Shocks, causality, regularization, weakly nonlinear theory;

Shocks and causality

The method of characteristics can be used to find the solution to a single quasi-linear PDE in two dimensions. As we have seen the solution is found parametrised by the new variables r and s. We have seen that it can be difficult to find a explicit solution given the implicit function $x(r,s)$, $t(r,s)$ and $u(r,s)$. The more significant difficult is that the mapping between x, t and r, s may not be one-to-one. In particular the projected characteristics my intersect and then the solution is multivalued in x, t. Such behaviour can also occur for systems of quasi-linear PDEs. If the problem is hyperbolic we will assume that the solution to the PDE is valid up to the "time" when the intersection occurs. We now explore how we can extend the solution to the problem past such a point (formally the solution to the PDE problem ceases to exist)

Note there are two types of discontinuous behaviour in quasi-linear PDEs. The first type relates to discontinuities in the initial data that propagate but have differentiable behaviour along characteristics (see for example the equation of a string with discontinuous initial data) which are typically called contact discontinuities (they also occur commonly in gas dynamics). The second type relates to discontinuities that are created by the nonlinear behaviour of the problem which are commonly called shocks. Here we examine shocks.

We now consider, weak solutions of the PDE problem and allow the solution to have discontinuities. For these weak solutions to be physically reasonable we need to return to the original conservation laws that underlie the problem. (beware: the same PDE can be extended to have many possible different forms for the weak solution)

Previously we could have derived the conservation of mass in the form

$$\frac{\partial}{\partial t}\iiint_V \rho \, dV = \iint_{\partial V} \rho \mathbf{u} \cdot d\mathbf{S}$$

and we then integrate the surface integral by parts. However, we are now interested in the case where u may be discontinuous. Hence if there is a discontinuity we consider a region V that covers the discontinuity and allow this region to shrink to the line containing the discontinuity.

One alternative approach to finding the behaviour at a shock, and one then ensures that we only physically relevant shocks in the solution is the method of "viscous solutions" or "entropy". Consider the case where the physical conservation law is

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \epsilon \frac{\partial^2 u}{\partial x^2}$$

for some "flux function" $f(u)$. Note that the crucial idea here is that there is some underlying dissipation due to diffusivity and that it is critical to have the correct form of the PDE as otherwise we can introduce discontinuities that only conserve other quantities across them and not the physically relevant one.

On physical grounds we assume that the parameter ϵ is extremely small and hence anticipate that we should be able to solve the simple hyperbolic equation

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

This is a valid approach in regions where the solution is smooth but if the hyperbolic equation predicts that the solution gradient gets large (and a discontinuity is forming) then we need to reconsider the problem. consider the discontinuity to be forming on a curve given locally by $x = Vt + C$, where V is the local speed of the shock. If we rescale to be near this point the we take

$$\eta = \epsilon(x - Vt + C)$$

and then seek a travelling wave solution with the properties that
i) as $\eta \to -\infty$ $u \to u^-$
ii) as $\eta \to +\infty$ $u \to u^+$
where u^- and u^+ are constants determined by the smooth behaviour of the hyperbolic equation. Using this variable and sending $\epsilon \to 0$ we get the ODE

$$-Vu_\eta + (f(u))_\eta = u_{\eta\eta}$$

which integrates to give

$$-Vu + f(u) = u_\eta + D\ .$$

Now we impose that boundary conditions noting that in both cases $u_\eta \to 0$ at large distances and hence we require

$$-Vu^+ + f(u^+) = D \text{ and } -Vu^- + f(u^-) = D\ .$$

Hence we conclude that such a travelling wave is only possible if

$$-Vu^+ + f(u^+) = -Vu^- + f(u^-).$$

If follows therefore that we need to have the speed of the shock V at any point determined by the behaviour on either side of the shock and that

$$V = \frac{[u]_-^+}{[f(u)]_-^+}$$

This relation is called the "Rankine-Hugoniot" condition and allows us to extend the solution of the conservation law to regions where the solution has discontinuities which travel at this speed V.

Note also that this derivation requires that the travelling wave satisfy the ODE

$$-Vu + f(u) = u_\eta + D \, .$$

and this will only hold for certain combinations of the u^+ and u^- because of the sign of u_η. There are physically irrelevant solutions which do not satisfy this ODE and typically these irrelevant solutions have characteristics that leave the shock as time increases (rather than the physically relevant solutions where characteristics enter the shock). For example if we linearise around u^+ and around u^- assuming $f(u)$ is differentiable we find that in order for a physically relevant travelling wave to exist we need at least to have

$$f'(u^-) > V \text{ and } f'(u^+) < V.$$

Charpit's method

The previous discussion was about quasi-linear systems of PDEs in two dimensions. We now turn to more complicated problems and consider a single dependent variable where the governing equations simply give a relation between the the two dependent variables, the dependent variable and the two partial derivatives. Such problems can be written in the form

$$F(p, q, u, x, y) = 0, \tag{3.1}$$

where we use the notation

$$\frac{\partial u}{\partial x} = p, \quad \frac{\partial u}{\partial y} = q$$

as shorthand. We now discuss how to solve such problems using Charpit's method. We start by noting the consistency condition that

$$\frac{\partial p}{\partial y} = \frac{\partial q}{\partial x} \qquad \text{from } u_{xy} = u_{yx}. \tag{3.2}$$

If we differentiate (3.1) with respect to x and y, we obtain

$$\begin{aligned} \frac{\partial F}{\partial p}\frac{\partial p}{\partial x} + \frac{\partial F}{\partial q}\frac{\partial q}{\partial x} &= -\frac{\partial F}{\partial x} - p\frac{\partial F}{\partial u}, \\ \frac{\partial F}{\partial p}\frac{\partial p}{\partial y} + \frac{\partial F}{\partial q}\frac{\partial q}{\partial y} &= -\frac{\partial F}{\partial y} - q\frac{\partial F}{\partial u}, \end{aligned}$$

or, using (3.2),

$$\frac{\partial F}{\partial p}\frac{\partial p}{\partial x} + \frac{\partial F}{\partial q}\frac{\partial p}{\partial y} = -\frac{\partial F}{\partial x} - p\frac{\partial F}{\partial u}, \tag{3.3}$$

$$\frac{\partial F}{\partial p}\frac{\partial q}{\partial x} + \frac{\partial F}{\partial q}\frac{\partial q}{\partial y} = -\frac{\partial F}{\partial y} - q\frac{\partial F}{\partial u}. \tag{3.4}$$

So, if we define *characteristics* or *rays* as curves $(x(\tau), y(\tau))$ satisfying

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = \frac{\partial F}{\partial p}, \quad \frac{\mathrm{d}y}{\mathrm{d}\tau} = \frac{\partial F}{\partial q}$$

then, along these curves,

$$\begin{aligned} \frac{\mathrm{d}p}{\mathrm{d}\tau} &= \frac{\partial p}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}\tau} + \frac{\partial p}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}\tau} = -\frac{\partial F}{\partial x} - p\frac{\partial F}{\partial u}, \\ \frac{\mathrm{d}q}{\mathrm{d}\tau} &= \frac{\partial q}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}\tau} + \frac{\partial q}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}\tau} = -\frac{\partial F}{\partial y} - q\frac{\partial F}{\partial u}, \end{aligned}$$

by (3.3), (3.4). We therefore have a system of four ODEs for x, y, p and q satisfied along the rays. Recall, though, that in general F depends on u also, so to close the system we also need an ODE for u along the rays, namely

$$\frac{\mathrm{d}u}{\mathrm{d}\tau} = \frac{\partial u}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}\tau} + \frac{\partial u}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}\tau} = p\frac{\partial F}{\partial p} + q\frac{\partial F}{\partial q}.$$

In summary, we have the following system of ODEs for x, y, p, q and u, known as *Charpit's equations*:

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = \frac{\partial F}{\partial p}, \qquad \frac{\mathrm{d}y}{\mathrm{d}\tau} = \frac{\partial F}{\partial q},$$

$$\frac{\mathrm{d}p}{\mathrm{d}\tau} = -\frac{\partial F}{\partial x} - p\frac{\partial F}{\partial u}, \qquad \frac{\mathrm{d}q}{\mathrm{d}\tau} = -\frac{\partial F}{\partial y} - q\frac{\partial F}{\partial u}, \qquad \frac{\mathrm{d}u}{\mathrm{d}\tau} = p\frac{\partial F}{\partial p} + q\frac{\partial F}{\partial q}. \tag{3.5}$$

Boundary data

We now consider how to impose boundary conditions on a solution found by Charpit's method. We assume that the conditions are given as Cauchy data which specifies u along some curve Γ in the (x, y)-plane:

$$x = x_0(s), \quad y = y_0(s), \quad u = u_0(s), \tag{3.6}$$

for s in some (possibly infinite) interval. We also require initial conditions for p and q, say $p = p_0(s)$, $q = q_0(s)$, which are obtained by differentiating u_0 with respect to s and using the PDE (3.1):

$$\frac{\mathrm{d}u_0}{\mathrm{d}s} = p_0\frac{\mathrm{d}x_0}{\mathrm{d}s} + q_0\frac{\mathrm{d}y_0}{\mathrm{d}s}, \quad F(p_0, q_0, u_0, x_0, y_0) = 0. \tag{3.7}$$

The two equations (3.7) may be solved (in principle, if not explicitly) for p_0 and q_0 provided the condition

$$\frac{\mathrm{d}x_0}{\mathrm{d}s}\frac{\partial F}{\partial q_0} - \frac{\mathrm{d}y_0}{\mathrm{d}s}\frac{\partial F}{\partial p_0} \neq 0 \tag{3.8}$$

is satisfied. This is the same as insisting that Γ not be parallel to a ray.

Charpit's method consists of solving the ODEs (3.5) for (p, q, u, x, y), with (3.6) and (3.7) as initial data at $\tau = 0$. This gives (p, q, u, x, y) all as functions of s and τ and, in principle, allows us to reconstruct the solution surface $u = u(x, y)$.

Example 1. Sugar on a spoon
Consider sugar piled up on a spoon such that its height is given by $u(x, y)$. At criticality, just before the sugar would start to slide off the spoon, the sugar makes a constant angle (the "angle of repose") γ with the horizontal, that is

$$|\boldsymbol{\nabla} u|^2 = \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 = \tan^2\gamma.$$

After normalisation, (such as taking $u = \tan\gamma\ \bar{u}$) this can be written as the *Eikonal equation*

$$\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 = 1, \tag{3.9}$$

which is of the form (3.1) with

$$F(p, q) = \tfrac{1}{2}\left(p^2 + q^2 - 1\right).$$

Charpit's equations for this particular F are

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = p, \quad \frac{\mathrm{d}y}{\mathrm{d}\tau} = q, \quad \frac{\mathrm{d}p}{\mathrm{d}\tau} = 0, \quad \frac{\mathrm{d}q}{\mathrm{d}\tau} = 0, \quad \frac{\mathrm{d}u}{\mathrm{d}\tau} = p^2 + q^2 = 1.$$

Notice that p and q are constant along rays and, hence, given by their boundary values:

$$p = p_0(s), \quad q = q_0(s).$$

The remaining ODEs are then readily integrated to give

$$x = x_0(s) + p_0(s)\tau, \quad y = y_0(s) + q_0(s)\tau, \quad u = u_0(s) + \tau.$$

Notice that the slope of a ray is given by $q_0(s)/p_0(s)$ which is constant along each ray. Thus the rays are *straight lines*, along which u increases linearly with τ.

At the edge of the spoon, the height is zero, so $u_0(s) = 0$. Then we have the system

$$\frac{\mathrm{d}x_0}{\mathrm{d}s} p_0 + \frac{\mathrm{d}y_0}{\mathrm{d}s} q_0 = 0, \quad p_0^2 + q_0^2 = 1$$

for p_0 and q_0, whose solution is

$$p_0 = \frac{\mp y_0'}{\sqrt{(x_0')^2 + (y_0')^2}}, \quad q_0 = \frac{\pm x_0'}{\sqrt{(x_0')^2 + (y_0')^2}}, \tag{3.10}$$

where $'$ is used as shorthand for $d/\mathrm{d}s$. The vector (p_0, q_0) is the *unit normal* to the boundary Γ. Hence the rays are straight lines perpendicular to Γ and $u(x, y)$ is simply the *distance* of the point (x, y) from Γ.

Notice that there are two possible solutions corresponding to the $\pm$ in (3.10). The correct solution is chosen by ensuring that the rays propagate *into* the region of interest, not out of it. So, in (3.10), we have to choose (p_0, q_0) to be the *inward* pointing normal. Otherwise the solution corresponds to the sandpile outside a spoon-shaped hole in a table.

If the spoon is elliptical, then we can write

$$x_0(s) = a\cos(s), \quad y_0(s) = b\sin(s), \quad 0 \le s < 2\pi,$$

for some constants a and b, and the solution is given parametrically by

$$x = a\cos(s) - \frac{b\tau\cos(s)}{\sqrt{a^2\sin^2(s) + b^2\cos^2(s)}}, \quad y = b\sin(s) - \frac{a\tau\sin(s)}{\sqrt{a^2\sin^2(s) + b^2\cos^2(s)}}, \quad u = \tau.$$

The rays and solution surface are shown in Figure 3.1. Notice that a ridge line, across which p and q are discontinuous, forms along the x-axis, between the $x = -(a^2 - b^2)/a$ and $x = +(a^2 - b^2)/a$. In this figure $a = 2$ and $b = 1$; if $a < b$ then the ridge at the corresponding position along the y-axis.

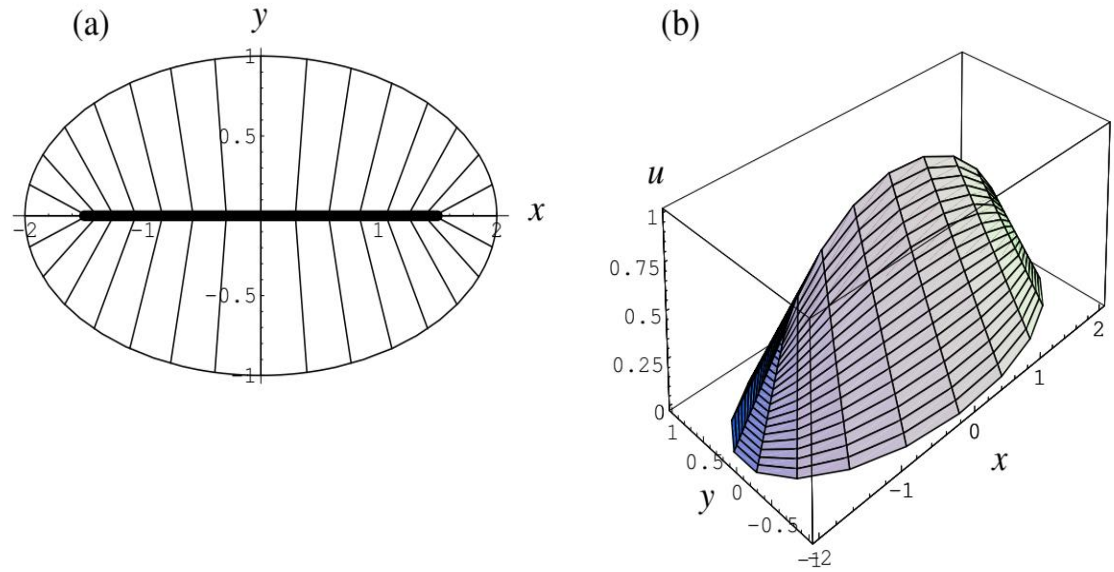

Figure 3.1: (a) Rays for a sugar heap on an elliptical spoon with $a = 2$ and $b = 1$; the bold line marks the ridge. (b) The corresponding pile height $u(x, y)$.

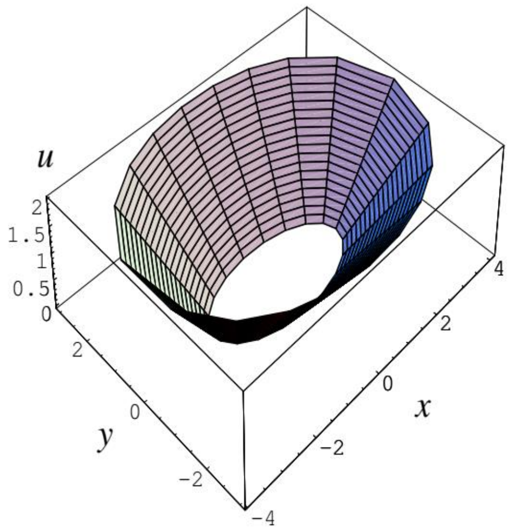

Figure 3.2: The height $u(x, y)$ of a sandpile outside an elliptical hole with $a = 2$ and $b = 1$.

If the other root is taken for p and q, then the rays propagate *out* of the ellipse as τ is increased from zero, and the parametric solution is now

$$x = a\cos(s) + \frac{b\tau\cos(s)}{\sqrt{a^2\sin^2(s) + b^2\cos^2(s)}}, \quad y = b\sin(s) + \frac{a\tau\sin(s)}{\sqrt{a^2\sin^2(s) + b^2\cos^2(s)}}, \quad u = \tau.$$

This corresponds to a sandpile on a table with an elliptical hole, as shown in Figure 3.2.

Discontinuities

Example 1 illustrates that it is possible for rays to intersect. This happens first where the Jacobian J of the transformation for x, y first becomes zero. Note that this reproduces the criterion (3.8) for Cauchy data *not* to determine a unique solution on Γ. If rays are allowed to cross, then the solution becomes multi-valued, which is clearly unphysical for a pile of sugar. Instead, we must allow shocks to form across which the solution is discontinuous. Recall that, for nonlinear PDEs, shocks are different from characteristics. The conditions that must be applied across a shock depend on the physical situation being modelled. For the sugar heap problem, it is clear that u must be continuous everywhere, since a discontinuity in u (corresponding to a vertical "cliff") cannot be sustained. This forces the shock, *i.e.* the ridge line, to be along the x-axis as shown in Figure 3.1. In general, the region of validity of the solution obtained by Charpit's method is bounded by curves on which $J = 0$.

Example 2. Solve the PDE

$$\frac{\partial u}{\partial x} = \left(\frac{\partial u}{\partial y}\right)^2$$

subject to $u = u_0(y)$ on $x = 0$.

Set $F = p - q^2$ and parametrise the initial conditions via

$$x = 0, \ y = s, \ u = u_0(s), \ p = p_0(s), \ q = q_0(s),$$

where

$$q_0(s) = u_0'(s), \quad p_0(s) = q_0(s)^2 = \left(u_0'(s)\right)^2.$$

Charpit's equations are

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = 1, \quad \frac{\mathrm{d}y}{\mathrm{d}\tau} = -2q, \quad \frac{\mathrm{d}p}{\mathrm{d}\tau} = \frac{\mathrm{d}q}{\mathrm{d}\tau} = 0, \quad \frac{\mathrm{d}u}{\mathrm{d}\tau} = p - 2q^2 = -p,$$

and the solution is

$$x = t, \quad y = s - 2tu_0'(s), \quad p = \left(u_0'(s)\right)^2, \quad q = u_0'(s), \quad u = u_0(s) - t\left(u_0'(s)\right)^2.$$

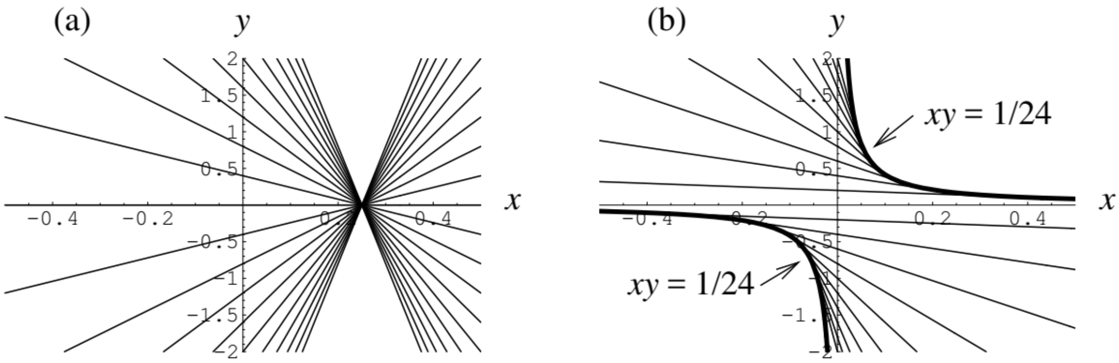

Figure 3.3: Rays for Example 2. (a) $u_0(s) = s^2$; (b) $u_0(s) = s^3$.

The rays are straight lines given by

$$y + 2xu_0'(s) - s = 0,$$

and their envelope is found parametrically by differentiating with respect to s:

$$x = \frac{1}{2u_0''(s)}, \quad y = s - \frac{u_0'(s)}{u_0''(s)}.$$

For example, if $u_0(s) = s^2$, then the solution in explicit form is

$$u = \frac{y^2}{1 - 4x}.$$

The rays in this case are given by $y = s(1 - 4x)$ so, as illustrated in Figure 3.3(a), they all pass through the point $(1/4, 0)$, and the solution is defined in $x < 1/4$.

If $u_0(s) = s^3$, then the solution is

$$u = s^3(1 - 9xs), \quad \text{where} \quad s = \frac{1 - \sqrt{1 - 24xy}}{12x}.$$

The rays are given by $y = s - 6s^2x$, and their envelope is the curve $24xy = 1$, as illustrated in Figure 3.3(b). The solution is therefore defined in the region $24xy < 1$ (which is where s is real).

References and further readings

1 A. R. Conn, N. I. M. Gould and Ph. L. Toint, Trust-Region Methods, SIAM 2000.

2. J. Dennis and R. Schnabel, Numerical Methods for Unconstrained Optimization and Nonlinear equations, (republished by) SIAM, 1996.

3. R. Fletcher, Practical Methods of Optimization, 2nd edition Wiley, 1987 (republished in 2000).

4. P. Gill, W. Murray and M. H. Wright, Practical Optimization, Academic Press, 1981.

5. N. I. M. Gould, An Introduction to Algorithms for Continuous Optimization, 2006. Available for download at http://www.numerical.rl.ac.uk/nimg/course/lectures/paper/paper.pdf.

6. J. Nocedal and S. J. Wright, Numerical Optimization, Springer Verlag, 1999 (1st edition) or 2006 (2nd edition).

7. Mathematical Modeling and Computation of Real-Time Problems: An Interdisciplinary Approach (Mathematical Engineering, Manufacturing, and Management Sciences) 1st Edition by Rakhee Kulshrestha, Chandra Shekhar, Madhu Jain, Srinivas R. Chakravarthy