Computing solution surfaces of quasilinear PDE's by continuation

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Summary. In this work we compute the solution surfaces of first order quasilinear PDE's as families of orbit segments of an associated dynamical system. The approach is to obtain these orbit segments as solutions of a boundary value problem solved by continuation methods. We illustrate this technique with an example that arises in the study of one-dimensional neutron transport theory.

Mathematical setting

We consider first order partial differential equations (PDEs) of the form

$$P(x,y,z)\frac{\partial z}{\partial x} + Q(x,y,z)\frac{\partial z}{\partial y} = R(x,y,z), \tag{1}$$

where $\mathbf{x} = (x,y,z) \in \Omega \subset \mathbb{R}^3$, and $P, Q, R : \Omega \to \mathbb{R}$ are sufficiently smooth functions. In general the functions P, Q, R may depend on the unknown z, hence (1) is known as a quasilinear PDE. This kind of PDEs arises in many applications ranging from traffic flow and gas dynamics to high energy physics and birth/death processes; see [4, 6, 8] and the references therein. The classical theory [1] tells us that a solution $z = z(x,y)$ of (1) in Ω can be represented as a smooth surface

$$S = \{(x,y,z) \in \Omega |\ z = z(x,y)\}$$

whose normal vector $n_S = (z_x, z_y, -1)$ is orthogonal to the vector field $X = (P,Q,R)$ at every point $(x,y,z) \in S$. Therefore, the solution surface S of (1) is an integral surface of X. (Notice that the same consequence holds if the surface S is given implicitly by $f(x,y,z) = 0$ provided $f_z \neq 0$.) Hence, geometrically, the surface S consists of orbits of a dynamical system defined by the set of ordinary differential equations

$$X : \left\{ \begin{array}{rcl} \dot{x} &=& P(x,y,z), \\ \dot{y} &=& Q(x,y,z), \\ \dot{z} &=& R(x,y,z). \end{array} \right. \quad \text{or equivalently} \quad \dot{\mathbf{x}} = X(\mathbf{x}). \tag{2}$$

An initial value problem for (1) consists on finding a solution surface S that contains a given "initial" curve

$$C = \{(x,y,z) \in \Omega |\ x = x_0(s), y = y_0(s), z = z_0(s),\ s \in [a,b]\}.$$

Provided the vector field X is not tangent to C, then the initial value problem is well-posed, i.e., there is a unique solution surface S that contains the curve C [1]. In such case, the method of characteristics allows one to obtain a functional expression for S. However, in a general context, this task may demand hard algebraic work; and even if one manages to get a formula by this method, its practical usefulness is not assured. Instead of taking this more traditional formulaic approach, in this work we take advantage of the geometric association between S and the vector field X to solve the initial value problem: We compute a solution surface S as a family of orbit segments of X obtained as solutions of a boundary value problem (BVP) solved by continuation methods in AUTO [3]. More concretely, we find orbit segments $\{\mathbf{u}(t) \in \Omega |\ 0 \leq t \leq 1\}$ that satisfy a rescaled version of (2) given by

$$\dot{\mathbf{u}} = TX(\mathbf{u}(t)),$$

(where T is the integration time of an orbit segment of X) subject to the boundary condition $\mathbf{u}(0) \in C$. This BVP defines a unique (s,T)-family of orbit segments. For any fixed $T = T_0$ we have a uniquely defined one-parameter family of orbit segments (parameterized by $s \in [a,b]$) with fixed integration time T_0 that constitutes an accurate approximation of the corresponding piece of the surface S that contains the initial curve C.

Application: Neutron transport theory

Neutron transport theory deals with the study of the location, velocity and motion directions of neutrons and their interactions with various media. Take for instance, the presence of neutrons in nuclear reactor cores and experimental or industrial neutron beams as some applications [5, 7].

As an illustration of our method, here we consider the problem of reflection and transmission of neutrons in a one-dimensional rod. Let $p_n(x)$ be the probability that exactly n neutrons emerge over all time from the left end of an homogeneous rod of length x as a result of one neutron entering at the left end at time zero. These probabilities can be obtained from the associated generating function

$$u(x,y) = \sum_{n=0}^{\infty} p_n(x) y^n, \quad 0 \leq x \leq L,\ 0 \leq y \leq 1,$$

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by means of the identity

$$p_n(x) = \frac{1}{n!}\frac{\partial^n u}{\partial y^n}(x,0). \tag{3}$$

Under the assumptions that there is no energy or velocity dependence and that collisions between neutrons can be disregarded, the following first order quasilinear PDE was derived in [2] for the generating function u:

$$\frac{\partial u}{\partial x} + y(1-u)\frac{\partial u}{\partial y} = (y-1)u, \tag{4}$$

with the boundary conditions

$$u(x,0) = p_0(x), \quad u(x,1) = 1, \quad u(0,y) = 1. \tag{5}$$

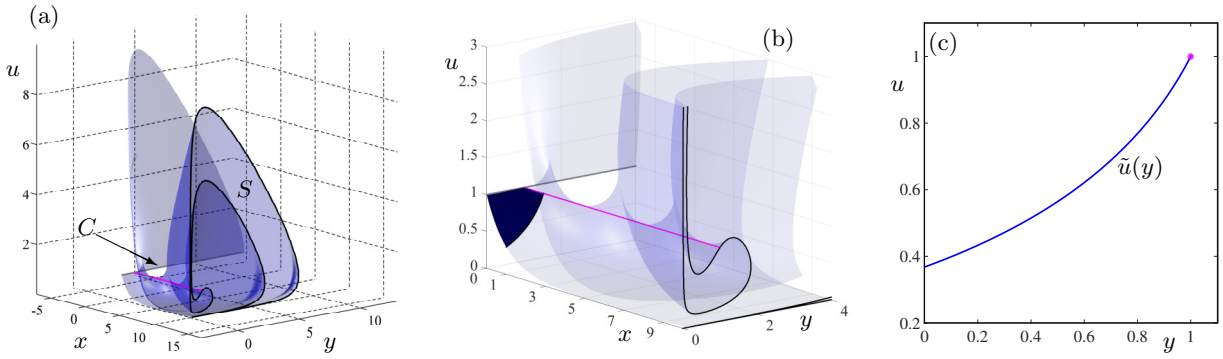

Figure 1: The solution of (4)–(5) computed as the integral surface of a nonlinear dynamical system in panel (a), and the intersection of this surface with the plane $x = 10$ in panel (b) —with an enlargement in panel (c)— give us information about the probabilities $p_n(x)$.

Figure 1(a) shows a computed piece of the integral surface S of the nonlinear dynamical system of the form (2) associated to (4). Here the initial data lies only on the (gray) line segment $C = \{(x,y,u)|\, x(s) = 0, y(s) = s, u(s) = 1,\ s \in [0,10]\}$ and corresponds to the boundary condition $u(0,y) = 1$. On the other hand, the other boundary conditions in (5) are also readily fulfilled: The surface S contains the (pink) line that corresponds to the boundary condition $u(x,1) = 1$. Moreover, the (a priori unknown) probability distribution $p_0(x)$ corresponds to the intersection curve of S with the plane $y = 0$.
In order to highlight the practical aspects of the method, Figure 1(b) shows the graph of the solution $u(x,y)$ contained in S in a darker shade up to the plane $x = 1$. The corresponding intersection of this portion of S with the plane $x = 1$ is a curve shown in Figure 1(c). This intersection curve is the graph of the (unique) solution $\tilde{u}(y) = u(1,y)$ that satisfies (4)–(5) for fixed $x = 1$. Moreover, from (3) and from the graph of $\tilde{u} = u(1,y)$ one can recover (and estimate) the probabilities $p_n(1)$ associated to a rod of length $x = 1$ for any $n = 0, 1, 2, \ldots$.

Conclusions

We have introduced the method of computing integral surfaces of first order quasilinear PDEs as families of orbit segments of an associated dynamical system by continuation. The technique is illustrated with an example that arises in neutron transport theory which gives geometric insight into the probability distribution of neutrons in a one-dimensional rod. In this example the method also proved to be quite flexible and adaptable in that it automatically satisfied additional boundary conditions that were not imposed a priori in our continuation scheme. The method is versatile enough to be applied in many other different contexts where qualitative, geometric knowledge is needed to shed light on the nature of quantities governed by this kind of PDEs. Current plans also include to extend the method to the case of nonlinear PDEs of first order.

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