions, state constraints

1 Introduction

In [1] a new way to study molecular evolution has been proposed. According to this way dynamics of the Crow – Kimura model for molecular evolution can be analyzed via the following HJE

$$\partial u/\partial t + H(x, \partial u/\partial x) = 0, \tag{1}$$

where the Hamiltonian $H(\cdot)$ has the form

$$H(x, p) = -f(x) + 1 - \frac{1+x}{2}e^{2p} - \frac{1-x}{2}e^{-2p}. \tag{2}$$

The function $f(\cdot)$ in (2) is given and called fitness. Equation (1) is considered for $t \geq 0$, $-1 \leq x \leq 1$. It is also assumed that an initial function $u_0 : \mathbb{R} \to \mathbb{R}$ is given such that

$$u(0, x) = u_0(x), \quad x \in [-1; 1]. \tag{3}$$

In [1] problem (1)-(3) was studied for input data $u_0(x) = -a(x - x_0)^2$, $a > 0$, $f(x) = x^2$ and physical interpretations were used.

The classical method for solving PDE of the first order in Cauchy problem is the method of characteristics (see, e.g. [2]). This method reduces integration of PDEs to integration of the characteristic system of ODEs.
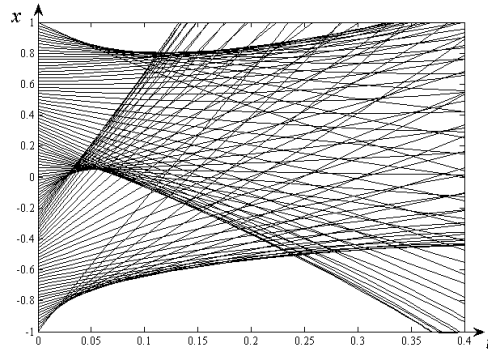
The characteristic system for problem (1)-(3) has the form

$$\dot{x} = H_p(x, p) = -(1 + x)e^{2p} + (1 - x)e^{-2p},$$

$$\dot{p} = -H_x(x, p) = f'(x) + (e^{2p} - e^{-2p})/2, \qquad (4)$$

$$\dot{z} = pH_p(x, p) - H(x, p),$$

with initial conditions

$$x(0, y) = y, \quad p(0, y) = u_0'(y), \quad z(0, y) = u_0(y), \qquad y \in [-1; 1]. \qquad (5)$$

Here $H_x(x, p) = \partial H(x, p)/\partial x$, $\quad H_p(x, p) = \partial H(x, p)/\partial p$, $\ f'(x) = \partial f(x)/\partial x$. Solutions of the system (4)-(5) are called characteristics. Components $x(\cdot, y)$, $p(\cdot, y)$ and $z(\cdot, y)$ of the solution are called state, conjugate, and value characteristics, respectively.

Fig. 1. State characteristics for the case $f(x) = -0.25x^2$, $u_0(x) = 0.25(x - 0.5)^2 - 0.1\cos 2\pi x$.

The method of characteristics can be applied to constructions of solutions for problem (1)-(3) in such a neighborhood of the initial manifold (5) where state characteristics don't cross. As a rule, characteristics for problem (1)-(3) are nonextendable to the whole time axis and can cross each other. Moreover, there are points in strip $t \geq 0$, $-1 \leq x \leq 1$. where solution of (1)-(3) should be found, and where the state characteristics do not pass. An example of such a behavior of state characteristics is presented on Fig. 1.

So, one can see that solutions of the problem (1)-(3) should be understood in a generalized sense.

In [3], we introduced a concept of continuous generalized solutions (see Definition 1 below) and proved it's existence in problem (1)-(3) using tools of Nonsmooth Analysis and results of the Optimal Control Theory. It was also shown that the generalized solution is not unique.

In this paper, we consider problem (1)-(3) with additional requirements to the structure of solutions, see [4] and [5]. Namely, we need to construct a continuous solution in the strip $t \geq 0$, $-1 \leq x \leq 1$ in such a way that it coincides with a solution obtained by the method of characteristics in a domain part where the characteristics defined by (4) and (5) pass.

The paper is organized as follows. In Section 2, the definition of a continuous generalized solution is introduced, and the results on its existence are presented. In Section 3 we state the problem of constructing the generalized solution with prescribed properties, give sufficient conditions under which the problem can be solved, and formulate auxiliary results on which solving is based. A scheme for constructing the generalized solution and results of a simulation are presented in Section 4 and Section 5 respectively. And, in Section 6, we compare our generalized solution with viscosity solutions.

2 Continuous Generalized Solutions to the Problem with State Constraints

2.1 The Problem with State Constraints and Definition of a Generalized Solution

Let $T > 0$ be such an instant that characteristics (4), (5) are extendable up to T, and $x(\cdot, y)$, $p(\cdot, y)$, $z(\cdot, y)$ are continuous on $[0, T]$ for all $y \in [-1; 1]$. Exact estimates for intervals of extendibility are obtained in [4, 6].

We consider problem (1)-(3) on the restricted closed domain

$$\overline{\Pi}_T = [0; T] \times [-1; 1],$$

and also use the notations

$$\Pi_T = (0; T) \times (-1; 1), \quad \Gamma_T = \{(t, x) | \ t \in (0, T), \ x = \pm 1\}.$$

In the HJEs' theory various concepts of generalized solutions have been introduced (see, e.g. [7–9]). Note that definitions of generalized solutions to HJEs in open areas were applied to problems with state constraints as additional requirements to solutions on the border were imposed. These requirements play a role of boundary conditions. Unfortunately, results of the theories of generalized solutions are inapplicable to the problem (1)-(3). In particular, one of the key conditions under which the known theorems on existense of a generalized viscosity solution [8, 10] has been proved is the coercivity of the Hamiltonian (see (22) below). And the theory of minimax solutions [9] is not developed for problems with state constraints. So, below a new definition of a generalized solution is introduced [3]. This definition is based on the minimax and viscosity approahes and uses the following tools of nonsmooth analysis [10, 11].

Let W be a set in $\mathbb{R}^2$. Denote by $\overline{W}$ the closure of this set, by $C(W)$ — the class of functions continuous on the set W.

Let $u(\cdot) \in C(\overline{W})$ and $(t,x) \in \overline{W}$. The subdifferential of the function $u(\cdot)$ at (t,x) is the set

$$
D^- u(t,x) = \left\{ (a,s) \in \mathbb{R} \times \mathbb{R} \;\middle|\; \liminf_{\substack{(\tau,y) \to (t,x) \\ (\tau,y) \in \overline{W}}} \frac{u(\tau,y) - u(t,x) - a(\tau - t) - s(y - x)}{|\tau - t| + |y - x|} \geq 0 \right\}.
$$

The superdifferential of the function $u(\cdot)$ at (t,x) is the set

$$
D^+ u(t,x) = \left\{ (a,s) \in \mathbb{R} \times \mathbb{R} \;\middle|\; \limsup_{\substack{(\tau,y) \to (t,x) \\ (\tau,y) \in \overline{W}}} \frac{u(\tau,y) - u(t,x) - a(\tau - t) - s(y - x)}{|\tau - t| + |y - x|} \leq 0 \right\}.
$$

Let $\mathrm{Dif}(u)$ be the set of points where the function $u(\cdot) \in C(\overline{W})$ is differentiable. For a given set $M \subset \mathbb{R}^2$, the symbol $\mathrm{co}M$ means its convex hull [13]. Let us define the set

$$
\partial u(t,x) = \mathrm{co}\Big\{ (a,s) \;\Big|\; a = \lim_{i \to \infty} \frac{\partial u(t_i,x_i)}{\partial t}, \; s = \lim_{i \to \infty} \frac{\partial u(t_i,x_i)}{\partial x};
$$
$$
(t_i,x_i) \to (t,x) \text{ as } i \to \infty, \quad (t_i,x_i) \in \mathrm{Dif}(u) \Big\}.
$$

Definition 1. *A continuous function $u(\cdot) : \overline{\Pi}_T \to \mathbb{R}^2$ is called a generalized solution to problem (1)–(3) iff it satisfies the initial condition (3) and the following relations are true*

$$
a + H(x,s) \leq 0, \quad \forall (a,s) \in D^+ u(t,x), \forall (t,x) \in \Pi_T, \tag{6}
$$

$$
a + H(x,s) \geq 0, \quad \forall (a,s) \in D^- u(t,x), \forall (t,x) \in \Pi_T, \tag{7}
$$

$$
a + H(x,s) \geq 0, \quad \forall (a,s) \in D^- u(t,x) \cap \partial u(t,x), \forall (t,x) \in \Gamma_T. \tag{8}
$$

2.2 Existence of Generalized Solutions

The following statement was proved in [4] by using tools of Mathematical Theory of Optimal Control [14] and the method of generalized characteristics [15, 16].

Theorem 1. *Let input data $u_0(\cdot) : [-1,1] \to \mathbb{R}$ and $f(\cdot) : [-1,1] \to \mathbb{R}$ be continuously differentiable functions. Let a function $\varphi(t,x) : \mathbb{R}^2 \to \mathbb{R}$ be also continuously differentiable and satisfy the relations*

$$
\varphi(0,x) = u_0(x) \quad \forall\, x \in [-1,1];
$$

$$
\frac{\partial \varphi(t,\pm 1)}{\partial t} + H\Big(\pm 1, \frac{\partial \varphi(t,\pm 1)}{\partial x}\Big) = 0 \quad \forall\, t \geq 0. \tag{9}
$$

Then there exists a solution $u(t,x)$ of problem (1)–(3) in sense of definition 1. The solution has the form

$$
u(t,x) = \max_{x(t,y^\sharp)=x} \left[\varphi(t^\sharp, y^\sharp) + \right.
$$

$$+ \int_{t^\sharp}^t p(\tau, y^\sharp) H_p(x(\tau, y^\sharp), p(\tau, y^\sharp)) - H(x(\tau, y^\sharp), p(\tau, y^\sharp)) d\tau \Big], \qquad (10)$$

for all $(t, x) \in \overline{\Pi}_T$, *where* $t^\sharp \in [0, T]$. *If* $t^\sharp = 0$ *then* $y^\sharp = y \in [-1, 1]$; *if* $t^\sharp > 0$, *then* $y^\sharp = \pm 1$. *The functions* $(x(\cdot, y^\sharp), p(\cdot, y^\sharp)) : [t^\sharp, t] \to \mathbb{R}^2$ *are solutions for the system composed of the first two equations of characteristic system* (4) *with initial conditions*

$$x(t^\sharp, y^\sharp) = y^\sharp, \quad p(t^\sharp, y^\sharp) = \frac{\partial \varphi(t^\sharp, y^\sharp)}{\partial y} = p_0(t^\sharp, y^\sharp).$$

To obtain $u(t, x)$ in accordance with (10), one should consider the set of all state characteristics $x(\cdot, y^\sharp)$ passing through the point (t, x), namely, $x(t, y^\sharp) = x$. Note that the generalized solution to problem (1)–(3) is not unique because of wide choice of functions $\varphi(\cdot)$ in Theorem 1.

3   Solutions with Prescribed Properties

Here, we consider a problem to construct the generalized solution of some particular structure.

Let $x^-(t) = x(t, -1)$ and $x^+(t) = x(t, +1)$, $t \in [0, T]$ be the state characteristics started at $t = 0$ from the points $x = -1$ and $x = 1$, respectively. Below, we assume that the following condition is satisfied.

A. For the state characteristics $x(\cdot, y)$ with initial conditions (5) at $t = 0$ the inequalities are valid

$$-1 \le x^-(t) \le x(t, y) \le x^+(t) \le 1, \quad \forall \ y \in [-1, 1], \forall \ t \in [0, T].$$

Define the subdomains

$$G_0 = \big\{ (t, x) | t \in [0, T], \ x^-(t) \le x \le x^+(t) \big\}.$$
$$G_+ = \{ (t, x) | \ t \in [0, T], \ x^+(t) \le x \le 1 \}, \qquad (11)$$
$$G_- = \{ (t, x) | \ t \in [0, T], \ -1 \le x \le x^-(t) \}.$$

So, under the assumption **A**, we get

$$\overline{\Pi}_T = G_+ \cup G_0 \cup G_-.$$

The goal of the work is to construct the generalized solution to problem (1)–(3) such that it has the following form in G_0:

$$u(t, x) = \max_{x(t, y) = x} [u_0(y) + \int_0^t p(\tau) H_p(x(\tau), p(\tau)) - H(x(\tau), p(\tau)) d\tau], \qquad (12)$$

where $x(t) = x(t, y), \quad p(t) = p(t, y), \ t \ge 0$, are state and conjugate characteristics, respectively, which satisfy at $t = 0$ the initial conditions

$$x(0, y) = y, \quad p(0, y) = u_0'(y), \quad y \in [-1, 1].$$

3.1 Sufficient Conditions

To solve the problem (1)–(3) with the requirement (12) we introduce the following additional assumptions on input data.

B1. The derivative $u_0'(\cdot) : [-1, 1] \to \mathbb{R}$ is continuous and satisfies the inequalities

$$u_0'(1) < 0, \quad u_0'(-1) > 0.$$

B2. The derivative $f'(\cdot) : [-1, 1] \to \mathbb{R}$ is continuous and monotone nondecreasing. It satisfies the inequalities

$$2f'(1) + e^{2u_0'(1)} < e^{-2u_0'(1)}, \quad -2f'(-1) + e^{-2u_0'(-1)} < e^{2u_0'(-1)}.$$

3.2 Auxiliary Problems of Calculus of Variations

Consider the following two problems of Calculus of Variations over the set of all continuously differentiable functions $x(\cdot) : [0, T] \to \mathbb{R}$

$$I(x(\cdot)) = \int_0^{\bar{t}} H^*(x(\tau), \dot{x}(\tau)) d\tau \mapsto \max \tag{13}$$

$$x_1(0) = 1, \quad x_1(\bar{t}) = \bar{x}, \quad (\bar{t}, \bar{x}) \in G_+; \tag{14}$$

$$x_2(0) = -1, \quad x_2(\bar{t}) = \bar{x}, \quad (\bar{t}, \bar{x}) \in G_- \tag{15}$$

where

$$H^*(x(t), \dot{x}(t)) = \inf_{p \in R} [p\dot{x}(t) - H(x(t), p)]. \tag{16}$$

The following assertions are proven in $[4, 5]$, where conditions **B1-B2** are essential.

Theorem 2. *For any interior point $(\bar{t}, \bar{x}) \in G_+$ there exists a unique extremal $x = x(t)$ of the problem (13),(14),(16). The extremal coinsides with a state characteristic $x(\cdot; 0, 1, p_0)$ satisfying the initial conditions $x(0) = 1$, $p(0) = p_0 \in (-\infty, u_0'(1))$ where initial value p_0 can be defined uniquely from the condition $x(\bar{t}) = \bar{x}$. The functional (13) attains its strong maximum at this extremal.*

Theorem 3. *For any interior point $(\bar{t}, \bar{x}) \in G_-$ there exists a unique extremal $x = x(t)$ of the problem (13),(15),(16). The extremal coinsides with a state characteristic $x(\cdot; 0, -1, p_0)$ satisfying the initial conditions $x(0) = -1$, $p(0) = p_0 \in (u_0'(-1), \infty)$ where initial value p_0 can be defined uniquely from the condition $x(\bar{t}) = \bar{x}$. The functional (13) attains its strong maximum at this extremal.*

Theorem 4. *For any boundary point $(\bar{t}, 1), 0 < \bar{t} \leq T$ in G_+, the maximum of functional (13), (16) is attained at a state characteristic $x(\cdot; 0, 1, p_0)$, such that the characteristics $x(\cdot; 0, 1, p_0)$, $p(\cdot; 0, 1, p_0)$ are nonextendable from the interval $[0, t^*(p_0) = \bar{t})$ to the right. The maximum of functional (13), (16) is equal to $I(x(\cdot; 0, 1, p_0)) = (f(1) - 1)\bar{t}$.*

Theorem 5. *For any boundary point $(\bar{t}, -1), 0 < \bar{t} \leq T$ in G_-, the maximum of the functional (13)-(16) is attained at a state characteristic $x(\cdot; 0, -1, p_0)$, such that characteristics $x(\cdot; 0, -1, p_0), p(\cdot; 0, -1, p_0)$ are nonextendable from the interval $[0, t^*(p_0) = \bar{t})$ to the right. The maximum of functional (13),(16) is equal to $I(x(\cdot; 0, -1, p_0)) = (f(-1) - 1)\bar{t}$.*

4   Construction of the generalized solution

The generalized solution of the problem (1)-(3) with the prescribed property (12) has the following form in G_0:

$$u(t,x) = \max_{x(t,y)=x} \left[\int_0^t p(\tau)H_p(x(\tau), p(\tau)) - H(x(\tau), p(\tau))d\tau + u_0(y) \right], \quad (17)$$

where $x(t) = x(t, y), \quad p(t) = p(t, y), \ t \geq 0$, are state and conjugate characteristics satisfied initial conditions

$$x(0, y) = y, \quad p(0, y) = \partial u_0(y)/\partial x, \quad y \in [-1, 1].$$

Let $(t_*, x_*) \in G_+$ and $x_* < 1$. We assign

$$u(t_*, x_*) = u_0(1) + \int_0^{t_*} \left[p(\tau)H_p(x(\tau), p(\tau)) - H(x(\tau), p(\tau)) \right] d\tau, \quad (18)$$

where $x(t) = x^+(t, p_0(t_*, x_*)), \ p(t) = p^+(t, p_0(t_*, x_*))$ is the solution of the problem of Calculus Variations (13),(14),(16).

For $x_* = 1, 0 \leq t_* \leq T$, we set

$$u(t_*, 1) = u_0(1) + (f(1) - 1)t_*. \quad (19)$$

Let $(t_*, x_*) \in G_-$ and $x_* > -1$. We assign

$$u(t_*, x_*) = u_0(-1) + \int_0^{t_*} \left[p(\tau)H_p(x(\tau), p(\tau)) - H(x(\tau), p(\tau)) \right] d\tau, \quad (20)$$

where $x(t) = x^-(t, p_0(t_*, x_*)), \ p(t) = p^-(t, p_0(t_*, x_*))$ is the solution of the problem of Calculus Variations (13),(15),(16).

For $x_* = -1, 0 \leq t_* \leq T$, we set

$$u(t_*, -1) = u_0(-1) + (f(-1) - 1)t_*. \quad (21)$$

So, we have defined function $u(\cdot)$ for all points from $\overline{\Pi}_T$ by relations (17)-(21). Following the Cauchy method of characteristics [2], one can show that $u(\cdot)$ is continuously differentiable at any interior point $(t, x) \in G_+ \cup G_-$, and the

gradient of $u(\cdot)$ is equal to $(-H(x, p(t)), p(t))$. Theorems 2-5 imply that $u(\cdot)$ is continuous in $\overline{\Pi}_T$, and inequalities (6)-(7) are valid. Below, in section 6.2, we will show that $D^- u(t, x) \cap \partial u(t, x) = \varnothing, \quad (t, x) \in \Gamma_T$. So, $u(\cdot)$ is a generalized solution of problem (1)-(3) in sense of Definition 1. It follows from (17) that $u(\cdot)$ satisfies the prescribed property (12).

5   Numerical example

Results of simulation for the input data $u_0(x) = -0.02x^2 + 0.001 \cos 2\pi x$, $f(\cdot) = -0.5x^2$ are presented in Fig. 2. One can easily check that these input data satisfy the conditions **B1**, **B2**.
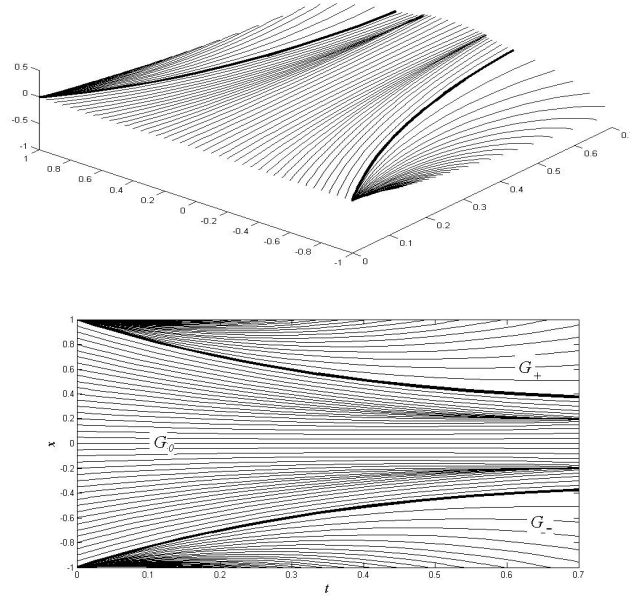
Fig. 2. The graph of the generalized solution and its projection on the (t, x)-plane for the input data $u_0(x) = -0.02x^2 + 0.001 \cos 2\pi x$, $f(x) = -0.5x^2$.

6   Comparison with Viscosity Solution

One can see that Definition 1 coincides with the definition of viscosity solution in the interior points of the region $\overline{\Pi}_T$. The difference between these definitions is evident at boundary points, namely, on the set Γ_T. In condition (8), the

inequality holds for such points (a, s) of the subdifferential $D^- u(t, x)$ which at the same time belong to the set $\partial u(t, x)$. In contrast to Definition 1, the notion of viscosity solution [10] for equation (1) on the set $\overline{\Pi}_T$ requires that this solution satisfies inequality (8) at the boundary points $(t, x) \in \Gamma_T$ for all $(a, s) \in D^- u(t, x)$.

6.1   On coercivity condition

Conditions ensuring existence and uniqueness for viscosity solutions on the compact domain were obtained in [10]. One of the key conditions for the existence of viscosity solutions (see [10, 12]) is the coercivity of the Hamiltonian:

$$H(x, p) \to +\infty \quad \text{as} \quad |p| \to \infty \tag{22}$$

It can be easily checked that the Hamiltonian (2) does not satisfy condition (22), for example, at $x = 1$ and $x = -1$. Therefore, the existence theorems for viscosity solutions in the sense of paper [10] cannot be used in the problem (1)-(3).

Moreover, the notion of generalized viscosity solution is inapplicable to the initial value problem (1)–(3) on the compact set $\overline{\Pi}_T$: If a viscosity solution would satisfy the condition $D^- u(t_*, x_*) \neq \varnothing$ at some point $(t_*, x_*) \in \Gamma_T$, then inequality (8) would not hold in this case. Indeed, let $0 \leq t_* \leq T$ and, for definiteness, $x_* = 1$. Let $(a, s) \in D^- u(t_*, x_*)$. One can use the above definition of subdifferential to get the following inclusion:

$$(a, s + k) \in D^- u(t_*, x_*) \quad \forall k \geq 0.$$

So, if condition (8) would hold then

$$a + H(1, s + k) = a - f(x) + 1 - e^{2(s+k)} \geq 0, \qquad \forall k \geq 0,$$

which is obviously unfair. Therefore, we use the intersection of the subdifferential with the set $\partial u(t, x)$ (see condition (8)) in Definition 1 of a continuous generalized solution to the initial value problem (1)–(3) on the compact set $\overline{\Pi}_T$.

6.2   Structure of subdifferentials on the border

Let's consider the structure of the sets $D^- u(t, x)$ and $\partial u(t, x)$ for the function $u(\cdot)$ defined by (17)-(20) if $(t, x) \in \Gamma_T$.

In the case $0 < t < T, \quad x = 1$, we have
$D^- u(t, x) = D^- u(t, 1) = \{(f(1) - 1, s) \mid s \in R, s \geq 0\}$,
$\partial u(t, x) = \partial u(t, 1) = \{(-H(1, -\infty), -\infty)\} = \{(f(1) - 1, -\infty)\}$.

In the case $0 < t < T, \quad x = -1$, we have
$D^- u(t, x) = D^- u(t, -1) = \{(f(-1) - 1, s) \mid s \in R, s \leq 0\}$,
$\partial u(t, x) = \partial u(t, -1) = \{(-H(-1, \infty), \infty)\} = \{(f(-1) - 1, \infty)\}$.

Thus, for generalized solution (17)-(20)

$$D^- u(t, x) \cap \partial u(t, x) = \varnothing, \quad (t, x) \in \Gamma_T.$$

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