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A Variational Formulation for a Class of First Order PDE's

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ABSTRACT

This paper proves that a class of first order partial differential equations, which include scalar conservation laws with concave (or convex) equations of state as special cases, can be formulated as calculus of variations problems. Every well-posed problem of this type, no matter how complicated, even in multi-dimensions, is reduced to the determination of a tree of shortest paths in a relevant region of space-time where “cost” is predefined. Thus, problems of this type can be practically solved with fast network algorithms. The new formulation automatically identifies the unique, single-valued function, which is stable to perturbations in the input data. Therefore, an auxiliary “entropy” condition does not have to be introduced for the conservation law.

In traffic flow applications, where one-dimensional conservation laws are relevant, constraints to flow such as sets of moving bottlenecks can now be modeled as shortcuts in space-time. These shortcuts become an integral part of the network and affect the nature of the solution but not the complexity of the solution process. Boundary conditions can be naturally handled in the new formulation as constraints/shortcuts of this type.

1. INTRODUCTION

This paper is concerned with problems that are described by the following first order partial differential equation for an unknown function N of arguments t and $x = (x_1, x_2, \dots, x_n)$, usually associated with time and space:

$$N_t = Q(-N_x, t, x). \quad (1a)$$

The subscripts t and x denote partial derivatives, N_x is an n -tuple, and Q is a differentiable function which is concave in $-N_x$.¹ We will abbreviate N_t by q and $-N_x$ by k . Thus, (1a) will also be written as:

$$q = Q(k, t, x). \quad (1b)$$

In applications where $n = 1$, e.g., traffic flow, N can be interpreted as a cumulative count of items such as cars, fluid units, etc. over one-dimensional space, and the rate at which N changes with distance as the negative of the (scalar) item density, $k = -N_x$. The identity $N_{xt} = N_{tx}$ becomes

$$k_t + q_x = 0, \quad (2)$$

which is the well-known conservation equation in one space dimension. A second way of writing (2) in terms of the density alone is obtained by substituting (1b) for q in (2):

$$k_t + Q_k k_x + Q_x = 0. \quad (3)$$

Equation (3) is the differential form of a one-dimensional “conservation law.” Conservation laws have been extensively studied; see Lax (1973) and LeVeque (1992) for background.

Multidimensional versions of (1) arise with certain geophysics problems (see e.g., Luke, 1972) and the one-dimensional version with fluids such as automobile traffic (see e.g., Lighthill and Whitham, 1955, and Richards, 1956).

Newell (1993) has shown the considerable practical advantage of using (1) for solving traffic flow problems, instead of the conservation law form. Independently, he and Luke proposed that if N has been defined on a boundary surface $\mathbf{D}$, then the value of N at a point P is given by the rule:

$$N_P = \min \{B_{\mathcal{W}} + \Delta_{\mathcal{W}}; \quad \forall \mathcal{W} \in \mathbf{W} \cap \mathbf{P}_P\} \quad (4)$$

In this expression and elsewhere in this paper script letters such as $\mathcal{W}$ are reserved for space-time paths, $x(t)$, directed in the direction of increasing time with specific beginning and ending times. Boldfaced, $\mathbf{P}_P$

¹ The results in this paper can also be used with convex Q 's because if we use $N' = -N$ as the unknown then Q is transformed into a concave function.

is the set of all paths from $\mathbf{D}$ to P and $\mathbf{W}$ is the set of all directed wave paths emanating from $\mathbf{D}$. The symbol $B_{\mathcal{W}}$ is the N -value at the beginning of the path (a data point) and $\Delta_{\mathcal{W}}$ is the predicted change in N along the wave path with the method of characteristics. The following facts and definitions from the theory of partial differential equations are used in (4) and elsewhere in this paper; see e.g., Garabedian (1964) for more details.

(i) The solution of (1) is a surface in $n+2$ dimensional space formed by a family of “characteristic” curves whose coordinates (N, t, x) satisfy the following system of ordinary differential equations, which includes k and q as unknowns:

$$x' = Q_k ; \quad (5a)$$

$$N' = q - k \cdot Q_k ; \quad (5b)$$

$$q' = Q_t ; \quad (5c)$$

$$k' = -Q_x . \quad (5d)$$

Primes denote differentiation with respect to time, and the dot in (5b) the dot product. Note that x' , Q_k , k , k' and Q_x are n -tuples.

(ii) In applications we look for the set of characteristics that will be consistent with the values of N continuously specified along a surface, $\mathbf{D}$, in space-time; e.g., the plane $t = 0$. For physically well-posed problems there are unique values of q and k satisfying (1) along the boundary, and therefore there is a unique characteristic associated with each boundary point. The projections of these characteristics onto space-time are curves $x(t)$ that are called waves. A directed portion of any such curve, beginning at the boundary and ending at a specific point is a wave path, $\mathcal{W}$. The set of wave paths for a given problem is $\mathbf{W}$. For well-posed problems, the solution of (1) in terms of characteristics is unique. It can be found by integrating (5) for every point on the boundary. The change in N along a specific wave path is the quantity we had denoted $\Delta_{\mathcal{W}}$; note that this quantity only depends on the values of t , x , q and k (the data) at the root of the wave.

(iii) Finally, if a problem is physically well posed a wave should pass through every space-time point P in the solution domain. Thus, the set $\mathbf{W} \cap \mathbf{P}_P$ is not empty. There can be more than one wave reaching point P , however, so that in general the surface $N(t, x)$ obtained as outlined in (ii) is multi-valued.

Luke (1973) and Newell (1993) proposed the minimum operation in (4) as a way of selecting the unique and correct value for N at every point in space-time without proving it. It should be noted in this respect that a “correct”, i.e. physically meaningful, solution of the problem must have two additional properties besides single-valuedness: (i) continuity everywhere, although there can be “shocks” where the

derivatives of N are discontinuous, and (ii) stability, in the sense that perturbations to the boundary data are never amplified into the solution. (Stability implies uniqueness.)

Thus, to establish that (4) always provides physically meaningful results one should show that the solutions it identifies are continuous and stable. Newell (1993) pointed out that (4) produces continuous solutions since it is the lower envelope of a continuously varying family of smooth curves, and Luke (1973) took continuity for granted. While both references are correct, the idea needs some elaboration.² Newell and Luke, again, did not comment on stability. While one could argue that stability is obvious in view of the argument in footnote 2, it would seem desirable to see if it can be established more directly.

We do know from the theory of conservation laws that in the one-dimensional case with concave Q the stable solution is the only one satisfying an “entropy” condition, which essentially means that the value of N at each point is determined by a characteristic from the boundary. The proof of this result is rather lengthy (see Lax, 1973). Therefore, if we were to show that (4) satisfies the entropy condition (which it does) we would have shown that it is stable. We will take a different tack, however. We will instead show directly that (4) must be stable (for any n), in this way furnishing a different proof of the existence, uniqueness and stability of the solutions to (1) and (3).

While (4) represents a significant advance over previous methods to solve (1) or (3), it is still cumbersome for general problems because identifying the relevant set of paths $\mathbf{W} \cap \mathbf{P}_P$ is not easy, except in special cases. Both Luke and Newell successfully applied the minimum principle to homogeneous, time-independent problems where $Q(k, t, x) = Q(k)$ because in these instances the characteristics are straight lines; see (5). But application of the principle to general problems is tedious, as illustrated by the solutions of Lighthill and Whitham’s bottleneck problem in Newell (1999).

This paper will attempt to simplify matters. We will first prove that if Q is concave $\Delta_{\mathcal{W}}$ can be written as the integral over time of a function, $R(x', t, x)$, independently of the input data. To stress that $\Delta_{\mathcal{W}}$ is just a functional of $\mathcal{W}$, we will write it as $\Delta(\mathcal{W})$. This functional can be applied to any “valid” path, and not just waves. A path is valid if it is directed with increasing time, continuous, piecewise differentiable and such that x' is everywhere in the range of possible wave speeds. Then, we will show that (4) can be replaced by:

$$N_P = \min \{ B_{\mathcal{P}} + \Delta(\mathcal{P}) : \forall \mathcal{P} \in \mathbf{V} \cap \mathbf{P}_P \} \quad (6)$$

² We know that multi-values can only arise from $N(t, x)$ in an interval $(t, t + dt)$ in the neighborhood of a location where waves converge into the solution. Because Q is concave, this only happens where $N(t, x)$ is concave in x . Because $N(t, x)$ is concave, the lower envelope of its characteristics (and not the upper envelope) defines a continuous, concave surface for $N(t+dt, x)$. When Q is not concave then the lower envelope will in general be discontinuous.

where $\mathbf{V}$ is the set of all valid paths. Finally, we will then prove in a very simple way that the solutions produced by (6) and (4) are stable. Note that $\mathbf{V} \supset \mathbf{W}$. The significance of enlarging the set of paths is that $\mathbf{V} \cap \mathbf{P}_p$ is independent of the boundary data and it is convex. These properties, and the expression of $\Delta(\mathcal{W})$ as an integral functional independent of the input data, open the door to variational methods, which cannot be used with (4). More specifically, if we interpret $R(x', t, x)$ as a “cost” per unit time and $B_{\mathcal{P}}$ as a starting cost, we see that (6) is just the formulation of a least cost (shortest) path problem. Thus, even the most complicated problems can be treated in a simple way with (6). Section 2, below, proves (6) and Sec. 3 discusses its implications.

2. A VARIATIONAL PRINCIPLE

We consider a solution of (4), $N(t, x)$, which is a continuous solution of (1), and start by looking for the functional $\Delta(\mathcal{W})$.

Where N is differentiable it must satisfy (5a)-(5d). In connection with these equations, it will be convenient to abbreviate the n -tuple Q_k by u

$$u = Q_k(k, t, x), \quad (7)$$

and the scalar N' by r so that (5b) becomes,

$$r = q - k \cdot u. \quad (8)$$

This scalar, which denotes the rate at which N changes with time along the wave, will play an important role. [In traffic applications r is the rate at which cars overtake an observer moving with the wave.]

Since (1) holds where N is differentiable, q can be eliminated from (8) and r becomes:

$$r = Q(k, t, x) - k \cdot u, \text{ for any pair } (k, u) \text{ satisfying } u = Q_k(k, t, x). \quad (9)$$

We now show that k can also be eliminated from (9) when Q is concave. Then, the rate at which N changes along the wave becomes a function of u , t and x , alone; i.e.

$$r = R(u, t, x). \quad (10)$$

Note that R is an intrinsic property of Q and does not depend on the boundary data or the solution.

To prove (10) it suffices to show that if $k^{(1)} \neq k^{(2)}$ are such that $u^{(1)} = u^{(2)}$ then $r^{(1)} = r^{(2)}$ according to (9). Since a concave Q cannot protrude above its tangent plane at $k^{(1)}$ we can write $q^{(2)} \leq q^{(1)} + (k^{(2)} - k^{(1)}) \cdot u^{(1)}$, in accordance with (9), which in turn implies $r^{(2)} \leq r^{(1)}$ (since $u^{(2)} = u^{(1)}$). Conversely, since Q must also be below the tangent plane at $k^{(2)}$, we also find that $r^{(1)} \leq r^{(2)}$. Thus, $r^{(1)} = r^{(2)}$, as claimed.

The significance of this is that the quantity $\Delta_{\mathcal{W}}$ in (4) becomes the path integral:

$$\Delta_{\mathcal{W}} = \Delta(\mathcal{W}) = \int_{t_B}^{t_P} R(x', t, x) dt, \quad \text{if } \mathcal{W} \in \mathbf{W}, \quad (11)$$

where $x(t)$ is the trajectory of $\mathcal{W}$, and t_B and t_P are its beginning and ending times. Note that, given $x(t)$, (11) does not involve the boundary data or the solution. The expression is a functional that can be applied to any $\mathcal{P} \in \mathbf{V}$.

By definition, when $\Delta(\mathcal{W})$ is applied to one of the waves that minimize (4) it gives the actual change in N ; i.e.:

$$\Delta(\mathcal{W}^*) = N_P - B_{\mathcal{W}^*}, \quad \text{if } \mathcal{W}^* \text{ is a minimum of (4).} \quad (12)$$

However, if $\mathcal{P} \in \mathbf{V}$ is an arbitrary path, not necessarily differentiable and possibly crossing shocks, $\Delta(\mathcal{W})$ does not give the actual change. Since N cannot have discontinuities, the correct general formula for any path $\mathcal{P}$ going from B to P is the integral of the rate at which N changes along the path, $dN/dt = N_t + N_x \cdot x' = q - k \cdot x'$. Since $q = Q(k, t, x)$, this is:

$$N_P - N_B = \int_{t_B}^{t_P} [Q(k, t, x) - k \cdot x'] dt, \quad \text{where } x(t) \text{ is the trajectory of } \mathcal{P}. \quad (13)$$

We now show that the correct change in item number (13) is bounded from above by $\Delta(\mathcal{P})$.

Lemma: A continuous solution of (1) satisfies $N_P - N_B \leq \Delta(\mathcal{P})$ for any $\mathcal{P} \in \mathbf{V}$ going from B to P . ■

Proof: An upper bound to (13) is obtained if its integrand is replaced by $\sup_k \{Q(k, t, x) - k \cdot x'\}$.

Because Q is concave the supremum is achieved for any k such that $Q_k = x'$. Thus, the supremum is

$$\sup_k \{Q(k, t, x) - k \cdot x'\} = Q(k, t, x) - k \cdot x', \quad \text{for any } k \text{ such that } x' = Q_k. \quad (14)$$

This is the definition of $R(x', t, x)$, according to (9) and (10). Since the integral of $R(x', t, x)$ is the definition of $\Delta(\mathcal{P})$ —see (11)—we conclude that $\Delta(\mathcal{P})$ is the sought upper bound. ■

A corollary of the lemma in combination with (12), is that every valid path to a point P satisfies:

$$B_{\mathcal{P}} + \Delta(\mathcal{P}) \geq N_P = B_{\mathcal{W}^*} + \Delta(\mathcal{W}^*); \quad \forall \mathcal{P} \in \mathbf{V}. \quad (15)$$

Thus, we can now state the main result of this paper.

Theorem: Equations (6) and (4) are equivalent. ■

Proof: Since $\mathcal{W}^* \in \mathbf{W} \subset \mathbf{V}$ is a valid path, we see from (15) that $\mathcal{W}^*$ minimizes (6). ■

It turns out that it is very easy to prove the stability of (6) and, by association, the stability of (4). To see that (6) is stable let Δ_{BP} denote the minimum of $\Delta(\mathcal{P})$ across all valid paths from $B \in \mathbf{D}$ to P so (6) becomes:

$$N_P = \min \{ N_B + \Delta_{BP} ; \forall B \in \mathbf{D} \}. \quad (16)$$

Note that the Δ_{BP} 's are fixed quantities, obtained from R by minimizing (11); e.g., with the calculus of variations. Since the Δ_{BP} 's are independent of the boundary data, (16) implies that if $\{N_B\}$ and $\{N'_B\}$ are two valid data sets, then the two solutions satisfy:

$$|N_P - N'_P| \leq \max \{ |N_B - N'_B| ; \forall B \in \mathbf{D} \}, \quad (17)$$

clearly showing that two solutions can never deviate from each other at any point any more than they deviate somewhere on the boundary. Thus, the solution obtained with (6) is stable.

It is shown in the appendix that if the equation of state is strictly concave then the minimum of (6) is a wave. If Q is merely concave then piecewise differentiable paths (with corners), which are not waves, can minimize (6), but there always is a differentiable $\mathcal{W}^*$ that also yields the minimum cost.

Note that the appendix proves that (6) solves (1) without using the continuity of (4) as an assumption. Since (16) provides continuous solutions – it is the lower envelope of continuous surfaces parametrized by “B” – the appendix indirectly proves that the solutions of (6) are continuous. Since, as we have just seen, the solutions of (6) are also stable, the appendix proves in a different way that (6) is the correct solution of (1).

With the new formulation, determining if a meaningful solution exists is also very easy. For a solution to exist there must be a shortest path with finite cost to every point in the solution domain, and every point on the boundary should be on a shortest path to itself. (If this were not to happen $N(t, x)$ would be discontinuous at the point in question and a proper solution to the problem could not exist.) Note that this always happens for the initial value problem. The conditions are easy to check a posteriori in other cases.

These results show that the class of problems discussed in this paper belong to the family of physics problems (e.g., Hamilton-Jacobi theory; optics) that can be described equally well by a partial differential equation or by a variational principle. Our problems have the additional feature of uniqueness, which allows the variational formulation to rule out all unstable solutions of the partial differential equation, automatically generating the physically relevant shocks.

3. PRACTICAL ISSUES: NETWORKS AND BOUNDARY CONSTRAINTS

The results in Sec. 2 establish that our problems can be solved approximately by first overlaying a dense but discrete network in the solution region, with a cost $\Delta_{PP'} \approx R\Delta t$ for each arc PP' , then connecting a fictitious origin to all points B on the boundary with a cost N_B for each arc, and finally finding the “shortest” tree from this origin to all nodes. These methods can be quite accurate. In particular, the network solution will be exact if the network can be guaranteed to contain one of the shortest paths in the continuum. Daganzo (2003) shows how this can be done for an important class of problems of relevance to traffic flow. In other cases we can ensure that the network contains a near-optimum path by ensuring that it is dense and that the set of links PP' incident on every node P contains a full complement of slopes, x' , within the range of validity. Since networks of this type contain no cycles, the full tree for a network with L links can be found in time $O(L)$; e.g., with dynamic programming.

Under the conditions of the appendix, the tree of shortest paths from the origin to all the nodes gives the waves. Its branches end either at the boundary of the solution region or at a “shock.” Shocks are those regions in solution space that can be reached by more than one path. In traffic flow applications, the equi-cost contours of the network—lines with the same item number—are the vehicle trajectories.

Formulation (6) has a further advantage over conventional (kinematic wave theory) formulations because it provides a natural framework for the treatment of discrete constraints (e.g., due to point bottlenecks in traffic flow) without the nuisance of having to check for stability during the solution process. To clarify, suppose we are given a set of paths $\{C_i(t)\}$ along which there is a maximum possible passing rate $\{R_i(t)\}$. (Think of a snowplow passing through a traffic signal or two trucks passing each other.) To solve this problem we simply add short links to the underlying network matching the $\{C_i(t)\}$ as well as possible and then assign to them unit costs (per unit time) close to $R_i(t)$. The problem (with constraints) is then solved by finding the shortest tree for the expanded network. The new low-cost links act as shortcuts through space-time. These shortcuts obviously change the solution but do not materially alter the solution effort. Note that the inclusion of shortcuts can only lower the cost of reaching a node. This is expected, since in kinematic wave theory, the inclusion of a bottleneck can only *lower* the item number reaching a node. Boundary conditions can be naturally modeled in this theory as constraints of this type. For example, constraints of the form $\{C_f(t) = x_f; R_f(t)\}$ can be used to model a road that meets a junction at location x_f .

We may ask if this solution with constraints is stable, unique, etc... but we need not worry. Since the solution continues to be the minimum of a shortest path problem it is unique and stable; it is the correct solution and no entropy conditions need to be checked. In practical applications one can allow the passing rates to depend on endogenous data (e.g., from other roads sharing a junction) according to some

meaningful rule. In this case, the rules should be tested for stability. But if they are stable boundary data will remain bounded, and the solution to the continuum problem will still exist, be unique and stable.

Daganzo (2003) presents a number of examples and discusses further simplifications, with emphasis on cases where *exact* solutions can be obtained in time $O(M)$, where M is the number of points at which the solution is sought.

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APPENDIX

This appendix shows that if Q is strictly concave then only waves can be shortest paths. It is assumed that (6) holds for all $P \in \mathbf{D}$, and that the problem is well posed in the sense that every point in the solution domain is reached by a wave.

We will prove this in two steps. First we will show that if $\mathcal{P}^*$ is a solution of (6) and goes from $B^* \in \mathbf{D}$ to P , then $\mathcal{P}^*$ satisfies (5) between B^* and P , although not necessarily at B^* itself. This will be proven in the second step, where it will be shown that x' must match the value of Q_k specified at the boundary.³ Thus, $\mathcal{P}^*$ is a wave.

³ For the initial value problem $Q_k(k, t, x)$ is easily found for any point on the boundary since N varies over the boundary with a fixed t , readily yielding the boundary values of $k = -N_x$. For more general problems one must first find a value of k which along with $Q(k, t, x)$ is consistent with the rate of variation of N along the boundary, and from this k the value of $Q_k(k, t, x)$.

Step 1. $\mathcal{P}^*$ satisfies (5): If $\mathcal{P}^*$ is a global minimum of (6) starting a B^* , it should be a global minimum of $\Delta(\mathcal{P})$ as given by (11), conditional on B^* . This sub-problem is a basic problem in the calculus of variations for which the Euler necessary condition for optimality (among the set of differentiable paths) is $R_x = dR_x/dt$. We see from the right side of (9) or (14) that $R_x = Q_x$ and $R_x = -k$. Thus, in terms of Q the Euler condition is $Q_x = d(-k)/dt = -k'$ which is (5d). Of course, k satisfies $Q_k = x'$, which is (5a). Since $Q_x = -k'$ and $Q_k = x'$, we see that $dQ/dt = Q_x \cdot x' + Q_k \cdot k' + Q_t = Q_t$, and $dN/dt = N_t + N_x \cdot x' = q - k \cdot Q_k$, which are (5c) and (5b). Thus, if $\mathcal{P}^*$ is differentiable it satisfies (5).

To complete this step we must establish that that piecewise differentiable paths (with corners) cannot be optimal. We demonstrate this by checking the Weierstrass-Erdmann corner conditions. They state that R_x must be equal on both sides of any corner; i.e., $\Delta R_x = 0$. It is well known that if Q is a strictly concave and differentiable function in k , changes in its gradient Q_k are related to changes in k by $\{\Delta k = 0 \Leftrightarrow \Delta Q_k = 0\}$. However, we have already shown that $-k = R_x$ and $Q_k = x'$. Thus, strict concavity for Q implies that R satisfies $\{\Delta R_x = 0 \Leftrightarrow \Delta x' = 0\}$. Since $\Delta R_x = 0$ at any corner, we see that $\Delta x' = 0$ at any such corner; i.e., there can be no corners. Thus, $\mathcal{P}^*$ satisfies (5).

Step 2. $\mathcal{P}^*$ is consistent with the boundary data: It suffices to show that if $\mathcal{P}^*$ was not a wave, there would be a point on it, P' , from which there is a shortcut to the boundary with less cost than $\mathcal{P}^*$.

Since the problem is well posed there must be a point on $\mathcal{P}^*$, P' , within a time dt of the boundary which is reached by a boundary wave, $\mathcal{W}$, emanating from some point, $B' \in \mathbf{D}$. Thus, $N_{P'} = N_{B'} + \Delta(\mathcal{W})$; i.e., there is a path from the boundary to P' with final cost $N_{P'}$. To conclude the step we shall show that if $\mathcal{P}^*$ is not a wave; i.e., $x' \neq Q_k(k_B, t_B, x_B)$, then the portion of $\mathcal{P}^*$ going from B' to P' , which we denote $\mathcal{P}'$, predicts an unacceptably large cost for P' : $N_{B'} + \Delta(\mathcal{P}') > N_{P'}$; i.e., $\mathcal{P}^*$ could not be a minimum path. Thus, it suffices to show that $\Delta(\mathcal{P}') > N_{P'} - N_{B'}$. The left side of this inequality is $R(x', t_B, x_B)dt = \sup_k \{Q(k, t_B, x_B) - k \cdot x'\}dt$. The right side is the differential of N in the neighborhood of B , which is: $(N_x + N_t \cdot x')dt = \{Q(k_B, t_B, x_B) - k_B \cdot x'\}dt$. Since the objective function of $\sup_k \{Q(k, t_B, x_B) - k \cdot x'\}dt$ is strictly concave and we are assuming that $x' \neq Q_k(k_B, t_B, x_B)$, i.e., the derivative of the objective function at $k = k_B$ is non-zero, we see that $\{Q(k_B, t_B, x_B) - k_B \cdot x'\}dt$ cannot be a global maximum of the function; i.e., $R(x', t_B, x_B) > Q(k_B, t_B, x_B) - k_B \cdot x'$. Thus, $\Delta(\mathcal{P}') > N_{P'} - N_{B'}$. ■
