

Chapter 3

Modeling Methods and Examples

As is usually the case models are first generated to describe physical processes which are stripped-down to their most important characteristic. If for instance we are to model traffic on the road we might start by assuming, at the beginning at least, that the weather will not be a factor, or that we only have 1 lane on the road, or that there are no traffic lights (a highway), or even that there are no entrances or exits. Naturally all these assumptions are too severe if we were to model the traffic in reality but at least by eliminating all these extra factors we have a better chance of obtaining a good initial model for traffic where still other important variables are accounted for. Once we are convinced that our initial model is good enough and compares well to expectations and traffic observations then we can enrich it with further and finer in detail extra factors (weather, extra traffic lanes, traffic lights etc.).

Similarly, when forecasting the weather we have some underlying simple models which help us into our predictions. These models initiate from some amazingly simple assumptions. If for instance you are trying to obtain a global weather model you might try and do a good job at predicting the weather mainly in the equator. It has been observed that the weather in the rest of the world is highly influenced and therefore dependent on equator weather. So this in effect decreases drastically the size of your domain. Further though we can simplify the situation even more by assuming that there is a stratification effect in the altitude of the atmosphere. In a way this allows us to treat the atmosphere as 2-dimensional planes one on top of the other instead of the much more complicated 3-dimensional domain which it really is. This assumption although significant is also not unrealistic for most cases as long as you allow these 2-dimensional planes to “talk” or “see” each other so that weather can flow through them. All in all these assumptions help in relieving the complications associated with such a complicated mathematical undertaking as modeling the weather.

These are only a few of the several examples where simplifying assumptions are commonly used in order to simplify the modeling process. We will follow these ideas and present some of those simple models. They may not immediately make perfect sense but we will revisit them later and try to understand the reasons behind their derivations.

3.1 One-dimensional Traffic flow

We consider a one-dimensional highway without entrances or exits. This may seem unreal but in fact it is common to start the model from such a very simple situation and even today active research is occurring with exactly these type of assumptions. A very realistic example of such a situation would

correspond to the Holland tunnel (or any other tunnel for that matter) in New York. Normally you are not supposed to change lanes while in the tunnel and therefore for all practical purposes you are essentially driving on a one-lane highway. Also it is clear that there are no entrances or exits for such a situation.

We will start by assigning variables to some of the quantities of interest which we believe are important to monitor through our mathematical model. This is usually not a very easy task. We must find as few variables as possible which on the other hand will be able to capture as much or most of the pertinent information about the traffic on the highway.

It seems necessary that the number of vehicles on the highway should be an important variable which we will denote by c and call “density”. Naturally density measures the number of vehicles per mile. Similarly vehicle velocities v ought to be important when trying to model the flow of traffic. Velocity is measured in miles per hour (at least for American highways). There are in fact several other variables we can probably think. For instance flow should be an important variable when trying to obtain a model for vehicular traffic flow. We denote flow as q and is measured in vehicles per hour. Notice however that once you know the vehicles densities (in vehicles per mile) and their velocities (in miles per hour) then you automatically know the flow (in vehicles per hour) since

$$q = cv. \quad (3.1)$$

In other words it seems unnecessary to create a model where all three such variables are included since knowing any two of them automatically would produce the third.

The simplest possible model for vehicular traffic flow is just a description of how any two of those variables interact mathematically in time and produce realistic results for a stream of vehicles. This simple and well-known model is called the Lighthill-Whitham-Richards model,

$$\frac{\partial c}{\partial t} + \frac{\partial q}{\partial x} = 0 \quad (3.2)$$

and was discovered in 1955 by these three researchers. This equation falls under the general category of scalar “conservation law”. It is called scalar because, as is clear in this case at least, we are modeling one-dimensional flows. It is a conservation law on the other hand because it describes the fact that total mass (or density of vehicles) is conserved. In other words no vehicles will be created or destroyed (at least we hope so) on the highway. This idea of conservation of mass is in fact responsible and gave rise to equation (3.2) itself.

3.1.1 Derivation of conservation laws

When trying to create a general model describing a given physical process it is natural to want to keep intact certain properties of that process which are considered so important that violating them would imply that your model is useless. Clearly if (3.2) ended up producing more vehicles through time or on the other hand we somehow ended up losing all the vehicles we started with then that would be a clear indicator that our equation is not really describing the problem we wished for in the first place. Thus realizing how important this conservation of mass (or vehicles) property is we in fact would want to create a model which in its very creation assures this property. We therefore start from

$$m(t) = \int_{x_1}^{x_2} c(x, t) dx \quad (3.3)$$

for a given time t . In this equation we are integrating density c in space $[x_1, x_2]$. You may think of an integral as a summation. Thus we are summing up all the density in a given interval in our one-dimensional space. For our application in vehicular traffic this is equivalent to summing up all the vehicles in our tunnel at a given time t and finding out that the total vehicles (or total mass) is m .

Imagine once again the idea of vehicles in a tunnel. We can then understand how the number of vehicles (or mass) is changing inside the tunnel if we know how many vehicles enter and how many vehicles leave the tunnel. Recalling the fact that mass (or vehicles) flow is based on equation (3.1), $c(x, t)v(x, t)$, we can obtain the following relation describing how vehicles (or mass) is changing in time,

$$\frac{d}{dt} \int_{x_1}^{x_2} c(x, t) dx = c(x_1, t)v(x_1, t) - c(x_2, t)v(x_2, t) \quad (3.4)$$

which is the difference of the number of vehicles exiting the tunnel subtracted from the number entering the tunnel. This is one form of the mass conservation law given in integral form.

This gives an understanding of the total density in the tunnel at any time t . Equation (3.4) which describes the rate of change for mass or otherwise how the number of vehicles is changing in time is also called *flux*. Thus equation (3.4) is measured in vehicles per hour when we relate it to our traffic flow model.

To obtain the usual mass conservation law (3.2) we now integrate in time equation (3.4). Note that we must apply the fundamental theorem of calculus when integrating in time the left hand side of (3.4). The result is as follows,

$$\int_{x_1}^{x_2} c(x, t_2) dx - c(x, t_1) dx = \int_{t_1}^{t_2} c(x_1, t)v(x_1, t) - c(x_2, t)v(x_2, t) dt \quad (3.5)$$

Note also that the following is true by use of the fundamental theorem of calculus,

$$c(x, t_2) - c(x, t_1) = \int_{t_1}^{t_2} \frac{d}{dt} c(x, t) dt.$$

We can then replace the left-hand side of (3.5) as,

$$\int_{x_1}^{x_2} \int_{t_1}^{t_2} \frac{d}{dt} c(x, t) dt dx = \int_{t_1}^{t_2} c(x_1, t)v(x_1, t) - c(x_2, t)v(x_2, t) dt \quad (3.6)$$

Assuming that all variables of interest c and v are differentiable we can apply the fundamental theorem of calculus in the following equation,

$$\frac{d}{dx} \int_{x_1}^{x_2} c(x, t)v(x, t) dx = c(x_2, t)v(x_2, t) - c(x_1, t)v(x_1, t). \quad (3.7)$$

Substituting equation (3.7) into the right-hand side of (3.6) we obtain,

$$\int_{x_1}^{x_2} \int_{t_1}^{t_2} \frac{d}{dt} c(x, t) dt dx + \int_{t_1}^{t_2} \frac{d}{dx} \int_{x_1}^{x_2} c(x, t)v(x, t) dx = 0$$

Rewriting the above we obtain,

$$\int_{x_1}^{x_2} \int_{t_1}^{t_2} \left(\frac{d}{dt} c(x, t) + \frac{d}{dx} c(x, t)v(x, t) \right) dt dx = 0$$

Since the above must be zero *for any* space $[x_1, x_2]$ and time interval $[t_1, t_2]$ the only possibility is for the interior (the integrand) to be identically zero! Thus we obtain our well-known *differentiation* form of our mass (or vehicles) conservation law,

$$\frac{\partial c}{\partial t} + \frac{\partial(cv)}{\partial t} = 0 \quad \text{conservation of mass.}$$

It is interesting to note however that no matter how great this simple model of vehicles might look in fact it is also useless! This is a single equation with **two** unknowns, either c and v or if you replace $cv = q$ in c and q . In either case we have learned in several classes that in order to solve anything the number of equations must equal the number of unknowns. In other words in order to solve this famous model we are still missing one more equation relating our main variables.

It is not unusual therefore when we are looking at models for traffic flow to observe that people assume a certain extra relation between c and v . In traffic flow for instance the most common assumption is that

$$v = v_{max} \left(1 - \frac{c}{c_{max}} \right) \quad (3.8)$$

In other words there is a convex type of relationship between velocity and density. So that for low densities (few vehicles) the velocity is high and in fact stays maximum. If however the density increases more then the velocity start decreasing first slowly and then faster. This does make some sense in terms of what we would expect to hold true in real life. Note therefore that by use of this extra equation (3.8) we have two equations, (3.2) and (3.8) with respect two two variables v and c . This system we can solve!

In other applications (fluid flows, weather predictions etc.) or even more detailed models for vehicular traffic we wish to obey more physical laws than just the conservation of mass. For instance it is not uncommon to believe that weather behaves in accordance to the laws of thermodynamics. So that the total heat or energy for the system should not change. Similarly there are several applications where momentum should not change. When trying to describe or model rarefied gasses for instance the following equations known as the *Euler equations* must be therefore satisfied:

$$\begin{aligned} c_t + (cv)_x &= 0 && \text{conservation of mass} \\ (cv)_t + (cv^2 + p)_x &= 0 && \text{conservation of momentum} \\ E_t + (v(E + p))_x &= 0 && \text{conservation of energy} \end{aligned}$$

Here p refers to the gas pressure while E corresponds to energy. Note once again that this is a system of 4 unknowns (assuming we known $f(x)$ for rarefied gases) but only 3 equations. So in order to solve it we still need one more equation. This is called the *equation of state* and related p to the other variables in this system.

It is common to write this system of equations in a simpler looking form as follows:

$$u_t + f(u)_x = 0 \quad (3.9)$$

where now the quantities are given as vectors instead of scalars,

$$u = \begin{pmatrix} c \\ cv \\ E \end{pmatrix} \quad \text{and} \quad f = \begin{pmatrix} cv \\ cv^2 + p \\ v(E + p) \end{pmatrix}$$

In general the form of equation (3.9) is what we consider to be that of a general conservation law. So any equation that can be written in this manner regardless for the specifics of the exact function f will imply that it corresponds to a conservation law.

3.2 Linear Advection Models

As we show in Section 3.1.1 properties such as conservation of mass, momentum and energy, together with several others, play a fundamental role in the modeling process. We will concentrate our study, for the time being at least, to the study of one dimensional models similar to the one we derived in Section 3.1.1 based on the conservation of mass.

In general any equation or system of equations which has the form

$$c_t + q(c)_x = 0$$

is called a *conservation* law. We will try to examine this equation and reveal its properties as a way of understanding it. Equation (3.2) is a *hyperbolic* partial differential equation with variable coefficients. In general any equation or system of equations with the form

$$Ac_t + Bc_x = C \quad \text{is hyperbolic if it has distinct eigenvalues}$$

where A, B and C do not have to be just scalars (numbers) but can even be matrices. Equations of this type are said to be hyperbolic if $P(\lambda) = \det(A - \lambda B)$ has n real distinct zeros where n denotes the number of equations in the system.

In the special case where $q(c)$ is known to depend on density in a simple fashion such as, $q(c) = ac$, for a a constant, our conservation law becomes,

$$c_t + ac_x = 0 \quad \text{a linear advection equation.} \tag{3.10}$$

In fact any equation which has a first order time derivative and a first order space derivative is an advection equation or otherwise also called a *one-way wave equation*. Given any type of initial density $c(x, 0) = g(x)$ this equation has the following solution

$$c(x, t) = g(x - at).$$

Check it by substituting it back into our advection equation! (We will see how this solution is arising in the next chapter when we study the method of characteristics.) The solution itself however ought to justify the reason for this equation being called a one-way wave equation. Notice that essentially the initial density $g(x)$ moves forward as time goes by. In other words a wave moving in one direction. This is typical behavior for advection equations. In fact even the speed of this motion is known and it can be shown to be equal to the coefficient a . In general this equation should be a good starting candidate for modeling basic waves.

3.3 Linear Advection-Diffusion Models

If you would really like to model water waves however the idea of a moving wave which would retain its altitude for ever, never getting smaller, does not seem very realistic. This is really what you

would get if you used the linear advection equation (3.10) presented in Section 3.2. Most people would agree that a realistic wave ought to lose some of its amplitude as it travels in time. This effect is modeled by adding a *diffusive* term in our original equation. A diffusive term in mathematics is represented with a second derivative in space,

$$\frac{\partial^2 c}{\partial x^2}.$$

In general we incorporate this diffusion effect by slightly altering the function $f(c)$ as follows,

$$q(c) = ac - Dc_x$$

where D is a constant. Given this function our conservation law becomes,

$$c_t + (ac - Dc_x)_x = 0$$

which simplifies to,

$$c_t + ac_x = Dc_{xx} \quad \text{an advection-diffusion equation.}$$

This may come as a surprise to you but this is no longer a hyperbolic type equation. In fact it is a *parabolic* PDE. We will study its solutions shortly but first a few words in terms of recognizing or classifying some general types of PDEs.

3.4 Classification of PDEs

Suppose that you have a system of n equations and you can obtain eigenvalue and eigenvector information about the corresponding matrices. Then classifying PDEs is relatively straight forward. We first find the eigenvalues of the system through the characteristic polynomial $P(\lambda) = \det(A - \lambda I)$ where I denotes the n dimensional Identity matrix and A corresponds to the matrix of the PDE system. The classification system outlined below depends on two parameters:

Z – the number of zero eigenvalues found,
 P – the number of positive eigenvalues.

Then if,

$Z = 0$ and $P = 1$ or $Z = 0$ and $P = n - 1$	PDE is hyperbolic
$Z = 0$ and $1 < P < n - 1$	PDE is ultra-hyperbolic
$Z > 0$	PDE is parabolic
$Z = 0$ and $P = n$ or $Z = 0$ and $P = 0$	PDE is elliptic

Note that there is still a missing case of possibly both real and complex eigenvalues existing. In that case we can not conclusively know the type of PDE without further knowledge of the equation itself. Also if any of the coefficients of our PDE are not constant then the type of the PDE will vary with position!

If on the other hand we have a single PDE (not a system) the following set-up can be employed in order to discover its type,

$$au_{xx} + 2bu_{xy} + cu_{yy} + du_x + eu_y + fu = g$$

where a, b, c, d, e, f, g are given constants. Now based on the so called *discriminant*

$$D = b^2 - ac$$

we can find the type of PDE at hand as follows,

- if $D < 0$ then the PDE is elliptic
- if $D = 0$ then the PDE is hyperbolic
- if $D > 0$ then the PDE is parabolic

In general we can quickly infer as to the type of the PDE as follows:

- if terms of the form u_{xy} or $u_{xx} - u_{yy}$ then it is probably a hyperbolic PDE
- if terms of the form u_{xx} then it is probably a parabolic PDE
- if terms of the form $u_{xx} + u_{yy}$ then it is probably an elliptic PDE

Caution should be exercised however if more terms appear since then the only sure way to tell the type of PDE is by undergoing calculations such as the ones shown in the examples below.

Example 1:

Suppose the PDE

$$4u_{xx} + 2u_{xy} + 10u_{yy} + u_y = 0.$$

Find the type of this PDE.

Solution:

We simply calculate the determinant via,

$$b^2 - ac = 1^2 - 4 \cdot 10 = 1 - 40 < 0$$

Thus this is an elliptic PDE.

Alternatively we can transform it into a matrix PDE and try and find its type by first obtaining its eigenvalues. This equation will produce a 2×2 matrix which is,

$$A = \begin{bmatrix} 4 & 2 \\ 0 & 10 \end{bmatrix}$$

This matrix is tridiagonal and therefore extremely easy to find its eigenvalues. In this case the eigenvalues are $\lambda_1 = 4$ and $\lambda_2 = 10$. Thus, once again, based on our table above this is an elliptic type PDE.

Example 2:

Classify the type of PDE,

$$2u_{x_1x_1} + 2u_{x_2x_2} - 15u_{x_3x_3} + 8u_{x_1x_2} - 12u_{x_2x_3} - 12u_{x_1x_3} = 0$$

Solution:

We start by building a matrix corresponding to this system,

$$A = \begin{bmatrix} 2 & 4 & -6 \\ 4 & 2 & -6 \\ -6 & -6 & -15 \end{bmatrix}$$

Finding the eigenvalues for this matrix is enough in order to classify the PDE. To do this we obtain the characteristic polynomial,

$$P(\lambda) = \det(A - \lambda I) = \lambda^3 + 11\lambda^2 - 144\lambda - 324$$

Setting this to zero gives,

$$\lambda_1 = -18, \quad \lambda_2 = -2, \quad \text{and} \quad \lambda_3 = 9$$

In other words, based on the classification system described earlier, this PDE is hyperbolic!

3.5 Method of Characteristics

We explore further now our linear advection equation with constant speed of propagation a ,

$$u_t + au_x = 0$$

We will define the so called “Cauchy problem” to be this PDE together with a given initial condition as follows,

$$\text{Cauchy problem:} \quad \begin{cases} u_t + au_x = 0 & \text{for } -\infty < x < \infty \text{ and } t \geq 0 \\ u(x, 0) = g(x) & \text{for } -\infty < x < \infty \text{ while } t = 0 \end{cases}$$

We have already seen that this equation has an exact solution defined in all space and time which is

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

for all $t \geq 0$ and $-\infty < x < \infty$.

This solution propagates *unchanged* along the space-time lines $x - at = \text{constant}$.

These lines in fact have a well-known name. They are called *characteristics*!

But what does this statement really mean? You actually know what it means... This is exactly what we saw in class when we determined, via our simple Matlab simulation, that the original wave was moving in space as time progressed without changing its form.

In fact this very sentence can be translated into mathematics! As we have seen before, almost in our very first class day, we can write equations which correspond to explicit physical situations. Starting from the fact that along the characteristics,

$$x - at = \text{constant} \tag{3.11}$$

taking a derivative in time produces the following equation: $x_t = a$ since the derivate of any constant is zero. Let us examine the system

$$\begin{cases} x_t = a \\ x(0) = x_0 \end{cases} \tag{3.12}$$

further. The equation $x(0) = x_0$ is added to implement any initial condition we might like in case we wish to solve this system. In reality $x(0) = x_0$ is exactly equal to that constant specified in the original equation (3.11).

There is a very interesting property for our linear advection problem which occurs when it reaches these lines (or more generally curves) which are known as characteristics. The following can be proved,

Theorem 14. *The solution u of our linear advection equation remains unchanged along these curves (characteristics).*

Proof: Let us start by differentiating $u(x, t)$ and see if it changes or not. If it does not change then its derivative should be zero. Note that here u depends on two variables and we must therefore pay particular attention to take the derivative in each of those two variables. In other words partial derivatives will appear. So,

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

If now we assume that we are on these characteristics then according to (3.12) $dx/dt = a$. Thus the above equation can be written as,

$$\frac{d}{dt}u(x, t) = u_t + u_x \frac{dx}{dt} = u_t + u_x a = 0$$

where the zero comes from the definition of our linear advection equation. Overall this implies that the derivative of $u(x, t)$ with respect to time is zero and therefore it proves that $u(x, t)$ does not change in time!

In fact what we just proved hold true in the general case where the characteristic curves are not just straight lines but actual curves! So our statement should be further generalized to apply to linear advection equations with a variable velocity $a(x)$ which can also depend on x (in a smooth way) as follows,

$$u_t + (a(x)u)_x = 0.$$

So even for this type of advection equation it can be shown that the solution $u(x, t)$ will remain unchanged along the characteristic curves satisfying

$$\begin{cases} \frac{dx}{dt} = a(x) \\ x(0) = x_0 \end{cases}$$