Numerical Method for the Computation of Tangent Vectors to Hyperbolic Systems of Conservation Laws

Michael Herty and Benedetto Piccoli

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Key words: conservation laws, optimization, tangent vectors

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Institut für Geometrie und Praktische Mathematik
RWTH Aachen
Templergraben 55, D–52056 Aachen (Germany)
NUMERICAL METHOD FOR THE COMPUTATION OF TANGENT VECTORS TO HYPERBOLIC SYSTEMS OF CONSERVATION LAWS

MICHAEL HERTY AND BENEDETTO PICCOLI

ABSTRACT. We are interested in the development of a numerical method for solving optimal control problems governed by hyperbolic systems of conservation laws. The main difficulty of computing the derivative in the case of shock waves is resolved in the presented scheme. Our approach is based a combination of a relaxation approach in combination with a numerical scheme to resolve the evolution of the tangent vectors. Numerical results for optimal control problems are presented.

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1. Introduction

We are concerned with a numerical approach to optimization problems governed by (systems of) hyperbolic partial differential equations in a single spatial dimension. As a prototype, we consider a tracking type problem for a terminal state $y_d$ prescribed at some given time $t = T$ and the control acts as initial condition $u_0$. A mathematical formulation of this optimal control problem is reduced to minimizing a functional, and, for instance, it can be stated as follows:

\[(1.1) \min_{u_0} J(y(\cdot, T); y_d(\cdot)),\]

where $J$ is the given cost functional and $y \in \mathbb{R}^n$ is the unique entropy solution of the nonlinear conservation law

\[(1.2) \quad \begin{array}{l}
y_t + f(y)_x = 0, \quad x \in \mathbb{R}, \quad t > 0, \\
y(0,x) = u_0(x), \quad x \in \mathbb{R}.
\end{array}\]

There has been tremendous progress in both analytical and numerical studies of problems of type (1.1), (1.2), see, e.g., [1, 2, 3, 7, 26, 11, 8, 12, 18, 23, 28, 27, 19, 17, 21]. Its solution relies on the property of the evolution operator $S_t : u_0(\cdot) \rightarrow y(\cdot, t) = S_t u_0(\cdot)$ for (1.2). It is known that the semi-group $S_t$ generated by a nonlinear hyperbolic conservation law is generically nondifferentiable in $L^1$ even in the scalar one-dimensional (1-D) case (see, e.g., [11, Example 1]). A calculus for the first-order variations of $S_t u_0$ with respect to $u_0$ has been established in [11, Theorems 2.2 and 2.3] for general 1-D systems of conservation laws with a piecewise Lipschitz continuous $u_0$ that contains finitely many discontinuities. Therein, the concept of generalized first order tangent vectors has
been introduced to characterize the evolution of variations with respect to \(u_0\), see [11, equations (2.16)–(2.18)]. It has been further extended in [10] to establish continuous dependence of \(S_t\) on the initial data \(u_0\). This result has been extended to BV initial data in [7, 3] and lead to the introduction of a differential structure for \(u_0 \rightarrow S_t u_0\), called shift-differentiability, see e.g. [3, Definition 5.1]. Further extensions have also been discussed for example [16]. Related to that equations for the generalized cotangent vectors have been introduced for 1-D systems in [9, Proposition 4]. These equations (also called adjoint equations) consists of a nonconservative transport equation [9, equation (4.2)] and an ordinary differential equation [9, equations (4.3)–(4.5)] for the tangent vector and shift in the positions of possible shocks in \(y(x,t)\), respectively. Necessary conditions for a general optimal control problem have been established in [9, Theorem 1]. However, this result was obtained using strong assumptions on \(u_0\) (see [9, Remark 4] and [3, Example 5.5]), which in the 1-D scalar case can be relaxed as shown for example in [28, 12]. We note that the nonconservative transport part of the adjoint equation has been intensively studied also independently from the optimal control context. In the scalar case we refer to [28, 5, 6, 25] for a notion of solutions and properties of solutions to those equations. Analytical results for optimal control problems in the case of a scalar hyperbolic conservation law with a convex flux have also been developed using a different approach in [28]. The relation to the weak formulation has been discussed in [2] in the case of Burger’s equation.

Numerical methods for the optimal control problems have been discussed in [1, 19]. In [18], the adjoint equation has been discretized using a Lax-Friedrichs-type scheme, obtained by including conditions along shocks and modifying the Lax-Friedrichs numerical viscosity. Convergence of the modified Lax-Friedrichs scheme has been rigorously proved in the case of a smooth convex flux function. Convergence results have also been obtained in [28] for the class of schemes satisfying the one-sided Lipschitz condition (OSLC) and in [1] for implicit-explicit finite-volume methods. Other examples of finite volume methods and Lagrangian methods are given in [13, 22].

In [12], analytical and numerical results for the optimal control problem (1.1) coupled with the 1-D inviscid Burgers equation have been presented in the particular case of a least-square cost functional \(J\). Therein, existence of a minimizer \(u_0\) was proven, however, uniqueness could not be obtained for discontinuous functions \(y\). This result was also extended to the discretized optimization problem provided that the numerical schemes satisfy either the OSLC or discrete Oleinik’s entropy condition. Furthermore, convergence of numerical schemes was investigated in the case of convex flux functions and with a–priori known shock positions, and numerical resolution of the adjoint equations in both the smooth and non–smooth cases was studied. In [20] perturbations of initial data are studied using an additional spatial dimension. Numerical results as well as a formalism to derive the linearized equations have been presented therein. In the scalar case of a production model coupled to ordinary differential equations has been studied in [15]. Therein, convergence of the wave–front tracking approximation to the tangent vector equation is proven.

We contribute to the discussion by introducing a novel scheme which allows to include the arising discontinuities in an optimization framework and without an a–priori assumption on the location of the discontinuities. This is possible and computationally
efficient under three basic assumptions: first, we only compute derivatives with respect to piecewise constant controls \( u_0 \); second, the system (1.2) is not solved directly, but an \( \epsilon \)-relaxation approximation (2.4) is solved instead and last, we compute the exact derivative for the \( \epsilon \)-approximation of the system (2.4) using tangent vectors. The number of discontinuities in \( u_0 \) may herein be as large as \( \frac{1}{\Delta x} \), where \( \Delta x \) is the spatial width of the numerical grid. The overall algorithm requires the solution of two additional hyperbolic partial differential equations. The motivation and theoretical investigations are presented in section 2 and numerical results in section 3.

2. Motivation and theoretical results

In order to derive a numerical scheme we consider the relaxation approximation [24] to (1.2). For simplicity we consider only the Jin–Xin relaxation in the case \( n = 1 \) and on the full real line \( x \in \mathbb{R} \). Then, the hyperbolic relaxation for

(2.3) \[ y_t^{(1)} + f(y^{(1)})_x = 0, \quad y^{(1)}(0, x) = u_0(x), \]

is given by

(2.4) \[ y_t + \begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix} y_x = \begin{pmatrix} 0 \\ \frac{1}{\epsilon} (f(y^{(1)}) - y^2) \end{pmatrix} \]

and by the initial data

(2.5) \[ y^{(1)}(0, x) = u_0(x), \quad y^{(2)}(0, x) = f(u_0(x)). \]

We assume that the value \( a^2 \) fulfills the sub characteristic condition

(2.6) \[ a^2 - f'(y^{(1)})^2 \geq 0 \quad \forall y^{(1)}. \]

For positive \( \epsilon \) it is known that a solution \( y \) yields an approximation to (1.2) in the following sense. For \( \epsilon \) sufficiently small we have up to second order in \( \epsilon \)

\[ y_t^{(1)} + f(y^{(1)})_x = \epsilon \left( a^2 - f'(y^{(1)})^2 \right) y_x^{(1)}. \]

Formally we obtain the original conservation law for \( y^{(1)} \) in the limit \( \epsilon = 0 \). We refer to [4] for a detailed analysis. For \( \epsilon > 0 \) the method is known as a relaxing scheme. The main advantage of (2.4) over (1.2) is the linear transport which greatly simplifies the computation of associated tangent vectors (in particular the numerical resolution of the finite dimensional component is trivial for (2.4)).

In the following we will therefore discuss the optimization problem (1.1) with respect to (2.4). Still, the numerical computation of tangent vectors in general poses severe challenges addressed below. Therefore, we further simplify by only considering piecewise constant controls \( u_0 \). In the following \( TV(\cdot) \) denotes the total variation.

Given some \( C > 0 \), we consider problem 1.1 subject to (2.4) and (2.5) for controls \( u_0 \in \mathcal{U} \).

**Definition 2.1.** We indicate by \( \mathcal{U} := \{ u : \mathbb{R} \rightarrow \mathbb{R} : u \text{ measurable, } TV(u) \leq C, u \text{ piecewise constant } \} \) the set of admissible controls. For every \( u \in \mathcal{U} \) we indicate by \( x_k = x_k(u), k = 1, \ldots, N(u) \) the points of discontinuity of \( u \).
For \( y_d \in L^1(\mathbb{R}) \), some \( T > 0 \) and a bounded interval \( I \subset \mathbb{R} \) we consider as a prototype example an unregularized cost functional of tracking type

\[
J(y(\cdot, \cdot), y_d(\cdot)) = \int \chi_I(x) (y(T, x) - y_d(x))^2 \, dx.
\]

(2.7)

We now introduce the notion of tangent vectors, see [11] and [10]. In (2.4) we assume \( \epsilon > 0 \) fixed and \( f \in C^4(\mathbb{R}) \) and \( a^2 \) fulfills the subcharacteristic condition. For a function \( u \in U \) a generalized tangent vector consists of two components \((v, \xi)\) where \( v \in L^1(\mathbb{R}) \) describes the \( L^1 \) infinitesimal displacement and \( \xi \in \mathbb{R}^{N(u)} \) describes the infinitesimal displacement of \( N(u) \) discontinuities. A distance on the space of tangent vectors \( T_u := L^1(\mathbb{R}; \mathbb{R}^n) \times \mathbb{R}^{N(u)} \) is given by

\[
\| (v, \xi) \| := \|v\|_{L^1} + \sum_{i=1}^{N(u)} |\Delta_i u| \ |\xi_i|
\]

(2.8)

where \( \Delta_i u = u(x_i+) - u(x_i-) \) denotes the jump in \( u \). The distance depends \( u \) through the number of points of discontinuities. Tangent vectors may be used to describe variations of \( u \), see Figure 2.1. For \( \delta > 0 \) an infinitesimal displacement \( u_\delta \) of \( u \) is given by

\[
u_\delta = u + \delta v + \sum_{i=1}^{N(u)} \chi_{[x_i+, \delta \xi_i, x_i+, x_{i+1}+\delta \xi_{i+1}]}(x) u(x_i+).
\]

(2.9)

\( u_\delta \) is obtained from \( u \) by shifting the function values by \( \delta v \) and the \( i \)th discontinuities by \( \delta \xi_i \). For \( \delta \) sufficiently small \( u_\delta \) has the same number of discontinuities as \( u \). Note that if \( \xi \neq 0 \) then the function \( \delta \to u_\delta \) is not differentiable in \( L^1 \) as the ratio \( \frac{u_\delta + \delta v - u_\delta}{\delta} \) does not

Figure 2.1. Construction of a tangent vector \((\xi_\alpha, v_\theta)\) to \( u_\theta \) having a discontinuity at \( x_\alpha^\theta \)
converge to any limit in $L^1$ for $h \to 0$. However, the previous limit remains meaningful if interpreted as a weak limit in a space of measures with a singular point mass located at $x_1$ and having magnitude $|\Delta_i u \xi_i|$. Therefore, in [11] a class of variations $\delta \to u_\delta$ is described up to first order by (generalized) tangent vectors $(v, \xi)$.

We introduce some notation and definitions (see [11, 10]) already in view of the special system (2.4). Let $u \in L^1(\mathbb{R}; \mathbb{R}^n)$ be a piecewise Lipschitz continuous function with $N$ jumps. Consider $\Sigma_u$ the family of all continuous paths $\gamma : [0, \delta_0] \to L_{loc}$ with $\gamma(0) = u$ with $\delta_0$ possibly depending on $\gamma$.

**Definition 2.2.** [11, Definition 1.3] The space of generalized tangent vectors to a piecewise Lipschitz function $u$ with jumps at the points $x_1 < x_2 \cdots < x_N$ is $T_u := L^1(\mathbb{R}; \mathbb{R}^n) \times \mathbb{R}^N$. A continuous path $\gamma \in \Sigma_u$ generates a tangent vector $(v, \xi) \in T_u$ if

$$\lim_{\delta \to 0} \frac{1}{\delta} \|\gamma(\delta) - \bar{\gamma}(\delta)\|_{L^1} = 0$$

for

$$\bar{\gamma} := u + \delta v - \sum_{i, \xi_i > 0} \Delta_i u \chi_{[x_i, x_i + \delta \xi_i]} + \sum_{i, \xi_i < 0} \Delta_i u \chi_{[x_i + \delta \xi_i, x_i]}.$$ 

Let $u$ be a piecewise Lipschitz function with simple discontinuities [11, Definition 2]. Then, a path $\gamma \in \Sigma_u$ is a regular variation for $u$ if additionally all function $\gamma(\delta) = u_\delta$ are piecewise Lipschitz with simple discontinuities and the jumps $x_i^\delta$ depend continuously on $\delta$.

A regular variation $\gamma$ for $u$ generates a tangent vector $(v, \xi)$ by

$$\xi_i = \lim_{\delta \to 0} \frac{x_i^\delta - x_i}{\delta}, \quad \lim_{\delta \to 0} \int_a^b \left\| \frac{u(x_i^\delta + y) - u(x_i + y)}{\delta} - v(x_i + y) - \xi_i u_\delta(x_i + y) \right\| dy = 0$$

whenever $[x_i + a, x_i + b]$ does not contain any other point of discontinuity of $u$ except $x_i$. Further, the length of a regular path $\gamma$ can be computed by (2.8). We now consider the initial data $u_0$ and a regular variation generating the tangent vector $(v, \xi) \in T_u$. Under suitable regularity assumptions [11, Theorem 2.2] regular variations are locally preserved by the system (2.4) and linearized equations for the time evolution of the tangent vector $(v(t, \cdot), \xi(t))$ can be derived. We have:

**Lemma 2.1.** [11, Theorem 2.2] Let $y(t, \cdot)$ be a piecewise Lipschitz continuous solution to (2.4) and initial data (2.5) $y(0, \cdot) = \bar{y}$ piecewise Lipschitz with $N$ simple discontinuities. Let $(\bar{v}, \bar{\xi}) \in T_{\bar{y}}$ be a tangent vector to $\bar{y}$ generated by the regular variation $\delta \to \bar{y}_\delta$. Let $y_\delta(t, x)$ be the solution to (2.4) and initial data (2.5) $y_0(0, x) = y_\delta(\cdot)$. Then, there exists a time $t_0 > 0$ such that the path $\delta \to y_\delta(t, \cdot)$ is a regular variation of $y(t, \cdot)$ generating the tangent vector $(v(t), \xi(t)) \in T_{y(t)}$ and $(v, \xi)$ is the unique broad solution to

$$v(0, \cdot) = \bar{v}(\cdot), v_t + \begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix} v_x = \frac{1}{\epsilon} \begin{pmatrix} 0 \\ f'(y^{(1)}) y^{(1)} - v^{(2)} \end{pmatrix},$$

where $v = (v^{(1)}, v^{(2)})$ and outside of the discontinuities of $y$. For $i = 1, \ldots, N$ we have

$$\xi_i(t) = \bar{\xi}_i$$

and

$$l_j \cdot (\Delta_i v + \Delta_i y_x \xi_i) = 0 \quad j \neq k.$$
along each line of discontinuity $x_i(t)$ where $u$ has a discontinuity in the $k$th characteristic family. Here, $\Delta_j v = v(x_i(t)+, t) - v(x_i(t)-, t)$ and $l_j$ denotes the $j$th left eigenvector of the matrix $\begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix}$.

Some remarks are in order. According to [11, Definition 2] $\bar{u} \in \mathcal{U}$ is piecewise Lipschitz with simple discontinuities. The equations (2.11) and (2.12) are particularly simple due to the linear transport in the hyperbolic relaxation. In particular, the equation for $\xi_i$ is solved without any effort. Further, if we diagonalize (2.4) first and then apply the tangent vector calculus, the second equation (2.12) simplifies and we come back to this point later in the numerical scheme. It is important to note that in the previous result it is assumed that all variations $u_k$ possesses the same number of discontinuities which in the case of problem (1.1) is unknown a priori.

Tangent vectors and their property (2.10) can be used to compute the derivative of the cost functional (2.7).

**Lemma 2.2.** Assume the assertions of Lemma 2.1 hold true and let $J$ be given by (2.7) and assume $I$ is sufficiently large. Then, the variation of $J$ with respect to initial data $y(0, x) = (u_0(x), f(u_0(x)))$ is given by

$$\nabla_{u_0} J(y, y_d) = 2 \int \chi_T(x) \left( y(1)(T, x) - y_d(x) \right) v(1)(T, x) dx +$$

$$\sum_{i=1}^{N(u_0)} \left( \left( y(1)(T, x_i+) - y_d(x_i+) \right) + \left( y(1)(T, x_i-) - y_d(x_i-) \right) \right) \Delta_i y(1)(T, \cdot) \xi_i(T).$$

The proof is similar to [15, Proposition 1] and omitted.

Lemma 2.2 and equation (2.9) already suggests a numerical method for solving (1.1) with cost (2.7). Given some control $u_0$ and a stepsize $\rho > 0$ we obtain a new control $\bar{u}_0$ corresponding to smaller value of the cost functional $J$ by the following variation

$$\bar{u}_0(x) = u_0(x) - \rho v(0, x) - \sum_{i=1}^{N(u_0)} \chi(x_{i+1}, x_{i+1} + \rho \xi_i(0)) (x) u_0(x_{i+1})$$

where $v(0, x)$ is the solution at time $t = 0$ to (2.11) for terminal data

$$v(1)(T, x) = \left( y(1)(T, x) - y_d(x) \right), \quad v(2)(T, x) = 0,$$

and $\xi_i(0)$ the solution to (2.12) with terminal data

$$\xi_i(T) = \left( \left( y(1)(T, x_i+) - y_d(x_i+) \right) + \left( y(1)(T, x_i-) - y_d(x_i-) \right) \right) \Delta_i y(1)(T).$$

Obviously, the given choice for $(v(T, x), \xi(T))$ yields $J(\bar{u}_0) < J(u_0)$. Note that this requires to solve (2.11) backwards in time and to fulfill (2.12). The previous computations motivate a numerical scheme for approximately solving (1.1), (2.7) and (2.4).

Before stating the full discrete algorithm we reformulate and comment on some parts of the method. The system (2.4) is diagonalisable with eigenvalues $\lambda_{1,2} = \pm a$ and characteristic variables

$$\eta^{(1)} = y^{(2)} + ay^{(1)} \quad \text{and} \quad \eta^{(1)} = y^{(2)} - ay^{(1)}.$$
Also, in view of condition (2.12) it is numerically advantageous to consider the minimization problem for $J$ in characteristic variables $\eta = (\eta^{(1)}, \eta^{(2)})$. Furthermore, in view of (2.14) equation (2.11) will be solved backwards in time for given terminal data $v(T, x)$. We obtain for $\tilde{v}(t, x) = v(T - t, x)$ the system

$$
\tilde{v}(0, \cdot) = v(T, \cdot), \tilde{v}_t - \begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix} \tilde{v}_x = \frac{1}{\epsilon} \left( \tilde{v}^{(2)}(T) - f'(y^{(1)}(T - t, \cdot))\tilde{v}^{(1)}(t) \right)
$$

and eigenvalues $\lambda_{1,2} = \mp a$ and corresponding characteristic variables

$$
\varphi^{(1)} = \tilde{v}^{(2)} + a\tilde{v}^{(1)} \text{ and } \varphi^{(2)} = \tilde{v}^{(2)} - a\tilde{v}^{(1)}.
$$

Let $I = [0, 1]$, $T > 0$, $y_0$ and $\epsilon > 0$ be given. The cost functional $J$ is given by (2.7). We discuss the numerical discretization of problem (2.19) using a first-order finite volume scheme with periodic boundary conditions. Note that we leave (for the moment) both components of the initial data $y_0$ subject to optimization. For $\epsilon$ sufficiently small a solution to (2.4) will due to the relaxation term satisfy $\|f(y^{(1)}_0) - y^{(2)}_0\| << 1$.

$$
(2.19) \quad \min_{y_0 = (y^{(1)}_0, y^{(2)}_0)} J \text{ sbj to (2.4), } y(0, x) = y_0(x), \ y(t, 1) = y(t, 0), \ x \in I, \ t \geq 0.
$$

Fix $a^2$ such that the subcharacteristic condition (2.6) is fulfilled. Introduce an equidistant spatial grid $\{x_i\}_{i=0}^{N_x}$ on $I$ with $\Delta x = x_{i+1} - x_i$. We choose $\Delta t$ such that the CFL condition holds, i.e., $\Delta t|a| = \Delta x$, and denote by $t^n = \Delta t n$ for $n = 0, \ldots, N_t$. We write $x_{i+\frac{1}{2}} = x_i + \frac{\Delta x}{2}$ and for simplicity assume $x_{N_x} = 1$ and $t^{N_t} = T$. Also for notational convenience we denote by $x_{-\frac{1}{2}} = x_{N_x-\frac{1}{2}}$ and $x_{N_x+\frac{1}{2}} = x_{\frac{1}{2}}$. Let $\mathcal{T}^{-1} \in \mathbb{R}^{2 \times 2}$ be the transformation to characteristic variables (2.17), i.e.,

$$
\mathcal{T}^{-1} \begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix} \mathcal{T} = \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix}, \ \eta = \mathcal{T}^{-1}y.
$$

The cell average on $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ at time $t^n$ for any function $u(t, x)$ is denoted by $u^n_i = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u(t^n, x)dx$. As in [24] an operator splitting is used to discretize (2.4) and similarly for (2.11).

Then, a first–order Upwind discretization of problem (2.19) with an exact integration of the source term for the solution of (2.4) is given by (2.20) for $i = 0, \ldots, N_x$ and $n = 1, \ldots, N_t$.

$$
(2.20a) \quad y^0_i = (y_0)_i;
$$

$$
(2.20b) \quad \eta^{(1)}_i = (\mathcal{T}^{-1} y_{i-1}^{n-1})^{(1)}, \ \eta^{(2)}_0 = (\mathcal{T}^{-1} y_{N_x}^{n-1})^{(1)}, \ \eta^{(1)}_i = (\mathcal{T}^{-1} y_{i}^{n-1})^{(2)},
$$

$$
(2.20c) \quad \tilde{y}^{(1)}_i = (\mathcal{T} \eta^{(1)}_i)^{(1)}, \ \tilde{y}^{(2)}_i = \exp(-\frac{\Delta t}{\epsilon})((\mathcal{T} \eta^{(2)}_i)^{(2)} + (1 - \exp(-\frac{\Delta t}{\epsilon}))f(\tilde{y}^{(1)}_i)),
$$

$$
(2.20d) \quad \eta^{(2)}_i = (\mathcal{T}^{-1} \tilde{y}^{(2)}_{i+1})^{(2)}, \ \eta^{(2)}_{N_x} = (\mathcal{T}^{-1} y_0^{(2)}), \ \eta^{(1)}_i = (\mathcal{T}^{-1} y_i^{(1)}),
$$

$$
(2.20e) \quad y^n_i = \mathcal{T} \eta_i.
$$

The discretization (2.20) uses a different splitting compared to [24] which leads to more complicated update formulas above but will be advantageous later on. In the current splitting we do first transport in the first characteristic variable, then apply the source
term and finally transport the second characteristic variable. The transformation to characteristic variables \( \eta \) and the CFL condition allows to resolve the transport exactly.

As explained above instead of equation (2.11) we discretize equation (2.18) to solve for the variations \( \tilde{v} \). Similarly to (2.20), we transform (2.18) to characteristic variables \( \varphi \) and resolve the linear transport exactly. If the discretized initial data is denoted by \( \tilde{v}_i^0 \), then we obtain for \( i = 0, \ldots, N_x \) and \( n = 1, \ldots, N_t \);

\[
\begin{align*}
\varphi_i^{(2)} &= (T^{-1} \tilde{v}_{i-1}^{n-1})^{(2)}, \quad \varphi_0^{(2)} = (T^{-1} \tilde{v}_{N_x}^{n-1})^{(2)}, \quad \varphi_i^{(1)} = (T^{-1} \tilde{v}_i^{n-1})^{(1)} \\
\varphi_i^{(1)} &= (T \varphi_i)^{(1)}, \quad \varphi_i^{(2)} = \exp(\frac{\Delta t}{\epsilon})(T \varphi_i)^{(2)} + (1 - \exp(\frac{\Delta t}{\epsilon}))f'(y_i^{(1)})(\tilde{v}_i^{n-1})^{(1)} \\
\varphi_i^{(1)} &= (T^{-1} \tilde{v}_{i+1})^{(1)}, \quad \varphi_i^{(1)} = (T^{-1} \tilde{v}_i^{(1)}), \quad \varphi_i^{(2)} = (T^{-1} \tilde{v}_i^{(2)}), \\
\tilde{v}_i^n &= T \varphi_i.
\end{align*}
\]

Next we turn to the discretization of equation (2.12). Within a first–order finite volume scheme a piecewise constant approximation is used to recover the solution, i.e.,

\[
y(t, x) \approx \sum_{i=0}^{N_x} \chi_{[\tau_n, \tau_{n+1}] \times [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]}(t, x)y_i^n,
\]

and similarly for the initial data. Therefore, numerically solving problem (2.19) naturally leads to consider piecewise constant controls \( y_0 \in \mathcal{U} \) having discontinuities at possibly each cell boundary \( x_{i+\frac{1}{2}} \). Therefore, a shift in the position of the discontinuity \( \xi_i \) may occur on each boundary \( x_{i+\frac{1}{2}} \). As long as the spatial resolution is not modified the number of discontinuities is however fixed being a crucial assumption in Theorem 2.1. Since the conservative \( y \) and characteristic variables \( \eta \) are equivalent upon the linear transformation \( T \) we optimize in (2.19) for \( \eta_0 = T^{-1}y_0 \) instead of \( y_0 \). Furthermore, we consider as admissible controls piecewise constant \( \eta_0^{(i)} \in \mathcal{U} \) for \( i = 1, 2 \) having each only \( N_x \) points of discontinuity which are of the following type: the first component \( \eta_0^{(1)} \) may have a discontinuity only at \( x_{i+\frac{1}{2}} \) for some odd value \( i \) and the second component \( \eta_0^{(2)} \) may only have a discontinuity at \( x_{i+\frac{1}{2}} \) for some even value \( i \). We therefore choose \( \eta_0^{(i)} \) according to (2.22) but such that

\[
(\eta_0^{(1)})_{2i} = (\eta_0^{(1)})_{2i+1}, \quad (\eta_0^{(2)})_{2i-1} = (\eta_0^{(2)})_{2i}, \quad i = 0, \ldots, \frac{N_x}{2}.
\]

For fixed \( N_x \) the set of all admissible controls \( \mathcal{U}_{ad} \subset \mathcal{U} \) consists of all piecewise constant functions \( \eta_0(x) \) given by

\[
\eta_0^{(j)}(x) = \sum_{i=0}^{N_x} \chi_{[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]}(x)\eta^{(j)}_{0,i}, \quad j = 1, 2,
\]

which additionally fulfill (2.23). Note that for \( N_x \) sufficiently large the condition (2.23) still allows to approximate any piecewise constant function.

When computing the tangent vector to \( \eta_0 \) we now have the \( L^1 \)–variations \( \varphi_0 \) and the variation in the position of the discontinuities \( \xi_i \). We denote by \( \xi_i, \quad i = 0, \ldots, N_x \) the variation of the discontinuity at position \( x_{i+\frac{1}{2}} \). Hence, \( \xi_i \) for \( i \) odd (even) is the
variation of the discontinuity in the first (second) component of \( \eta_0 \). The discretization (2.20) introduces a splitting of the dynamics (2.4) and may be written for \( t \in [t^n, t^{n+1}] \) and in characteristic variables as follows

\[
\begin{align*}
\partial_t \eta^{(1)} + a \partial_x \eta^{(1)} &= 0, \\
\partial_t \eta^{(2)} &= S(\eta^{(1)}, \eta^{(2)}), \\
\partial_t \eta^{(2)} - a \partial_x \eta^{(2)} &= 0, \\
\partial_t \eta^{(1)} &= 0.
\end{align*}
\]

Due to the discretization of the linear transport term the initial discontinuities in \( \eta_0 \) propagate with speed \( \pm a \) and therefore during one time step \( \Delta t \) they are again located at the cell interfaces \( x_{i+\frac{1}{2}} \). Further within \( \Delta t \) the splitting does not introduce additional discontinuities due to the action of the source term \( S(\eta^{(1)}, \eta^{(2)}) = \frac{1}{2} \left( f((T\eta)^{(1)}) - (T\eta)^{(2)} \right) \) provided that \( \eta_0 \) fulfills (2.23). Note that the same holds true for \( \varphi \) provided that \( \varphi^0 = T^{-1} \tilde{v}_0^0 \) fulfills (2.23). The position of the discontinuity in the first component and second component of \( \eta \) at time \( t^n \) are given by

\[
x_{2i-1}(t^n) = x_{2i-1}(0) + a t^n, \\ x_{2i}(t^n) = x_{2i}(0) - a t^n, \quad i = 0, \ldots, N_x,
\]

where \( x_j(0) = x_{j+\frac{1}{2}} \) and where the discontinuities exiting at \( x = 1 \) (or \( x = 0 \)) enter again at \( x = 0 \) (\( x = 1 \)). We turn to the discussion of the second part of equation (2.12). In characteristic variables \( \ell_j \) is the \( j \)th unit vector. Let \( i \) be odd and \( \eta \) be computed by the previous splitting. Then, we observe \( \Delta \eta^{(2)} = 0 \) since \( \eta^{(2)} \) is constant across the position of the discontinuity in the first family \( x_{2i-1}(t^n) \). Provided we discretize \( J \) such that \( \varphi_j^0 := T^{-1} \tilde{v}_j^0, \ j = 0, \ldots, N_x \) in (2.21) also fulfills (2.23), then, we have \( \Delta \eta \varphi^{(2)} = 0 \). The same is true for \( i \) even and, therefore, the second part of equation (2.12) is fulfilled trivially within the previous scheme.

Finally, we consider \( J(\eta, y_d) = J(Ty, y_d) \) and obtain the gradient of \( J \) in terms of the characteristic variables \( \eta \) and its associated tangent vectors \( (\phi, \xi) \) as

\[
\nabla_{\eta_0} J(\eta, y_d) = \frac{1}{2} \int \chi_i(x) \left( \frac{\eta^{(1)}(T, x) - \eta^{(2)}(T, x)}{2a} - y_d(x) \right) \phi^{(1)}(T, x) dx + \\
- \frac{1}{2} \int \chi_i(x) \left( \frac{\eta^{(1)}(T, x) - \eta^{(2)}(T, x)}{2a} - y_d(x) \right) \phi^{(2)}(T, x) dx + \\
\frac{1}{2} \sum_{i=1}^{N_{(u)}} \left\{ \left( \frac{\eta^{(1)}(T, x_i) - \eta^{(2)}(T, x_i)}{2a} - y_d(x_i) \right) \right\} \xi_i(T) \left( \Delta \eta^{(1)}(T, \cdot) - \Delta \eta^{(2)}(T, \cdot) \right).
\]
Let $\varphi(t, x) = \phi(T - t, x)$. Then, similarly to (2.14) we may use (2.25) to determine a descent direction for $J$ by the following discretization for $i = 0, \ldots, N_x$,

\begin{align}
(2.29a) & \quad \varphi_{2i}^{(1),0} = \frac{\eta_{2i}^{(1), N_t} - \eta_{2i}^{(2), N_t}}{2a} - (yd)_{2i}, \quad \varphi_{2i+1}^{(1),0} = \varphi_{2i}^{(1),0}, \\
(2.29b) & \quad \varphi_{2i-1}^{(2),0} = -\left(\eta_{2i-1}^{(1), N_t} - \eta_{2i-1}^{(2), N_t}\right) - (yd)_{2i-1}, \quad \varphi_{2i}^{(2),0} = \varphi_{2i-1}^{(2),0}, \\
(2.29c) & \quad \xi_{2i} = -\frac{1}{2a}\left(\bar{\Delta}_{2i-1}(\mathcal{T}\varphi^{N_t})^{(1)} - \bar{\Delta}_{2i-1}yd\right)\Delta_{2i-1}\varphi^{(1), N_t}, \\
(2.29d) & \quad \xi_{2i} = -\frac{1}{2a}\left(\bar{\Delta}_{2i}(\mathcal{T}\varphi^{N_t})^{(1)} - \bar{\Delta}_{2i}yd\right)\Delta_{2i}\varphi^{(2), N_t},
\end{align}

where $\Delta_j w(\cdot) = w(x_{j+1}) - w(x_j)$ and $\bar{\Delta}_j w(\cdot) = \frac{1}{2}(w(x_{j+1}) + w(x_j))$.

Finally, we discretize (2.14) such that $\mathcal{T}^{-1}\eta_0 \in \mathcal{U}$ and fulfills (2.23). The tangent vector $(\varphi(T, \cdot), \xi(T))$ to $\eta_0(x)$ describes the $L^1$-variation as well as the variation of the position of discontinuities, respectively. Given a current control $\eta_i^0$ we obtain a new control $\eta_i^0$ for $i = 0, \ldots, N_x$, and $j \in \{0, \ldots, N_x\}$ odd, and $k \in \{0, \ldots, N_x\}$ even by equation (2.30).

\begin{align}
(2.30a) & \quad \Xi_{j-1}^1 = \Xi_j^1 = \min\{(-\bar{\xi}_j)^+, \Delta x\} \eta_{j-1}^{(1),0} + \max\{\bar{\xi}_j^{+} - \Delta x, 0\} \eta_{j-1}^{(1),0}, \\
(2.30b) & \quad (\Delta x - \min\{(-\bar{\xi}_j)^+, \Delta x\} - \max\{\bar{\xi}_j^{+} - \Delta x, 0\}) \eta_{j}^{(1),0}, \\
(2.30c) & \quad \Xi_{k-1}^2 = \Xi_k^2 = \min\{(-\bar{\xi}_k)^+, \Delta x\} \eta_{k+1}^{(2),0} + \max\{\bar{\xi}_k^{+} - \Delta x, 0\} \eta_{k-1}^{(2),0}, \\
(2.30d) & \quad (\Delta x - \min\{(-\bar{\xi}_k)^+, \Delta x\} - \max\{\bar{\xi}_k^{+} - \Delta x, 0\}) \eta_{k}^{(2),0}, \\
(2.30e) & \quad \bar{\eta}_i^{(1),0} = \eta_i^{(1),0} - \varphi_i^{(1), N_t} - \frac{\Xi_i^1}{\Delta x}, \\
(2.30f) & \quad \bar{\eta}_i^{(2),0} = \eta_i^{(2),0} - \varphi_i^{(2), N_t} - \frac{\Xi_i^2}{\Delta x}.
\end{align}

Here, we denote by $x^+ = \max\{x, 0\}$ and by $\bar{\xi}_i = \mathcal{P}(\xi_i)$ where $\mathcal{P}$ is the projection on $[-2\Delta x, 2\Delta x]$. Note that equation (2.30) corresponds to a gradient step in the $L^1$-variation but a scaled gradient step in the variation of the shock position in order to prevent shock variations to interact. In (2.30) a piecewise constant reconstruction of $\bar{\eta}$ is computed where for example in the case of the first component the discontinuity at $x_{i+\frac{1}{2}}$ is moved by $\xi_i$ and at $x_{i-\frac{1}{2}}$ by $\xi_{i-2}$. Since $\varphi$ fulfills (2.23) this holds true for $\bar{\eta}$.

The previous computation leads to an iterative algorithm for numerically solving (2.19) or equivalently

$$
\min_{\eta_0 \in \mathcal{U}} J(\mathcal{T}\eta, y_d) \text{ subj to } y = \mathcal{T}\eta, (2.4), \eta(0, x) = \eta_0(x), \eta(t, 0) = \eta(t, 1) \text{ and } (2.23).
$$

**Algorithm**

1. Set terminal time $T > 0$, $a^2 \geq \max_{y(1)}(f'(y(1))^2$ and choose an equidistant spatial discretization with $N_x$ gridpoints. Choose $\Delta t = \frac{\Delta x}{a}$ and $k = 0$. Let $\eta_{0,i}^{k} = \ldots = \eta_{N_x,i}^{k} = \eta_i$. 

\[
\left( (\eta^{(1)}_0)_{k,i}, (\eta^{(2)}_0)_{k,i} \right) \text{ for } i = 0, \ldots, N_x, \text{ be an arbitrary initial control such that } \eta^k_0 \text{ fulfills } (2.23). \text{ Let } (y_d)_i \text{ be a discretization of the given function } y_d(\cdot).
\]

2. Solve equations (2.20) with \((y_0)_i := T \eta^k_{0,i}\) to obtain \(\eta^N_i = T^{-1} y^N_i\).

3. Set initial data \(\phi^0_i\) and shock variations \(\xi_i\) by equation (2.29) where \(x_i(t^N_i)\) are given by equation (2.24).

4. Solve equations (2.21) for initial data \(\tilde{v}^0_i := T \phi^0_i\) to obtain \(\phi^N_i = T^{-1} \tilde{v}^N_i\).

5. Update the current iterate \(\eta^k_{0,i}\) by setting \(\eta^{k+1}_0 := \tilde{\eta}^k_0\) obtained from equation (2.30) with \(\eta^k_0 := \eta^k_{0,i}\).

6. Provided that \(J(T \eta, y_d)\) is sufficiently small we terminate. Otherwise set \(k \rightarrow k + 1\) and continue with step (2).

3. Numerical results

We present numerical results using the previous calculus for two cases. The simplest possible application is the optimal control of a linear system (2.4) \textit{without} source term. Second, we present results on the optimal control for the relaxation system (2.4) for Burgers flux \(f(w) = \frac{1}{2} w^2\). All spatial grids are equidistant on \(I = [0, 1]\) and the temporal discretization is such that the CFL condition [14] is satisfied. We use periodic boundary conditions in all cases. The cost functional \(J\) is discretized using the trapezoidal rule. All initial controls are constant with \(\eta_0(x) = \left(\frac{1}{2}, \frac{1}{4}\right)\).

![Figure 3.2. Solution \(y(T = 1, x)^{(1)}\) (red circle) computed by discretization (2.20) with initial data \(y_0^{(1)}(x)\) (blue cross) and \(y_0^{(2)}(x) = f(y_0^{(1)}(x))\) on a grid with \(N_x = 1600\) points in space and \(\epsilon = 10^{-6}\).](image-url)
3.1. Grid convergence example. We consider the discretization (2.20) and initial data given by \( y^{(1)}_0 = \sin(2\pi x) \) and \( y^{(2)}_0 = f(y^{(1)}_0) \). We set \( a^2 = 1 \) and compute the solution to the proposed scheme (2.20) at time \( T = 1, \epsilon = 10^{-6} \) and for \( N_x = 1600 \) points in the domain \( I \). The initial data \( y^{(1)}_0 \) as well as the solution \( y^{(1)}(1, \cdot) \) are depicted in Figure 3.2. Table 3.1 shows the grid convergence behavior of the discretization (2.20) in both components. As expected we observe first-order convergence and remark that the applied modifications do not alter the properties of the original scheme proposed in [24].

| \( N_x \) | \( ||y^*(1, \cdot) - y^{(1)}_{N_x}(1, \cdot)||_2 \) | Rate | \( ||y^*(2, \cdot) - y^{(2)}_{N_x}(1, \cdot)||_2 \) | Rate |
|----------|---------------------------------|------|---------------------------------|------|
| 50       | 1.2126e-02 (0.0000e + 00)       |      | 1.5248e-03 (0.0000e + 00)       |      |
| 100      | 5.8062e-03 (1.0442e + 00)       |      | 5.3919e-04 (1.4139e + 00)       |      |
| 200      | 2.6396e-03 (1.0998e + 00)       |      | 1.3022e-04 (2.0704e + 00)       |      |
| 400      | 1.0128e-03 (1.3031e + 00)       |      | 3.3623e-05 (1.9364e + 00)       |      |

Table 3.1. Grid convergence of the discretization (2.20). \( y^* \) is a fine grid solution of (2.20) with \( N_x = 1600 \) points in space. \( y_{N_x} \) is the numerical solution on the grid given in first column of the table.

3.2. Optimal control of a linear system. We consider problem (3.31) with periodic boundary conditions on the domain \( x \in I, T = 0.35 \) and \( a^2 = \frac{3}{4} \).

\[
\min_{u_0} \int_0^1 \left( y^{(1)}(T, x) - y_d^{(1)}(x) \right) \, dx \quad \text{sbj to} \quad y_t + \begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix} y_x = 0, \quad y(0, x) = (u_0(x), f(u_0)).
\]

(3.31)

In the example we initialize the control similar to (2.5) and \( f(w) = \frac{1}{2} w^2 \). The desired state \( y_d \) is depicted in Figure 3.3 (along with the obtained optimized state).

The algorithm is started with constant control \( \eta_0 \) and stopped after at most 2000 steps of iteration. The iteration history is depicted in the right part of Figure 3.3. With the proposed method we observe convergence until the grid resolution is reached. The dependence on the spatial grid in Table 3.2. As expected we observe first-order convergence is observed.

We compare the obtained results also with the case when the shock variations \( \xi_i \) are not taken into account. Hence, we consider the same example as before and run the same algorithm but setting \( \Xi_j^i \equiv 0 \) for \( j = 1, 2 \) in equation (2.30). The dependence on the spatial grid in this situation is depicted in Table 3.3. Comparing with Table 3.2 we observe a deterioration in the convergence rate from \( \approx 1 \) when including the shock variations to \( \approx \frac{1}{2} \) for the cost functional and \( \approx \frac{3}{4} \) for state when neglecting the this contribution.
Figure 3.3. Desired state (red cross) and optimized state (blue circles) for the linear system with $N_x = 200$ grid points in space for both components $(y^{(1)}, y^{(2)})$ in the left part of the figure. Iteration history in log−scale for the cost. The spatial resolution of the scheme is $\Delta x = 5 \times 10^{-3}$ and $\log_{10}(\Delta x) \approx -2.3$.

Table 3.2. Convergence history for different spatial grids with $N_x$ equidistant grid points. Reported are the value of the cost functional $J$ after optimization, the $L^2$−norm difference of both components $(y^{(1)}, y^{(2)})$ for the initial data $y_0 = y(0, x)$ and the desired state $y_d$. The optimized solution is denoted by $y_*(t, x)$. 

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>$J$</th>
<th>Rate</th>
<th>$|y_0^{(1)} - y_*^{(1)}|_2$</th>
<th>Rate</th>
<th>$|y_0^{(2)} - y_*^{(2)}|_2$</th>
<th>Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>$4.6936 e - 03$</td>
<td>(0.00)</td>
<td>$5.5364 e - 03$</td>
<td>(0.00)</td>
<td>$6.9206 e - 03$</td>
<td>(0.00)</td>
</tr>
<tr>
<td>100</td>
<td>$2.5878 e - 03$</td>
<td>(0.91)</td>
<td>$2.8922 e - 03$</td>
<td>(0.96)</td>
<td>$3.6152 e - 03$</td>
<td>(0.96)</td>
</tr>
<tr>
<td>200</td>
<td>$1.3510 e - 03$</td>
<td>(0.96)</td>
<td>$1.4739 e - 03$</td>
<td>(0.98)</td>
<td>$1.8424 e - 03$</td>
<td>(0.98)</td>
</tr>
<tr>
<td>400</td>
<td>$9.9964 e - 04$</td>
<td>(0.68)</td>
<td>$8.2176 e - 04$</td>
<td>(0.90)</td>
<td>$1.2031 e - 03$</td>
<td>(0.77)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>$|y_d^{(1)} - y_*^{(1)}|_2$</th>
<th>Rate</th>
<th>$|y_d^{(2)} - y_*^{(2)}|_2$</th>
<th>Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>$5.5364 e - 03$</td>
<td>(0.00)</td>
<td>$6.9206 e - 03$</td>
<td>(0.00)</td>
</tr>
<tr>
<td>100</td>
<td>$2.8922 e - 03$</td>
<td>(0.96)</td>
<td>$3.6152 e - 03$</td>
<td>(0.96)</td>
</tr>
<tr>
<td>200</td>
<td>$1.4739 e - 03$</td>
<td>(0.98)</td>
<td>$1.8424 e - 03$</td>
<td>(0.98)</td>
</tr>
<tr>
<td>400</td>
<td>$7.5945 e - 04$</td>
<td>(0.97)</td>
<td>$1.2666 e - 03$</td>
<td>(0.73)</td>
</tr>
</tbody>
</table>
Table 3.3. Convergence history for different spatial grids with $N_x$ equidistant grid points neglecting the effect of the shock variations $\xi_i$ on the optimal control. As in Table 3.2 we report the value of the cost functional $J$ after optimization, the $L^2$-norm difference of both components $(y^{(1)}, y^{(2)})$ for the initial data $y_0 = y(0, x)$ and the desired state $y_d$. The optimized solution is denoted by $y_*(t, x)$.
3.3. Optimal control of the relaxation approximation to Burgers Equation.
We consider problem (3.31) $T = 0.35$, $\epsilon = 10^{-4}$, $N_x = 400$ and $a = 5/4$. The desired state $y_d$ is the solution at time $T$ to (2.4) and (2.5) for $u_0(x) = \cos(2\pi x)$. The algorithm is started with constant control $\eta_0$ and stopped after the cost functional is below $10^{-4}$. We depict desired and optimized state in the original variables $y(T, \cdot)$ in Figure 3.4. The obtained optimized control $\eta_0^k$ and the function $u_0$ are depicted in Figure 3.4 and the iteration history in Figure 3.5.

![Figure 3.4](image1)

**Figure 3.4.** Desired state (red cross) and optimized state (blue circles) for the linear system with $N_x = 400$ grid points in space for the variable $y^{(1)}(T, x)$ in the left part of the figure and for $y^{(1)}(0, x)$ in the right part.

![Figure 3.5](image2)

**Figure 3.5.** Iteration history for the example of Figure 3.4 in log-scale for the value of the cost functional $J$. The stopping criteria is $J \leq 10^{-4}$ which is comparable with the spatial resolution of the scheme is $\Delta x = 2.5 \times 10^{-3}$.

We observe a good agreement in the recovered desired state $y_d$. The difference in the obtained control is due to the fact that the solution to (2.19) is not unique.

In Figure 3.6 and Figure 3.7 we present a similar example but with desired state $y_d$ obtained as solution to (2.4) and (2.5) for $u_0(x) = \chi_{[0.3,0.45]}(x)$. All other parameters are
as before. Similarly to the previous results we observe that there is no uniqueness in the control $u_0$ leading to $y_d$.

**Figure 3.6.** Desired state (red cross) and optimized state (blue circles) for the linear system with $N_x = 400$ grid points in space for the variable $y^{(1)}(T, x)$ in the left part of the figure and for $y^{(1)}(0, x)$ in the right part.

**Figure 3.7.** Iteration history for the example of Figure 3.4 in log-scale for the value of the cost functional $J$. The stopping criteria is $J \leq 10^{-4}$ which is comparable with the spatial resolution of the scheme is $\Delta x = 2.5 \times 10^{-3}$.

### 4. Summary

We present a numerical method for solving optimal control problems subject to the relaxation approximation to a scalar hyperbolic conservation law. Equations for the evolution of the corresponding tangent vector of the relaxation system are derived and a numerical discretization has been introduced. The tangent vector has been used to compute the analytical gradient of the reduced cost also in the presence of traveling discontinuities. A numerical discretization of the gradient has been implemented to solve some examples of linear and nonlinear optimal control problems. The computation of
the finite dimensional part of the tangent vector allows to obtain the expected order of convergence.

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References


