数学模型 Lecture Notes

Zhennan Zhou

2018 年 3 月 20 日

PRELIMINARY DRAFT. NOT FOR WIDE CIRCULATION.

2 自然科学中的微分方程选讲

从某种意义上说，微分方程在17世纪80年代已经出现在微积分创立者的著作中了。*微分方程*一词首次出现在Leibniz给Newton在1676年写的信中，并在1684年后被用于他的著作中。牛顿的《自然哲学的数学原理》中包含了很多微分方程，这些方程用于构造并集成于初等几何框架中。从那时起，基本的自然规律和技术问题在严格数学模型下的公式频繁地甚至很普遍地，以微分方式给出。

本堂课中，我们选讲三个方面：波现象方程，流体方程，肿瘤生长模型。

2.1 波动现象

2.1.1 最小作用量原理（least action principle）和欧拉-拉格朗日方程（Euler-Lagrange equation）

*哈密顿变分原理*或*最小作用量原理*：要确定具有一定动能$T(t,q,v)$和势能$U(t,q)$的力学系统的运动需要系统的质点轨迹提供作用量积分

$$S=\int_{t_1}^{t_2} L(t,q,v)\,dt$$

的极值，其中，（在常见的经典系统里面）$L(t,q,v)=T-U$称为系统的拉格朗日量（Lagrangian function）。这里，t表示时间，$q=(q_1,\cdots,q_s)$ 表示系统指点的坐标，$v=\dot{q}:=dq/dt$表示速度。

注意，运动轨迹是S的极值和经典系统里面$L(t,q,v)=T-U$是两个模型假设，我们不需要了解原因。但是我们接下来会做一些数学演算，之后大家会发现这背后的数学思想其实是一个全体到局部的过程（或者说积分到微分的广成）。

为了推导欧拉-拉格朗日方程，我们先学习一下泛函导数 (functional derivative) 的基本知识：

考虑一个元素为函数ρ的空间M （也就是说空间的每一个元素是一个函数，我们不妨假设 $\rho:\mathbb{R}\to\mathbb{R}^s$），和定义在上面的泛函

$$F:\quad M\to\mathbb{R}\quad\text{or}\quad\mathbb{C}.$$

需要提醒大家的是，我们不讨论一般泛函的定义，虽然泛函可以很抽象，但是在很多具体的问题中，泛函其实就是一个函数在某一点的赋值，一个函数的积分，或者函数的函数的积分。

The functional derivative of $F(\rho)$, denoted by $\delta F/\delta\rho$, is defined by

$$\int \frac{\delta F}{\delta\rho}(x)\phi(x)\,dx=\lim_{\varepsilon\to 0}\frac{F[\rho+\varepsilon\phi]-F[\rho]}{\varepsilon}=\left[\frac{d}{d\varepsilon}F[\rho+\varepsilon\phi]\right]_{\varepsilon=0},$$

where ϕ is an arbitrary function which vanishes at boundaries （想想为什么我们需要这个）. The quantity $\varepsilon\phi$ is called the variation （变分） of ρ. 在形式演算中，我们可以通过泰勒展开来求泛函导数。

Recall, $S = \int_{t_1}^{t_2} L(t,q,\dot{q})dt$, then

$$\begin{aligned}\int_{t_1}^{t_2} \frac{\delta S}{\delta q}(t)\phi(t)dt &= \left[\frac{d}{d\varepsilon}S[q+\varepsilon\phi]\right]_{\varepsilon=0} \\ &= \left[\frac{d}{d\varepsilon}\int L(t,q+\varepsilon\phi,\dot{q}+\varepsilon\dot{\phi})dt\right]_{\varepsilon=0} \\ &= \int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q}\cdot\phi + \frac{\partial L}{\partial v}\cdot\dot{\phi}\right)dt \\ &= \int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q}\cdot\phi - \left(\frac{\partial L}{\partial v}\right)_t\cdot\phi\right)dt \\ &= \int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q} - \left(\frac{\partial L}{\partial v}\right)_t\right)\cdot\phi dt.\end{aligned}$$

这里，分布积分的边界项消失了，因为ϕ在边界处为0。Therefore, by the principle of least action, we have derived the Euler-Lagrangian equation

$$\frac{\partial L}{\partial q} - \left(\frac{\partial L}{\partial v}\right)_t = 0.$$

If q is a function of $x = (x_1, \cdots, x_d)$, then the Euler-Lagrangian equation becomes

$$\frac{\partial L}{\partial q} - \sum_{j=1}^{d}\left(\frac{\partial L}{\partial q_{x_i}}\right)_{x_i} = 0.$$

Let's look at two more examples of functional derivatives:

Example 1. For the classical part of the electron-electron interaction, Thomas and Fermi employed the Coulomb potential energy functional

$$J[\rho] = \frac{1}{2}\int\int \frac{\rho(r)\rho(r')}{|r-r'|}drdr'.$$

From the definition of the functional derivative,

$$\begin{aligned}\int \frac{\delta J}{\delta\rho(r)}\phi dr &= \left[\frac{d}{d\varepsilon}J[\rho+\varepsilon\phi]\right]_{\varepsilon=0} \\ &= \left[\frac{d}{d\varepsilon}\frac{1}{2}\int\int \frac{(\rho(r)+\varepsilon\phi(r))(\rho(r')+\varepsilon\phi(r'))}{|r-r'|}drdr'\right]_{\varepsilon=0} \\ &= \frac{1}{2}\int\int\frac{\phi(r)\rho(r')}{|r-r'|}drdr' + \frac{1}{2}\int\int\frac{\rho(r)\phi(r')}{|r-r'|}drdr' \\ &= \int\left(\int\frac{\rho(r')}{|r-r'|}dr'\right)\phi(r)dr.\end{aligned}$$

Thus,

$$\frac{\delta J}{\delta\rho(r)} = \int\frac{\rho(r')}{|r-r'|}dr'.$$

Example 2*. Note that

$$\rho(r) = \int\rho(r')\delta(r-r')dr',$$

then

$$\frac{\delta\rho(r)}{\delta\rho(r')} = \delta(r-r').$$

Try to add the details by yourself. 标星号的例子可能超出了一些同学的只是范围，可以跳过。

2.1.2 绳索的微小振动

考虑在时间t距离平衡位置x的位移$u = u(x,t)$的微分方程。这里，$x \in \mathbb{R}$。我们仅考虑微小振动，$u(x,t)$及其导数的高阶项将被忽略。

令$\rho(x)$表示绳索的线密度，在时间t在位置x的动能密度为

$$T = \frac{1}{2}\rho(x)u_t^2.$$

微积分我们知道绳索微元长度 $ds = \sqrt{1+u_x^2}dx$, 所以形变长度为

$$ds - dx = (\sqrt{1+u_x^2} - 1)dx \approx \frac{1}{2}u_x^2 dx.$$

所以（with some elasticity theory）势能密度的表达式是

$$U = \frac{1}{2}\mu u_x^2,$$

这里μ是弹性系数。势能模型的建立需要更多的物理知识，所以我们只是把它当作一个模型假设。

绳索的作用积分为

$$S = \int L dt dx = \int (T-U) dt dx = \int \left(\frac{1}{2}\rho(x)u_t^2 - \frac{1}{2}\mu u_x^2\right) dt dx.$$

对应的 Euler-Lagrange equation 为

$$\frac{\partial L}{\partial u} - \left(\frac{\partial L}{\partial u_t}\right)_t - \left(\frac{\partial L}{\partial u_x}\right)_x = 0.$$

经过计算，我们得到

$$\frac{\partial L}{\partial u} = 0, \quad \frac{\partial L}{\partial u_t} = \rho(x)u_t, \quad \frac{\partial L}{\partial u_x} = -\mu u_x,$$
$$\left(\frac{\partial L}{\partial u_t}\right)_t = \rho(x)u_{tt}, \quad \left(\frac{\partial L}{\partial u_x}\right)_x = -\mu u_{xx}.$$

于是我们得到一维波动方程

$$\rho(x)u_{tt} = \mu u_{xx}.$$

如果绳索收到外力$f(x,t)$, 那么动能密度不变，势能密度变为

$$U = \frac{1}{2}\mu u_x^2 - f(x,t)u,$$

（Again, 势能模型的建立需要更多的物理知识，所以我们只是把它当作一个模型假设。）于是，我们可以得到一维受迫振动方程

$$\rho(x)u_{tt} = \mu u_{xx} + f(x,t).$$

2.1.3 极小曲面

考虑一个膜$(x, y, u(x,y)), \quad (x,y) \in V$，当这个膜的表面积

$$\int_V \sqrt{1+u_x^2+u_y^2}dxdy$$

有最小值的时候，极小曲面问题需要确定所有可能的膜外形。这个问题对应的拉格朗日量

$$L = \sqrt{1+u_x^2+u_y^2}.$$

为了得到对应的Euler-Lagrange equation，我们计算

$$\frac{\partial L}{\partial u}=0,\quad \frac{\partial L}{\partial u_x}=\frac{u_x}{\sqrt{1+u_x^2+u_y^2}},\quad \frac{\partial L}{\partial u_y}=\frac{u_y}{\sqrt{1+u_x^2+u_y^2}}.$$

于是我们得到

$$\left(\frac{u_x}{\sqrt{1+u_x^2+u_y^2}}\right)_x+\left(\frac{u_y}{\sqrt{1+u_x^2+u_y^2}}\right)_y=0,$$

或者化简为

$$(1+u_y^2)u_{xx}-2u_xu_yu_{xy}+(1+u_x^2)u_{yy}=0.$$

我们可以线性化此方程（扔掉高阶项），得到拉普拉斯方程（Laplace equation）：

$$u_{xx}+u_{yy}=0.$$

2.2 流体方程

Recall, if we denote the density function by $u(x,t)$ where $x\in\mathbb{R}$, the flux function by $f(u)$, we have derived

- Conservation law: $u_t+(f)_x=0$.

Actually, when $x\in\mathbb{R}^s$, then we have

$$u:\quad \mathbb{R}^{s+1}\to\mathbb{R}^d,\qquad f_i(u):\quad \mathbb{R}^d\to\mathbb{R}^d,\quad i=1,\cdots,s.$$

And the conservation law, becomes:

$$u_t+\sum_{i=1}^{s}(f_i)_{x_i}=0.$$

And sometimes, we write $f=(f_1,\cdots,f_s)$, and rewrite the conservation in a more compact form

$$u_t+\nabla_x\cdot f=0.$$

The Euler equations in the Froude limit are equivalent to a single conservation equation with conserved quantity and associated flux respectively:

$$u=\begin{pmatrix}\rho\\ j\\ E\end{pmatrix},\quad f=\begin{pmatrix}j\\ \frac{1}{\rho}j\otimes j+p\mathbf{I}\\ (E+p)\frac{j}{\rho}\end{pmatrix},$$

where

- ρ is the fluid density;
- $j=\rho u$ is the momentum, where u is the velocity;
- p is the pressure and E is the energy density;
- the Euler system is often completed by some equation of state $p(\rho,j,E)$.

Here, for two vectors u and v, $u \otimes v = uv^T$ denotes the outer product (special case of tensor product).

这里我们不需要理解为什么质量、动量、能量的flux function是怎么得来的。事实上，不同的流体方程的建模重点就是给出一个流体相对应的flux function，这需要反复的力学实验和数学修正。很多科学家、工程师终生的工作就是在流体模型的建立和修正上。

幸运的是，作为数学人，反而可以研究这个模型在抽象形式下的数学结构。不幸的是，这个模型的分析求解实在太难了！接下来，我们介绍一些这个模型的简化和改变。

The Euler equations are simplified by only considering the conservation of mass and momentum. And often we further assume that the flow is incompressible, namely $\nabla \cdot u = 0$. 回忆一下散度的意义（利用多元微积分中的高斯定理），想想为什么。

Then, the we get the incompressible Euler equation

$$\begin{cases} \rho_t + u \cdot \nabla \rho = 0, \\ u_t + u \cdot \nabla u = -\frac{\nabla p}{\rho}. \\ \nabla \cdot u = 0. \end{cases} .$$

If we assume the density function is a constant of space and time, i.e. $\rho \equiv \rho_0$, then we obtain the incompressible Euler equations with constant and uniform density

$$\begin{cases} u_t + u \cdot \nabla u = -\frac{\nabla p}{\rho_0}. \\ \nabla \cdot u = 0. \end{cases} .$$

By the way, we can add viscosity to the Euler equations to obtain the Navier–Stokes equations. For example, with constant and uniform density, the incompressible Navier–Stokes equations are

$$\begin{cases} v_t + v \cdot \nabla v = -\frac{\nabla p}{\rho_0} + \mu \Delta v. \\ \nabla \cdot v = 0. \end{cases} .$$

Here, μ is the viscosity constant.

Why are fluid equations interesting? Well, many answers... But let me show you one. Let's consider the one dimensional Burgers' equation

$$u_t + u u_x = 0.$$

Introduce the characteristic equation

$$\frac{dx(t)}{dt} = u(x(t), t), \quad x(0) = \xi.$$

Then

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

Therefore, $u(x(t), t)$ is constant along characteristics. 这里看起来很像刘维尔定理，但是下面我们会发现由于非线性的作用，方程的解会有意想不到的演化。

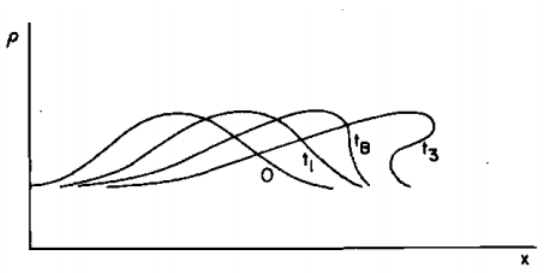
What about the characteristic velocity? Note that

$$u(x(t), t) = u(x(0), 0) = u(\xi, 0),$$

so we have

$$x(t) = u(\xi, 0)\, t + \xi.$$

This actually means possible formation of shocks!



2.3 肿瘤增长模型

这一部分，我们选讲法国数学家Benoît Perthame（院士）的部分工作，感兴趣的同学们请参考

`https://www.ljll.math.upmc.fr/perthame/cours_M2.pdf`

For the cell density model, we introduce the following notations

- $\rho(x,t)$ population density of tumor cells;
- $u(x,t)$ cell velocity;
- $p(x,t)$ pressure in the tumor tissue;
- $c(x,t)$ concentration of nutrient.

The governing equation is given by

$$\frac{\partial}{\partial t}\rho + \nabla\cdot\big(\rho u\big) = \rho G(c,p), \quad \mathbf{x}\in\mathbb{R}^d,\ t\geq 0.$$

Darcy's law for friction dominated flow

$$u = -\nabla_x p(\rho).$$

Constitutive law (m>1)

$$p(\rho) = \frac{m}{m-1}\rho^{m-1}. \tag{2.1}$$

大家注意，这其实是一个balance law模型。Flux function是ρu, 而source function是ρG.

也许大家会好奇压力方程p为什么会被选取成一个特殊的形式。除了实验上的原因之外，在数学上，这其实蕴含了一个很有趣的自由边界极限！

Multiplying the cell density equation by $p'(\rho)$, we find

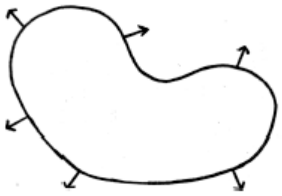
$$\frac{\partial}{\partial t}p = (m-1)p\Delta p + |\nabla p|^2 + (m-1)pG(c,p).$$

Sending $m\to\infty$ (we denote the limit of p by p_∞), we formally have the 'complementary relation'（互补关系）:

$$p_\infty\big(\Delta p_\infty + G(c,p_\infty)\big) = 0.$$

The normal velocity of the boundary $\partial\Omega$ is $v = -\nabla p_\infty\cdot\hat{n}$, where $\hat{n}(\mathbf{x},t)$ is the unit outer normal direction on the boundary.

$$-\Delta p_\infty = G(c,p_\infty), \quad \text{on}\,\Omega(t).$$





We elaborate the nutrient models in the following:

$$\tau \frac{\partial}{\partial t} c - \Delta c + \Psi(\rho, c) = 0,$$

where $\Psi(\rho, c)$ is the consumption function which takes different forms and τ is a time scaling constant. 这其实也是一个balance law模型。（flux和source分别是什么？）

When $\tau = 0$, the nutrient distribution $c(\mathbf{x}, t)$ effectively adjusts to its local equilibrium according to the cell density $\rho(\mathbf{x}, t)$. 在第四章的无量纲化部分，我们会探讨$\tau = 0$的具体含义。形式上看，我们可以认为t是肿瘤细胞的运动的特征时间，而$t' = t/\tau$是营养物质扩散的特征时间，而τ是这两个特征时间的比值。我们注意到

$$\frac{\partial}{\partial t'} c = \frac{\partial t}{\partial t'} \frac{\partial}{\partial t} c = \tau \frac{\partial}{\partial t} c, \quad \tau = \frac{t}{t'}.$$

所以$\tau = 0$的含义其实是，在肿瘤细胞运动的有限时间里，营养物质已经无限充分的扩散了，达到了局部均衡的状态。

We consider two specific models: the *in vitro* (活体外) model and the *in vivo* (活体内) model. In the following $c_B > 0$ is the nutrient concentration in the environment.

For the *in vitro* model, the nutrient equation reads

$$\begin{aligned} -\Delta c + \psi(\rho) c = 0, &\quad \text{for } \mathbf{x} \in D; \\ c = c_B, &\quad \text{for } \mathbf{x} \in \mathbb{R} \backslash D, \end{aligned}$$

where $D = \{\rho(\mathbf{x}) > 0\} = \{p(n) > 0\}$.

And for the *in vivo* model, the nutrient equation reads

$$-\Delta c + \psi(\rho) c = \chi_{\{\rho=0\}} (c_B - c) d.$$

（本节这部分是选读材料）我们下面要做一个模型检验。我们对营养浓度的建模，有一个基本要求，就是希望这个浓度不高于环境里面营养浓度的最大值，但是也不低于0。那么问题来了，因为很多微分方程我们是无法解析求解的，那么如何判断这样的基本要求是否被满足呢？

Actually, we can show that, if $\psi(\rho) \geq 0$, the in the in vitro model $0 \leq c(x, t) \leq c_B$ for $t \geq 0$ and $x \in \mathbb{R}^d$.

Write $c(x, t) = c_+(x, t) - c_-(x, t)$, where $c_\pm(x, t) \geq 0$ denote the positive part and the negative part of $c(x, t)$, respectively. Notice that at the boundary $c(x, t)|_{\partial D(t)} = c_B > 0$, thus $c_-(x, t)|_{\partial D(t)} = 0$.

Then multiply the nutrient equation by $-c_-(x, t)$, and integrate over $D(t)$, we have, upon integration by parts,

$$\int_{D(t)} |\nabla c_-|^2 + \psi(\rho) c_-^2 dx = 0.$$

Notice that by assumption, $\psi(\rho) \geq 0$. Then the above equation implies $c_-(x, t) = 0$ in $D(t)$, and thus $c(x, t) \geq 0$ in $D(t)$. Hence, $c(x, t) \geq 0$ in $\mathbb{R}^d$.

And with more knowledge in PDE, one can actually show that $c(x, t) \leq c_B$ in $\mathbb{R}^d$.

2.3.1 traveling wave solutions （行波解）

很多时候方程的解是有很多个（比如一元二次函数就有两个解）。对于微分方程来说，我们知道求解往往非常复杂，甚至不可实现。但是，我们与其把通解（甚至是弱解的集合）找出来，再挑一个跟应用相关的，有时候，我们不如直接去找一个跟应用相关的特解。下面介绍的行波解就是这么一个例子。

In this part, we consider a simplified one-dimensional tumor growth model, the reaction-diffusion model

$$u_t - u_{xx} = f(u).$$

Here $u \in [0,1]$ denotes the density function, and $f(u)$ is the growth rate satisfying

$$f(0) = f(1) = 0.$$

注意，这仍然是一个balance law。

A traveling wave is a solution of the type $u(x,t) = v(x - ct)$ for some $c \in R$ and $v(-\infty) = 1$, $v(+\infty) = 0$. The parameter c is called the speed of the wave.

Clearly, a traveling wave satisfies

$$-cv' - v'' = f(v), \quad v(-\infty) = 1, \quad v(+\infty) = 0.$$

We consider the following the ignition temperature model (点燃温度模型). For $\theta \in (0,1)$, and $\mu > 0$,

$$f(u) = \begin{cases} 0, & 0 \le u < \theta \\ \mu(1-u), & \theta < u \le 1. \end{cases}$$

Actually, we can show that there is a unique solution (c^*, v) such that v is decreasing, $v(0) = \theta$, and $c^* > 0$.

When $x < 0$, we have $u > \theta$, so the equation takes the following form

$$cv' + v'' + \mu(1 - v) = 0.$$

Since v is bounded at $-\infty$, we have

$$v(x) = 1 - (1-\theta)e^{\lambda_+ x}, \quad x < 0,$$

where

$$\lambda_+ = \frac{1}{2}(-c + \sqrt{c^2 + 4\mu}).$$

When $x > 0$, we instead have $u < \theta$, so the equation reads

$$cv' + v'' = 0.$$

The boundedness of v at ∞ implies

$$c = \theta e^{-cx}, \quad x \ge 0.$$

Note that, v'' has a jump at 0 because of the discontinuity of f at θ, but v' continuous at 0. This leads to

$$(1-\theta)\lambda_+ = \theta c.$$

With some elementary calculus analysis, we know there is indeed a unique solution $c^* > 0$, and the explicit formulas show that v is a decreasing function. （我们会在作业中再次碰到这个问题。）