Mat1062: Computational Methods for PDE

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March 4, 2008

Ownership

These notes are built upon those of Rob Almgren who taught an analogous course in 2003. Whatever you learn of value from them is due to him. All mistakes and sources of confusion are to be blamed on me.

Nonlinear problems

Now we consider the case in which the convection speed depends on u itself. For parabolic and for elliptic problems, we have only nodded in the direction of nonlinearity, and suggested that it can be handled by minor modifications of the linear schemes. But for conservation laws, we have an extensive theory describing them, both in the PDE and the numerical discretization.

Here conservation form will be absolutely essential. In the simplest case, we consider a scalar u, and a nonlinear function $f(u)$, and write the PDE

$$u_t + f(u)_x = 0. \tag{1}$$

If everything is smooth, then we may expand the derivative to write

$$u_t + a(u)\, u_x = 0, \qquad a(u) = f'(u).$$

This looks similar to the linear convection equation with variable coefficient

$$u_t + a(x,t)\, u_x = 0,$$

but depending on u is a completely different story than on u. Both convection equations say that u is constant along curves in the (x,t)-plane whose inverse slope is a: that is, the characteristic curves are $\xi(t)$ with $\xi'(t) = a$. If a depends only on x, t, then curves cannot cross, since when they come near the same location, their speeds become equal (this assumes $a(x,t)$ is smooth). But if a depends on u, and if the curves are carrying different values of u, then nothing prevents them from crossing.

A system has the same form, except that $u(x,t)$ is a vector of n components, and $f(u)$ is a function from $\mathbb{R}^n \to \mathbb{R}^n$. We require that the $n \times n$ gradient matrix $A(u) = \nabla_u f(u)$ have n real eigenvalues and a full set of eigenvectors; the eigenvalues are the propagation speeds.

Sometimes it will be convenient to write the system in the form

$$g(u)_t \;+\; f(u)_x \;=\; 0, \tag{2}$$

where the components of u are the state variables and the components of $g(u)$ are the conserved quantities. Of course it is in principle always possible to invert g and use its components as the state variables, but this is sometimes not convenient.

Blowup in finite time

Before giving some examples, let us explain very simply why these systems in general do not have smooth solutions. If $f(u)$ and hence $a(u)$ are smooth functions, and if smooth initial data $u_0(x)$ is given on $t = 0$, then it is reasonable to suppose that a smooth solution $u(x,t)$ exists for at least some $t > 0$; for example, you could certainly calculate such a solution by using explicit forward difference in t and any reasonable x-discretization. The claim is that this solution will fail to exist at some finite time $t_* > 0$. In particular, its derivatives will blow up, and so if we want to have a solution for $t > t_*$ we need to give some other definition of "solution."

All we have to do is imagine two locations x_1 and x_2, with $x_1 < x_2$, and corresponding initial values $u_1 = u_0(x_1)$ and $u_2 = u_0(x_2)$. Let us suppose that $a(u_1) > a(u_2)$, so that the characteristic lines coming from the left go faster than the ones on the right. (It will always be possible to find such points unless $a(u(x))$ is purely increasing in x.)

The characteristic line coming from x_1 has position $\xi_1(t) = x_1 + a(u_1)t$, and the line coming from x_2 has position $\xi_2(t) = x_2 + a(u_2)t$. We are supposed to have $u(x,t) = u_1$ along the first line, and $u(x,t) = u_2$ along the second. But the lines intersect, meaning that $\xi_1(t) = \xi_2(t)$, at time $t_* = (x_2 - x_1)/(a(u_1) - a(u_2)) > 0$. Since the characteristic construction assumed the existence of a smooth solution, we conclude that *no* smooth solution to the equation exists after time t_*.

To see the same thing a different way, differentiate (1) with respect to x, and let $v = u_x$. Then v satisfies $v_t + a(u)v_x = -a'(u)v^2$ which, along a characteristic line with $\xi'(t) = a(\xi(t), t)$ (note that u is constant along that line, so $a(u)$ and $a'(u)$ don't change) gives the ODE

$$\frac{dv}{dt} = -a'(u)\, v^2 \qquad \Longrightarrow \qquad v(t) = \frac{v_0}{1 + v_0\, a'(u)\, t}$$

This becomes infinite at $t_* = -1/(v_0 a'(u)) = -1/a(u_0)_x$. So anyplace along the initial axis where the propagation speed is *decreasing* as we move from left to right will give rise to a singularity.

Weak solutions

Assuming we have a function $u(x,t)$ that satisfies (1), we can integrate over a fixed region in space-time interval $[\alpha, \beta] \times [t_0, t_1]$ to write

$$\int_{t_0}^{t_1} \int_{\alpha}^{\beta} u_t(x,t)\, dx\, dt + \int_{t_0}^{t_1} \int_{\alpha}^{\beta} f(u(x,t))_x\, dx\, dt = 0.$$

It then follows that

$$\int_{\alpha}^{\beta} u(x,t_1)\, dx = \int_{\alpha}^{\beta} u(x,t_0)\, dx + \int_{t_0}^{t_1} f(u(\alpha,t))\, dt - \int_{t_0}^{t_1} f(u(\beta,t))\, dt. \quad (3)$$

That is, the amount of "stuff" in $[\alpha, \beta]$ at time t_1 is equal to the amount of stuff in $[\alpha, \beta]$ at time t_0 plus the amount of stuff that flowed into the interval through the $x = \alpha$ boundary between times t_0 and t_1 minus the amount of stuff that flowed out through the $x = \beta$ boundary between times t_0 and t_1.

A smooth solution of $u_t + (f(u))_x = 0$ will satisfy equation (3) for all $\alpha < \beta$ and all $t_0 < t_1$. If a function $u(x,t)$ satisfies equation (3) for all $\alpha < \beta$ and all $t_0 < t_1$ then we call u a *weak solution*. Most physical systems are originally derived in the integral form (3); the differential form (1) is derived under an assumption of smoothness. It is therefore reasonable to take (3) as the rule that must be preserved for discontinuous solutions when (1) does not apply. The differential form (2) has an analogous integral form with weak solutions; rather than considering $\int_\alpha^\beta u$ one considers $\int_\alpha^\beta g(u) dx$ and so on.

An alternate, but equivalent, formulation of weak solution with initial data $u_0(x)$ at time $t = 0$ is

$$\int_{\mathbb{R}} \int_0^\infty u(x,t)\, \phi_t(x,t) + f(u(x,t))\, \phi_x(x,t)\, dx\, dt = -\int_{\mathbb{R}} u_0(x)\, \phi(x,0)\, dx \quad (4)$$

where $\phi(x,t)$ is a differentiable function with compact support in $\mathbb{R}\times[0,\infty)$. If (4) holds for all such test functions ϕ then we say u is a weak solution.

Shock waves are weak solutions. The need to understand shock waves is one of the main reasons to consider weak solutions in the first place. The shock speed is dermined from the integral formulation (3) as follows. Suppose that $u(x,t)$ is smooth except for a simple jump discontinuity across the line $x=\xi(t)$ in the (x,t)-plane. Let

$$u_{\mathrm{L}}(t) \;=\; \lim_{x\to\xi(t)^-} u(x,t), \qquad u_{\mathrm{R}}(t) \;=\; \lim_{x\to\xi(t)^+} u(x,t)$$

be the values on the two sides of the discontinuity. Then by taking $t_1\to t_0$ in the integral form (3) we find that $u(x,t)$ is a weak solution if it satisfies

$$\frac{d}{dt}\int_\alpha^\beta u(x,t)\,dx \;=\; -f(u)\Big|_{x=\alpha}^{\beta} \;=\; f\big(u(\alpha,t)\big) \;-\; f\big(u(\beta,t)\big) \tag{5}$$

for all α, β, and t. Fix a time t and choose α and β on either side of $\xi(t)$. Then we can break the integral in (5) into two pieces, and apply (5) separately on the intervals $[\alpha,\xi(t)]$ and $[\xi(t),\beta]$. Thus

$$\begin{aligned}
\frac{d}{dt}\int_\alpha^\beta u\,dx \;&=\; \frac{d}{dt}\left(\int_\alpha^{\xi(t)} u\,dx \;+\; \int_{\xi(t)}^\beta u\,dx\right)\\
&=\; \xi'(t)\,u_{\mathrm{L}}(t) \;-\; f(u)\Big|_\alpha^{\xi(t)} \;-\; \xi'(t)\,u_{\mathrm{R}}(t) \;-\; f(u)\Big|_{\xi(t)}^\beta\\
&=\; \xi'(t)(u_{\mathrm{L}}-u_{\mathrm{R}}) \;-\; \big(f(u_{\mathrm{L}})-f(u_{\mathrm{R}})\big) \;-\; f(u)\Big|_\alpha^\beta\\
&= f\big(u(\alpha,t)\big) \;-\; f\big(u(\beta,t)\big)
\end{aligned}$$

The last equality must hold because u is satisfies (5). But we see that it can hold if and only if the discontinuity satisfies the Rankine-Hugoniot condition:

$$\xi'(t) \;=\; \frac{f(u_{\mathrm{L}})-f(u_{\mathrm{R}})}{u_{\mathrm{L}}-u_{\mathrm{R}}}. \tag{6}$$

That is, weak solutions can have discontinuities if the discontinuities propagate with the correct speed.

For example, a *stationary* discontinuity, with $\xi'(t)=0$, must have $f(u_{\mathrm{L}})=f(u_{\mathrm{R}})$: since none of the conserved quantity may accumulate on a thin line, the flux in from one side must exactly balance the flux out the other side.

If the discontinuity is moving this corresponds to some accumulation of material: the net accumulation must balance the net influx. For example,

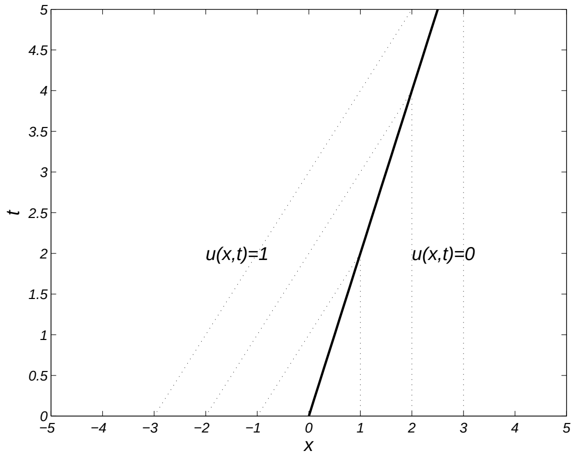

Figure 1: Bold line: the shock (discontinuity) travels on the line $t = 2x$. To the left, the solution is identically 1 and the characteristics (dotted lines) are travelling with speed 1. To the right, the solution is identically 0 and the characteristics (dotted lines) are stationary — they are vertical lines in the x-t plane. The characteristics run into the shock from both sides.

if we have initial data

$$u_0(x) = \begin{cases} 1 & x \leq 0 \\ 0 & \text{otherwise} \end{cases}$$

and the conservation law is $u_t + (u^2/2)_x = 0$ then the shock travels with speed

$$\xi'(t) = \frac{1/2 - 0}{1 - 0} = \frac{1}{2}$$

and the weak solution is

$$u(x,t) = \begin{cases} 1 & \text{if } x - t/2 < 0 \\ 0 & \text{otherwise} \end{cases}$$

Figure 1 shows this solution in the x-t plane.

Any smooth solution of $u_t + (u^2/2)_x = 0$ is also be a solution of the conservation law $(u^2)_t + 2/3\,(u^3)_x = 0$ and vice versa. These two conservation laws have the same smooth solutions. However, they have different weak solutions! For the same step-function initial data u_0, the Rankine-Hugoniot condition for $(u^2)_t + 2/3\,(u^3)_x = 0$ is:

$$\xi'(t) = \frac{2/3\ u_{\mathrm{R}}^3 - 2/3\ u_{\mathrm{L}}^3}{u_{\mathrm{R}}^2 - u_{\mathrm{L}}^2} = \frac{2}{3}$$

and so the weak solution is

$$u(x,t) = \begin{cases} 1 & \text{if } x - 2t/3 < 0 \\ 0 & \text{otherwise} \end{cases}$$

This shows that two hyperbolic conservation laws can have the same smooth solutions but have different weak solutions.

Physical examples

Before discussing more properties of these systems and how to solve them, it will be worthwhile to give a few examples. These are generally constructed by writing down all the quantities we know to be conserved, typically mass, momentum, energy, and then adding some constituitive relations to close the system.

Scalar equation: Traffic flow

Suppose $\rho(x,t)$ is the local density of traffic on a straight road (cars/km). The spacing is thus $1/\rho$, in km/car. Let $v(x,t)$ be the local speed (km/hour). We are implicitly assuming that local density and average velocity have a meaning; that is, we are not forced to write some kind of multi-agent model in which each vehicle acts completely independently.

The *flux* of cars is $q = \rho v$, the number of cars per hour passing a fixed point. Suppose we look at a fixed section of road $\alpha \le x \le \beta$. The total number of cars on this section is $\int_\alpha^\beta \rho(x,t)\,dx$. Conservation of cars says that cars do not appear or disappear in the middle of the road (there are no entrances or exits), so this number changes only due to fluxes in and out across the endpoints:

$$\frac{d}{dt}\int_\alpha^\beta \rho(x,t)\,dx \;=\; q(\alpha,t) \;-\; q(\beta,t).$$

Dividing by $\beta - \alpha$ and taking $\beta - \alpha \to 0$, with the assumption that $\rho(x,t)$ and $q(x,t)$ are smooth functions, gives the differential law

$$\rho_t \;+\; q_x \;=\; 0.$$

This is the canonical form of a conservation law with flux q. With our specific form, it becomes

$$\rho_t \;+\; (\rho v)_x \;=\; 0$$

which is also a standard form, when v transports the quantity represented by ρ. This is one PDE for two functions ρ, v. To solve it we must introduce another modeling assumption: a constituitive relation or "equation of state".

We assume that drivers choose their speed as a reaction to the local spacing of the cars around them: v is determined in terms of ρ by as function g, so that $v(x,t) = g\big(\rho(x,t)\big)$. This applies at each point of space, and each instant of time; the speed is assumed to respond instantly to changes of density. Then $q = \rho\, g(\rho) \equiv f(\rho)$, and we have the single conservation law

$$\rho_t \;+\; f(\rho)_x \;=\; 0$$

in the form (1). For comparison, we had obtained the diffusion equation by assuming that q depended on the *gradient* of ρ: the linear Fourier law $q = -\kappa\rho_x$ gives the heat equation.

The characteristic speed, the propagation speed of small disturbances, is $a(\rho) = f'(\rho) = \rho\, g'(\rho) + g(\rho)$. The maximum flux happens where f is maximized, at ρ_* such that $-g'(\rho_*) = g(\rho_*)/\rho_*$. This is why there are sometimes stoplights at the entrances to tunnels: if the oncoming traffic has $\rho > \rho_*$ then stopping cars lets them drive faster after they are freed, *increasing* the total flux through the tunnel.

Let's propose some specific choices for $g(v)$. We assume that it decreases from $g(0) = v_{\max}$, representing the speed of cars on a nearly empty road, to $g(\rho_{\max}) = 0$, representing bumper-to-bumper traffic in which no car is moving. It is plausible to assume that speed is not reduced very much by having only a few cars per km of roadway, so we suppose that $g'(0) = 0$. The simplest expression satisfying these conditions is the quadratic

$$g(\rho) \;=\; v_{\max}\left(1 - \left(\frac{\rho}{\rho_{\max}}\right)^2\right)$$

which gives the flux

$$q \;=\; f(\rho) \;=\; \rho\, v_{\max}\left(1 - \left(\frac{\rho}{\rho_{\max}}\right)^2\right)$$

and the characteristic speed

$$a(\rho) \;=\; f'(\rho) \;=\; v_{\max}\left(1 - 3\left(\frac{\rho}{\rho_{\max}}\right)^2\right)$$

The max flux is attained at $\rho_* = \rho_{\max}/\sqrt{3} \approx 0.577\rho_{\max}$. At that speed, small disturbances move neither forward nor backward relative to the roadway, although the cars are moving through them at speed $v_* = g(\rho_*) = (2/3)v_{\max}$. At low densities, $\rho \to 0$, disturbances propagate at speed $a(0) = v_{\max}$, along with the cars. At high densities, disturbances propagate *backwards* along the road at speed $-a(\rho_{\max}) = 2v_{\max}$. This backwards propagation is how you detect a traffic jam ahead of you, as we will see below.

Second-order system: Shallow-water equations

Imagine a thin layer of fluid on a rigid surface: the ocean (ignoring the shape of the bottom) or the water in your kitchen sink when the faucet is running and the drain is open. Let $h(x,t)$ denote the depth of the layer, and $v(x,t)$ its depth-averaged horizontal velocity. You may assume the velocity is constant as a function of depth but we need only the average. We suppose the layer is shallow enough that this average velocity tells us everything we need about the motion of the fluid (no vortices or turbulence). Thus, for example, this model does *not* describe ordinary surface waves on the ocean surface; it would apply to seismically generated waves (tsunami) whose wavelength is much longer than the ocean depth, so that the whole vertical column roughly slides forward and backward as a single unit.

By the definition of depth-averaging, the total mass moving from left to right past location x per unit time is $q = hv$. Then just as above, we have the conservation law

$$h_t \;+\; (hv)_x \;=\; 0. \tag{7}$$

Now, however, because the fluid has momentum its velocity is not simply determined in terms of the height or its gradients: we need a second dynamic equation to describe v.

The hydrostatic pressure in the fluid increases linearly from zero at the free surface to $\rho g h$ at the bottom of the layer, where ρ is the density. Thus the average pressure is $\frac{1}{2}\rho g h$, and the total force exerted by one parcel of fluid on its neighbor is $\frac{1}{2}\rho g h^2$. The momentum per unit x is $\rho h v$. Motion of the fluid carries momentum along with it, and momentum changes due to forces exercised on the fluid. We suppose that there is no viscous drag where the fluid moves over the bottom, so no momentum is transferred to the rigid surface. Then conservation of momentun says that for fixed α, β,

$$\frac{d}{dt}\int_\alpha^\beta \rho\, h\, v\, dx \;=\; \left[\rho h v^2 + \tfrac{1}{2}\rho g h^2\right]_{x=\alpha} \;-\; \left[\rho h v^2 + \tfrac{1}{2}\rho g h^2\right]_{x=\beta}$$

giving (the fluid is incompresible, so ρ is fixed and constant)

$$(hv)_t + \left(hv^2 + \tfrac{1}{2} g h^2\right)_x \;=\; 0. \tag{8}$$

This equation asserts that the "momentum flux" is $hv^2 + \frac{1}{2}gh^2$. This notion may take a little while to get used to: the first term $hv{\cdot}v$ represents transport of momentum just as though it were a physical quantity carried by the fluid. The second term represents hydrostatic force which is a more usual way to transfer momentum.

If you prefer, you may consider the end points $\alpha(t)$ and $\beta(t)$ to drift with the fluid, so that $\alpha'(t) = v\big(\alpha(t), t\big)$ and $\beta'(t) = v\big(\beta(t), t\big)$. Then the quantity of fluid between $\alpha(t)$ and $\beta(t)$ is a real physical chunk of material. Conservation of momentum then says

$$\frac{d}{dt}\int_{\alpha(t)}^{\beta(t)} \rho\, h\, v\, dx \;=\; -\Big[\tfrac{1}{2}\rho g h^2\Big]_{x=\alpha}^{\beta}.$$

Differentiating the integral, including the endpoints, gives the same results as above. This derivation seems to assume that v is constant through the fluid depth (so there is no leakage at the endpoints) but the result still holds as long as v is the average.

Eqs. (7,8) give a 2×2 system of the form (2) with

$$u = \begin{pmatrix} h \\ v \end{pmatrix}, \qquad g(u) = \begin{pmatrix} h \\ hv \end{pmatrix}, \qquad f(u) = \begin{pmatrix} hv \\ hv^2 + \frac{1}{2}gh^2 \end{pmatrix}$$

To write it in the form (1), we introduce the momentum $m = hv$, and get

$$u = \begin{pmatrix} h \\ m \end{pmatrix}, \qquad g(u) = u, \qquad f(u) = \begin{pmatrix} m \\ \dfrac{m^2}{h} + \dfrac{1}{2}\, gh^2 \end{pmatrix}$$

which you may or may not prefer.

Starting from the second form, we calculate the Jacobian matrix

$$A(h, m) \;=\; \nabla f \;=\; \begin{pmatrix} 0 & 1 \\ -\dfrac{m^2}{h^2} + gh & \dfrac{2m}{h} \end{pmatrix}.$$

Its eigenvalues are $(m/h) \pm \sqrt{gh} = v \pm \sqrt{gh}$. Small waves move with the fluid velocity, plus or minus the wave speed $\sqrt{gh}$. Like the 2×2 linear wave equation, this system has two characteristic modes corresponding to left- and right-going waves.

Isentropic gas dynamics

Suppose we have a compressible gas in a tube. We assume it undergoes one-dimensional motion, with no friction at the walls. If its local density is ρ, local pressure is p, and x-velocity is v, then conservation of mass and momentum give

$$\begin{aligned} \rho_t + (\rho v)_x &= 0 \\ (\rho v)_t + \left(\rho v^2 + p\right)_x &= 0. \end{aligned}$$

Just as for the shallow water equation, the momentum flux has two terms: the first term represents transport and the second is momentum transfer by forces exerted by one piece of fluid on its neighbor. If you prefer, the second equation may also be written (using the first one) as

$$v_t + v\, v_x = -\frac{1}{\rho}\, p_x.$$

This gives an explicit expression for v_t, but it is not in conservation form.

To close the system, an equation of state $p(\rho)$ must be specified. In doing this, we assume that the temperature does not need to be given separately; that is, each parcel of gas compresses and expands without exchanging any heat with its neighbors. If it did exchange heat, then we would have to introduce an additional thermodynamic variable to track the heat content.

For a polytropic ideal gas, the *isentropic* equation of state is $p = C\rho^\gamma$, where γ is the ratio of specific heats. It may be written $\gamma = (\alpha+2)/\alpha$, where α is the number of degrees of freedom of each gas molecule. For a monatomic gas (He,Ar) $\alpha = 3$ and $\gamma = 5/3$. For diatomic (N_2, O_2) $\alpha = 5$ and $\gamma = 1.4$. Setting $\gamma = 2$ recovers the shallow-water equations.

Nonisentropic gas dynamics

The gas may be nonisentropic, either due to inhomogeneous initial temperature, or chemical reactions that release heat energy directly into the gas. Then we have to account for the internal energy separately.

Let us denote E the total energy per unit mass. This is commonly written

$$E = \frac{1}{2}\rho v^2 + \rho e,$$

where the internal energy $e(p,\rho)$ comes from the equation of state; for an ideal gas, $e = c_v T = p/(\gamma - 1)\rho$. Then we get the 3×3 system

$$\begin{aligned} \rho_t \; + \; (\rho v)_x \; &= \; 0 \\ (\rho v)_t \; + \; \left(\rho v^2 + p\right)_x \; &= \; 0 \\ (\rho E)_t \; + \; \left(v(E+p)\right)_x \; &= \; 0. \end{aligned}$$

The additional mode corresponds to *contact discontinuities*, variations of temperature with uniform pressure and velocity.