Flux-Conservative Initial Value Problems

The prototypical Example: One-Dimensional Linear Advection

Models transport of a scalar quantity u (concentration, temperature...) in a medium flowing with velocity v (flow direction for $v > 0$ in positive x-diretion).

$$\begin{array}{ll} u_t + v u_x = 0 & \text{for } u = u(x,t); \quad 0 < x < 1, \quad t > 0; \\ & v \text{ given, constant;} \\ u(x,0) = u_0(x) & \text{initial condition for } t = 0, \quad 0 \le x \le 1; \\ u(0,t) = a & \text{boundary condition at } x = 0, \quad t > 0. \end{array} \tag{1}$$

Analytical solution

Executive Summary: The exact solution is the initial profile $u_0(x)$ moving with velocity v along the x-axis.

For constant v and an arbitrary function $u_0(x)$, define

$$u(x,t) = u_0(x - vt).$$

Assuming suitable differentiability, you will easily check that this $u(x,t)$ fulfills the differential equation (1) with initial condition $u(x,0) = u_0(x)$ for $0 \le x \le 1$, and the boundary condition $u(0,t) = u_0(-vt)$ for $t > 0$.

The solution of 1 therefore is

$$u(x,t) = \begin{cases} a & \text{for } 0 \le x < vt, \\ u_0(x - vt) & \text{for } vt \le x < 1. \end{cases} \tag{2}$$

Sample initial condition: a triangular spike

$$u_0(x) = \begin{cases} 10x & \text{for } 0 \le x < 0.1 \\ 2 - 10x & \text{for } 0.1 \le x < 0.2 \\ 0 & \text{else} \end{cases} \tag{3}$$

Even though this initial condition is not differentiable at $x = 0, x = 0.1$ and $x = 0.2$, we will consider $u_0(x - vt)$ as a solution of the PDE - wherever derivatives exists, it fulfils the PDE, and the differentiable pieces fit together. (In the next section, we will give an *integral formulation* with more relaxed differentiability conditions.)

Figure 1 shows profiles of this solution at two time levels in the xu-plane.

A solution $u(x,t)$ of the PDE in (1) defines a surface in xtu-space. Figure 2 shows this surface.

One way to represent a surface is by contour lines (isolines) in the xt-plane. Consider the family of straight lines

$$x - vt = c. \tag{4}$$

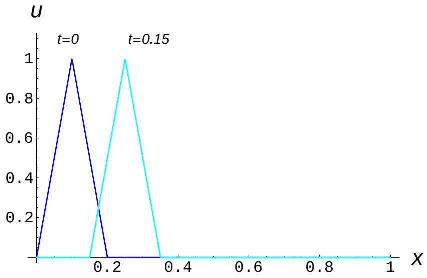


Figure 1: Initial condition and solution of $u_t + u_x = 0$ after $t = 0.15$. Zero boundary condition at left end. The spike travels with velocity $v = 1$ from left to right.

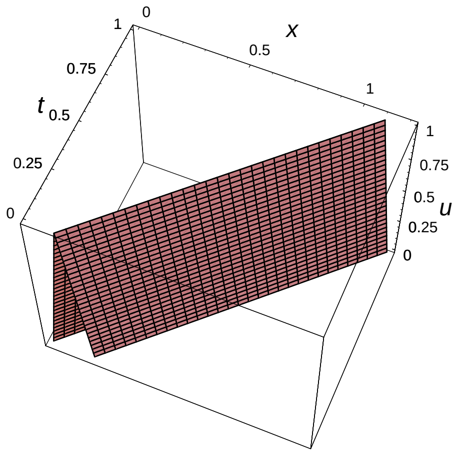


Figure 2: The solution, represented as a surface in xtu-space. Compare Figure 1, which shows cross sections of this surface along planes $t = 0$ and $t = 0.15$. Figure 3 shows isolines of this surface in the xt-plane.

Simple fact: If a function $u = u(x, t)$ solves the PDE in Equation (1), then the straight lines (4) are isolines. Proof: set $x(t) = c - vt$, insert in u: $u = u(x(t), t)$ and show that

$$\frac{d}{dt}u(x(t), t) = 0$$

Figure 3 shows isolines of this surface in the xt-plane. The straight lines defined by Equation (4) are an example of *characteristic lines*—see later!

Scalar conservation, integral and quasilinear form

The general form of a scalar conservation law is

$$u_t + f(u)_x = 0 \tag{5}$$

for a function $u = u(x, t)$, the *conserved quantity* (e.g. some sort of mass or energy density), and a *flux function* $f = f(u)$.

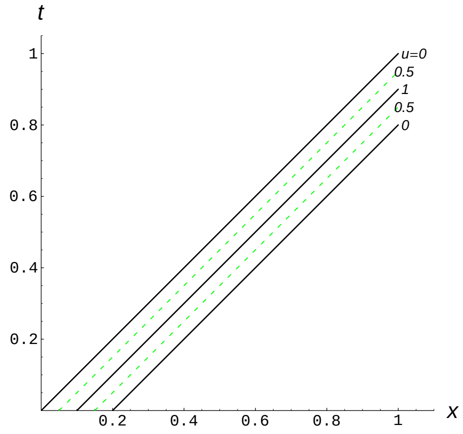


Figure 3: The solution of our simple advection problem, represented by contour lines in the xt-plane.

Integrate Equation (5) form $x = a$ to $x = b$:

$$\int_a^b u_t dx + \int_a^b f(u)_x dx = 0$$

Switch in the first term differentiation with respect to time with integration in x, and evaluate the second term to get

$$\frac{d}{dt}\int_a^b u dx = f(a) - f(b)$$

Interpretation: The rate of change for the total amount of u in the interval $[a, b]$ is the difference of inflow at a minus outflow at b.

Differentiating with the chain rule gives the *quasilinear form* of Equation (5)

$$u_t + f(u)_x = 0 \quad \longrightarrow \quad u_t + f'(u)u_x = 0 \qquad \text{(equivalent for differentiable } f \text{ and } u\text{).}$$

Explicit difference schemes for the linear advection problem

Exercises Derive difference schemes for the simple linear advection equation and try them for the spike initial condition.

Try also a linear advection equation with spatially variable velocity $v = v(x)$,

$$u_t + (v(x)u)_x = 0$$

Specifically, assume $v(x) = x$ or $v(x) = 1 + x(x - 1)$.

FTCS

FTCS = "Forward-in-Time, Centered-in-Space". For

$$C = \frac{v\Delta t}{h} \qquad \text{Courant Number}$$

the FTCS-Stencil is

$$\begin{array}{ccccc} & & 1 & & \\ & & \uparrow & & \\ \frac{C}{2} & — & 1 & — & -\frac{C}{2} \end{array}$$

- Straightforward, easy to derive, unstable and useless.
- Note, however, that FTCS works (conditionally stable) for the heat equation.

Lax-Friedrichs

replaces u_j^n in the FTCS scheme by the arithmetic average of its neighbors, $(u_{j-1}^n + u_{j+1}^n)/2)$.

$$\begin{array}{ccccc} & & 1 & & \\ & & \uparrow & & \\ \frac{1+C}{2} & — & 0 & — & \frac{1-C}{2} \end{array}$$

- Conditionally stable for $|C| \leq 1$
- second-order in space (theoretically), but very diffusive (practically)
- works for positive and negative v
- mesh decoupling
- $|C| = 1$ gives the exact solution; in practice, however, v is not constant, and you cannot have $|C| = 1$ everywhere in your problem)

Lax-Wendroff

adds just the necessary amount of diffusion to the FTCS scheme to make it conditionally stable.

$$\begin{array}{ccccc} & & 1 & & \\ & & \uparrow & & \\ \frac{C}{2} + \frac{C^2}{2} & — & 1 - C^2 & — & -\frac{C}{2} + \frac{C^2}{2} \end{array}$$

- Conditionally stable for $|C| \leq 1$
- second order in space, less diffusive than Lax-Friedrichs and Upwind

Upwind

One-sided formula for spatial derivative

$$\begin{array}{ccccc} & & 1 & & \\ & & \uparrow & & \\ C & — & 1 - C & — & \end{array}$$

- Conditionally stable for $0 \leq C \leq 1$

- standard first-order scheme for convective terms (especially in nonlinear problems).
- if v changes sign, you have to switch the upwind direction in the scheme
- motivated by underlying physics of hyperbolic PDEs: only data from the direction of incoming flow can causally influence the solution.

Beam-Warming

A two-point upstream scheme

$$\begin{array}{ccccc} & & & & 1 \\ & & & & \uparrow \\ -\frac{C}{2}+\frac{C^2}{2} & — & 2C-C^2 & — & 1-\frac{3C}{2}+\frac{C^2}{2} \end{array}$$

Method of characteristics for first-order PDEs

(I borrowed much of this paragraph from the English Wikipedia; the German Wikipedia article ,,Methode der Charakteristiken" links to a skript of ETH Zürich. It discusses characteristics for the advection equation, with just a bit more mathematics.)

For a first-order PDE the method of characteristics discovers curves (called *characteristic curves* or *characteristics*) along which the PDE degenerates into an ordinary differential equation (ODE). Once the ODE is found it can be solved along the characteristic curves and transformed into a solution for the original PDE.

Consider a first-order PDE of the general form

$$au_t + bu_x = c,$$

where a, b and c may be constant or functions of x, t and u. The advection equation $u_t + vu_x = 0$ is a very simple case with $a = 1$, $b = v$, $c = 0$.

We want to find a curve in the xtu-space in parametric form, depending on the parameter s,

$$\begin{aligned} x &= x(s) \\ t &= t(s) \\ u &= u(s) \end{aligned}$$

so that the PDE can be reformulated into an ODE along the curve; i.e. something of the form

$$\frac{d}{ds}u(x(s),t(s)) = F(u,x(s),t(s))$$

.

The curve $(x(s), t(s), u(s))$ (or just its projection in the xt-plane) is called a characteristic line. To find it, we differentiate by the chain rule.

$$\frac{d}{ds}u(x(s),t(s)) = u_x\frac{dx}{ds} + u_t\frac{dt}{ds}$$

Now, notice if we set $\frac{dx}{ds} = b$ and $\frac{dt}{ds} = a$ we get $au_t + bu_x$, which happens to be the left-hand side of the PDE we started with. Thus

$$\frac{d}{ds}u = au_t + bu_x = c.$$

In fact, we now have a coupled system of *three* ODEs to solve:

$$\frac{dx}{ds} = b$$
$$\frac{dt}{ds} = a$$
$$\frac{du}{ds} = c$$

In the case of the linear, constant-coefficient advection equation $u_t + vu_x = 0$, the ODEs are simple to solve.

$$\begin{aligned}
\frac{dt}{ds} &= 1, && \text{letting } t(0) = 0 \text{ we know } t = s \\
\frac{dx}{ds} &= v, && \text{letting } x(0) = x_0 \text{ we know } x = vs + x_0 \\
\frac{du}{ds} &= 0, && \text{letting } u(0) = u_0(x_0) \text{ and substituting from above } x_0 = x - vt, \\
& && \text{we get } u(x(s), t(s)) = u_0(x_0) = u_0(x - vt)
\end{aligned}$$

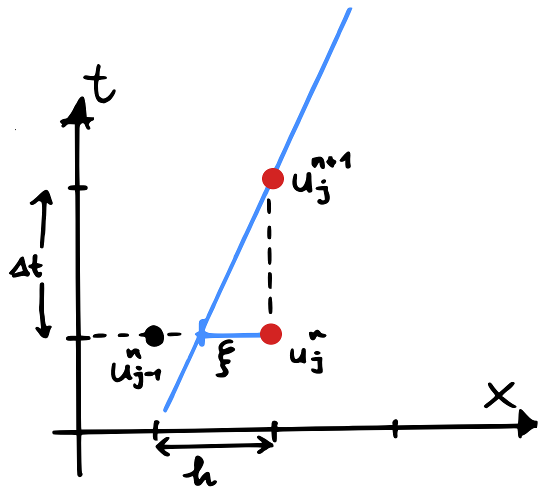
This set of equations defines characteristic curves as parametric curves in xtu-space. Sometimes (like in the Wikipedia article) also the projections of these curves in the xt-plane are called characteristics.

For our example, the linear, constant-coefficient advection equation, the characteristic lines in the xt-plane are straight lines with slope $1/v$. In general, they could be curves. The value of u remains constant along the curve — which means, they are contour lines of u. (This property holds only because $c = 0$).

Characteristics are a powerful tool for gaining qualitative insights into PDE. This kind of knowledge is useful when solving PDEs numerically as it can indicate which finite difference scheme is best for the problem.

Differenzenverfahren und Charakteristiken

Für die lineare Advektionsgleichung $u_t + vu_x$ sind die charakteristischen Kurven in der xt-Ebene Gerade mit Steigung $1/v$. Entlang dieser Geraden ist u konstant.



Die Abbildung zeigt Lösungswerte u_{j-1}^n, u_j^n, u_{j+1}^n, u_j^{n+1} in den Gitterpunkten eines Differenzenverfahrens (den „Stern“). Eingezeichnet ist auch die Charakteristik durch u_j^{n+1}. Das Zeitniveau n schneidet sie zwischen u_{j-1}^n und u_j^n. Dort lässt sich der Wert u_ξ auf der Charakteristik aus linearer Interpolation bestimmen:

$$u_\xi = u_j^n + \frac{\xi}{h}(u_{j-1}^n - u_j^n)$$

Weil u konstant entlang der Charakteristik ist, ergibt sich daraus $u_j^{n+1} = u_\xi$.

- Drücken Sie ξ durch v und Δt und anschließend $\frac{\xi}{h}$ durch die Courant-Zahl C aus. Stellen Sie eine explizite Formel für u_j^{n+1} auf.
- Vergleichen Sie: ist diese Formel neu oder entspricht sie einem bekannten Differenzenverfahren?
- Was erhalten Sie bei linearer Interpolation zwischen u_{j-1}^n und u_{j+1}^n?
- Und was ergibt quadratische Interpolation?

Other linear and quasi-linear examples

The advection equation is a simple example for a first-order linear partial differential equation. The general form for this type of equation for an unknown function $u(x_0, \ldots, x_n)$ would be

$$\sum_{i=0}^{n} a_i u_{x_i} = a,$$

where a_i and a are continuously differentiable functions of $x_0, \ldots, x_n$; in the case of a quasilinear equation the coefficients do not only depend on $x_0, \ldots, x_n$ but also on the unknown u.

In our first example, the advection equation, the independent variables are $x_0 = t$ and $x_1 = x$; the attribute “one-dimensional” refers to the spatial coordinate.

Spatially three-dimensional versions for a flow field $\mathbf{v} = \mathbf{v}(\mathbf{x})$ and a source term $S(\mathbf{x}, t)$ (conservation equation for a passive scalar):

$$u_t + \operatorname{div}(\mathbf{v}\, u) = S.$$

Quasi-linear relatives: inviscid Burgers' equation (models gravity waves in shallow water)

$$u_t + u\, u_x = 0.$$

Burgers' equation can be written in a different form (conservation form, see below), which is equivalent for smooth solutions.

$$u_t + \left(\frac{1}{2}u^2\right)_x = 0.$$

If we multiply the quasilinear equation by $2u$ first,

$$2u u_t + 2u^2\, u_x = 0,$$

the conservation form is

$$(u^2)_t + \left(\frac{2}{3}u^3\right)_x = 0.$$

Another formulation, also in conservation form: for solutions $u(x) \neq 0\ \forall x$ we could divide by u and write

$$(\log u)_t + u_x = 0$$

Now set $w = \log u$, then

$$w_t + (\exp w)_x = 0$$

is another conservation equation, equivalent for smooth solutions but giving different front positions when discontinuities develop.

Which of the three equations is "the right one"? This depends on the quantity that is conserved in physical reality: u, u^2 or $\log u$, respectively.

Exercises

Check difference schemes for a nonlinear advection equation $u_t + (v(u)u)_x = 0$ where v depends on u in the form $v = u/2$ (Burgers' equation). Try them for the spike initial condition.

Systems of conservation laws

General form of a *system of conservation laws* in one space dimension

$$\mathbf{u}_t + \mathbf{F}(\mathbf{u})_x = 0$$

In two- or three-dimensional space

$$\mathbf{u}_t + \operatorname{div} \mathbf{F}(\mathbf{u}) = 0$$

also written as

$$\mathbf{u}_t + \nabla \cdot \mathbf{F}(\mathbf{u}) = 0$$

The vector $\mathbf{u}$ contains the conserved quantities; their transport is governed by a *conserved flux* vector $\mathbf{F}(\mathbf{u})$. Meaning: for any component of $\mathbf{u}$ and any interval on the x-axis (or area or volume in space), accumulation equals the net flux across the boundary.

Remember Equation (5), the scalar equation $u_t + f(u)_x = 0$. Integrate it over an interval,

$$\int_a^b (u_t + f(u)_x) dx = 0, \quad \text{gives } \frac{d}{dt}\int_a^b u\, dx = f(a) - f(b)$$

for arbitrary intervals $[a, b]$ in the spatial domain of u.

Interpretation: The rate of change of the "total amount of u", i.e. the integral of u in some spatial domain is the difference of in- and outflow across the ends of the interval. The same statement holds in two or three space dimensions.

A difference scheme that preserves this property is called *conservative*.

For smoothly differentiable u this integral formulation is mathematically equivalent to the differential equation.

Weak solutions

Because $\frac{d}{dt}\int_a^b u\, dx$ is only defined for u sufficientltly smooth with respect to t, we integrate also over a time interval, so that the time derivative vanishes.

$$\int_{t_0}^{t_1}\int_a^b (u_t + f(u)_x)\, dxdt = 0, \quad \text{yields}$$

$$\int_a^b u|_{t=t_1}\, dx - \int_a^b u|_{t=t_0}\, dx = \int_{t_0}^{t_1} (f(b) - f(a))\, dt.$$

Verbal formulation: The difference of the "total amount" of u between t_0 and t_1 in some spatial domain equals the difference between in- and outflow during that time interval.

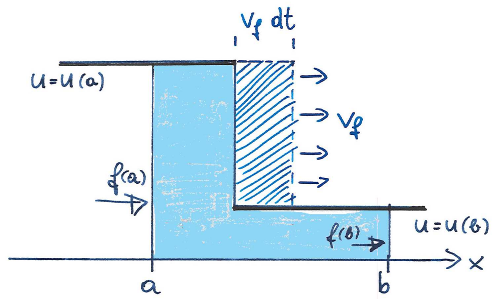
We define a *weak solution* of the conservation law as a function u which fulfils the integral form above for arbitrary $[a, b]$ and t_0, t_1 within the domain of u.

A weak solution is defined for a much larger class of problems and initial conditions than a solution of the PDE in the classical sense. In our example with the advection equation, the traveling triangular spike is not everywhere differentiable, so it is not really a classical solution of the PDE, but it clearly is a weak solution.

Rankine-Hugoniot Condition

Important features that may develop in weak solutions are *shock fronts*. These are discontinuities (steps, jumps), which travel along in time.

Let there be a front at a position $x_f = x_f(t)$ (between a and b in the drawing). The conservation law provides a relation, the *Rankine-Hugoniot condition*, between front speed $v_f = \frac{dx_f}{dt}$ and jump height.



The condition is

$$v_f = \frac{[f(u)]}{[u]},$$

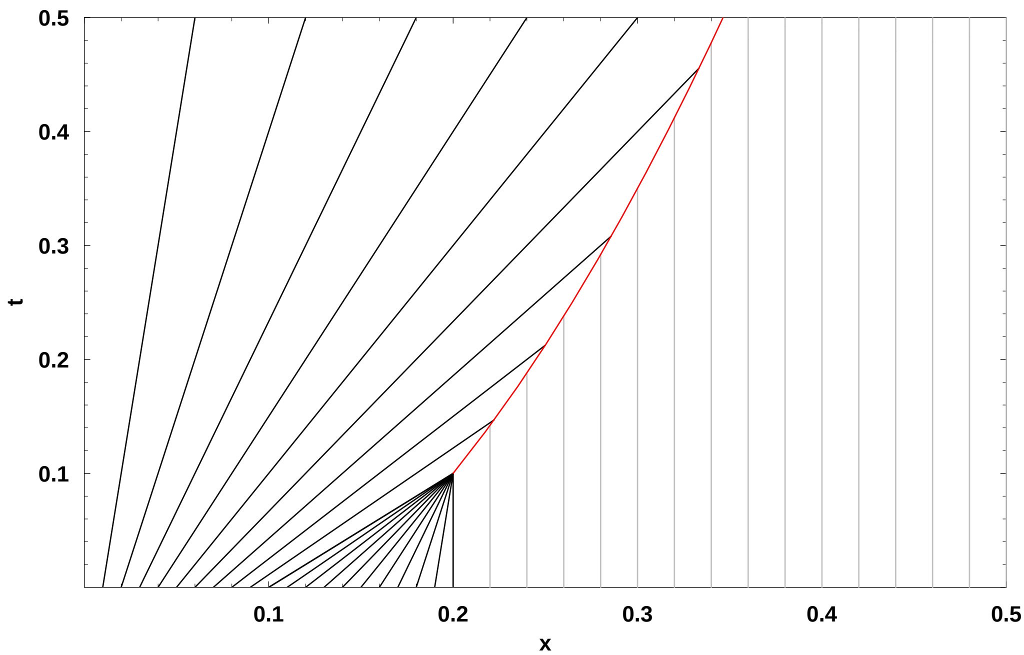
where the square brackets $[\cdot]$ denote difference between the limit values from left and right at the front.

Eine Lösung der Burgers-Gleichung im Charakteristiken-Diagramm

Für die Burgers-Gleichung $u_t + (u^2/2)_x = 0$ sind die Charakteristiken in der xt-Ebene Gerade mit Steigung $\frac{dx}{dt} = u$. Entlang einer Charakteristik ist der Wert von u konstant.

Das Diagramm zeigt Charakteristiken zu den Werten $u = 0, \frac{1}{10}, \frac{2}{10}, \ldots 1$ für eine dreieckige Zacke als Anfangsbedingung (linearer Anstieg von $u_0 = 0$ auf $u_0 = 1$ zwischen $x = 0$ und $x = \frac{1}{10}$, danach linearer Abfall auf $u_0 = 0$ bis $x = \frac{2}{10}$

Ab $t = \frac{1}{10}$ entsteht eine Schockfront. An ihr treffen Charakteristiken für $u > 0$ von links mit Charakteristiken für $u = 0$ von rechts zusammen.



- Beschriften Sie die Charakteristiken im linken Bereich, soweit es der Platz zulässt, mit den entsprechenden u-Werten.
- Skizzieren Sie den Verlauf der Lösung zur Zeit $t = \frac{1}{2}$ für $0 \leq x \leq 0.5$. Achten Sie insbesondere auf die korrekte Frontposition und -höhe.

- Zu $t = 0{,}45$ trifft von links die Charakteristik zu $u = 0{,}603$ auf die Front. Welche Frontgeschwindigkeit ergibt sich aus den Rankine-Hugoniot-Bedingungen?
- Die Steigung der Front-Linie im Charakteristiken-Diagramm hängt mit der Frontgeschwindigkeit zusammen. Die Gleichung der Kurve in diesem Diagramm lautet

  $$x_f = \frac{\sqrt{10t+1}}{5\sqrt{2}}$$

  Bestimmen Sie die Frontgeschwindigkeit für $t = 0{,}45$.

Examples for Nonlinear Systems of Conservation Laws

Euler's equations for one-dimensional gas flow

$$\begin{bmatrix} \rho \\ \rho v \\ E \end{bmatrix}_t + \begin{bmatrix} \rho v \\ \rho v^2 + p \\ v(E+p) \end{bmatrix}_x = 0$$

Here, p is defined via the polytropic equation

$$p = (\gamma - 1)(E - \frac{1}{2}\rho v^2), \quad \gamma = \frac{7}{5} \text{ in air .}$$

Isothermal flow (c is the sound speed)

$$\begin{bmatrix} \rho \\ \rho v \end{bmatrix}_t + \begin{bmatrix} \rho v \\ \rho v^2 + c^2 \rho \end{bmatrix}_x = 0$$

Shallow-water waves (φ stands for gh)

$$\begin{bmatrix} v \\ \varphi \end{bmatrix}_t + \begin{bmatrix} v^2/2 + \varphi \\ v\varphi \end{bmatrix}_x = 0$$

Although the system is frequently written in this form (which is in conservation form), it delivers the correct solution only as long as it remains smooth. For shock fronts (means breaking waves) the jump conditions come out wrong. Physically, not the velocity v but the momentum $v\varphi$ is the correct conserved quantity. Thus, the physically correct conservation form is

$$\begin{bmatrix} v\varphi \\ \varphi \end{bmatrix}_t + \begin{bmatrix} v^2\varphi + \varphi^2/2 \\ v\varphi \end{bmatrix}_x = 0$$

Hyperbolic systems

The system

$$\mathbf{u}_t + \mathbf{F}(\mathbf{u})_x = 0$$

is called *hyperbolic* if for all values $\mathbf{u}$ all eigenvalues of the Jacobian $\mathbf{F}'$ are real and the corresponding eigenvectors are linearly independent. Hyperbolic systems describe phenomena with *finite speed of propagation*. The solution $u(x, t)$ in some point (x, t) can be influenced by initial conditions in a *bounded* interval. Whatever the initial conditions may look like outside this interval, they have no bearing on the solution in (x, t).

Why this eigenvalue condition? For a general linear, constant coefficient one-dimensional system of partial differential equations

$$\mathbf{u}_t + A\mathbf{u}_x = 0$$

hyperbolicity means that all eigenvalues of A are real, and the corresponding eigenvectors are linearly independent. In this case, A can be written as

$$A = S \cdot D \cdot S^{-1}$$

where the columns of S are the eigenvectors of A and D is a diagonal matrix of corresponding eigenvalues. Then,

$$\begin{aligned} \mathbf{u}_t + A \cdot \mathbf{u}_x &= 0 \\ \mathbf{u}_t + S \cdot D \cdot S^{-1} \cdot \mathbf{u}_x &= 0 \qquad | \quad \cdot S^{-1} \\ S^{-1} \cdot \mathbf{u}_t + D \cdot S^{-1} \cdot \mathbf{u}_x &= 0 \end{aligned}$$

We can define a new vector of unknowns, $\mathbf{v} = S^{-1} \cdot \mathbf{u}$ and reduce the system to an uncoupled system of equations

$$\mathbf{v}_t + D\mathbf{v}_x = 0$$

Each equation of that system is then a one-dimensional advection equation of the form treated already.

In the general case, the eigenvectors and eigenvalues are no longer constant, and the transformation to an uncoupled system is more complicated (if possible at all). There are *characteristic curves* in the xt-plane, along which the *Riemann invariants* (functions of the dependent variables) remain constant. A Riemann invariant propagates quite like the solution of the prototypical one-dimensional advection equation.

The situation is different for parabolic equations. Take the prototypical example, the one-dimensional heat equation. Initial conditions far away from some point affect the solution there instantly (infinite signal speed; no contradiction to relativity, though, because this equation is not valid on the atomic scale). Still, as for hyperbolic equations, boundary conditions in the future do not affect the past.

For elliptic equations, the solution is influenced by the whole boundary (therefore a reasonable elliptic equation does not contain a time variable).