数学模型 Lecture Notes

Zhennan Zhou

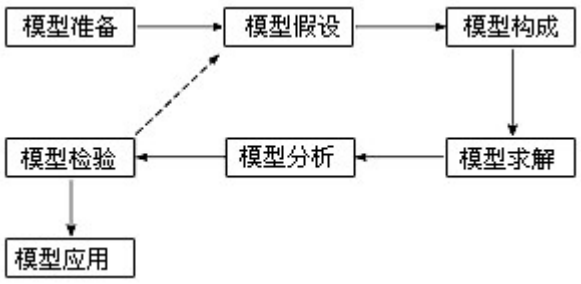
2018 年 3 月 8 日

PRELIMINARY DRAFT. NOT FOR WIDE CIRCULATION.

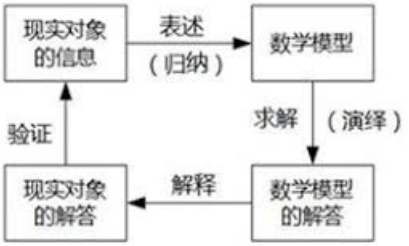
1 Preliminaries

1.1 Some Key concepts

- 原型（Prototype）：人们在现实世界里关心、研究或者从事生产管理的实际对象。
- 模型（Model）：为了某个特定目的将原型的一部分信息简缩、提炼而构造的原型替代物。
- 数学模型（Mathematical Model）：对于现实世界的一个特定对象，为了一个特定目的，根据特有的内在规律，做出一些必要的简化假设，运用适当的数学工具，得到一个特定的数学结构。
- 数学建模，或者建模（Mathematical Modeling）：建立数学模型的全过程。
- 数学建模的一般步骤



- 数学建模的全过程



1.2 Examples of mathematical models in physics/mechanics

- 守恒律模型（Conservation Law）。
  Let $u(x,t):\mathbb{R}\times\mathbb{R}\to\mathbb{R}^d$ be a density function. The total mass between between x_1 and x_2 at time t is given by $\int_{x_1}^{x_2}u(x,t)dx$, which changes with respect to time due to

  – flux/flow at x_1, x_2. $f(u):\mathbb{R}^d\to\mathbb{R}^d$, the flux function.

  – source/sink within $[x_1,x_2]$. $\psi(u):\mathbb{R}^d\to\mathbb{R}^d$, the source function.

  Therefore, we obtain

  $$\frac{d}{dt}\int_{x_1}^{x_2}u(x,t)dx=f|_{x=x_1}-f|_{x=x_2}+\int_{x_1}^{x_2}\psi dx=-\int_{x_1}^{x_2}(f)_x dx+\int_{x_1}^{x_2}\psi dx,$$

  which simplifies to

  $$\int_{x_1}^{x_2}\left(u_t+(f)_x-\psi\right)dx=0.$$

  Thus, we have derived

  – Balance law: $u_t+(f)_x=\psi$.

  – Conservation law: $u_t+(f)_x=0$.

  Some further examples:

  – $f=au$, $u_t+au_x=0$, advection equation （对流，传送）.

  – $f=-\beta u_x$, $u_t=\beta u_{xx}$, diffusion (heat) equation （扩散，热传导）.

  – $f=au-\beta u_x$, $u_t+au_x=\beta u_{xx}$, advection-diffusion equation.

  – $f=\frac{1}{2}u^2$, $u_t+uu_x=0$, (inviscid) Burgers' equation.

  – Euler equations (欧拉方程), etc.

  前两个例子很简单，但是道理还是很深刻的。如果flux是u的线性函数，那么我们的守恒律对应的是一个传送过程（速度为a），而如果flux是u_x的线性函数，那么我们的守恒律对应的是一个扩散过程（这个比例系数β也常被我们成为扩散系数）。

- 输运方程（Kinetic equation）。
  Let $f(x,v,t)$ be the density function (of e.g. dilute gas) on the phase space. The addition variable v stands for the momentum. The general equation can be written as

  $$\frac{df}{dt}=\left(\frac{\partial f}{\partial t}\right)_{\text{force}}+\left(\frac{\partial f}{\partial t}\right)_{\text{diffusion}}+\left(\frac{\partial f}{\partial t}\right)_{\text{collision}}.$$

  In particular, the Boltzmann equation (玻尔兹曼方程) takes the following form

  $$\frac{\partial f}{\partial t}+\frac{v}{m}\cdot\nabla_x f+F(x)\cdot\frac{\partial f}{\partial v}=\left(\frac{\partial f}{\partial t}\right)_{\text{collision}}.$$

  （注意，这里我们把v理解成了动量。）The collision terms describes interactions between $f(x,v,t)$ and $f(x,v',t)$. Due to the collision term, the Boltzmann equation is not time reversible.

- 哈密顿力学方程（Hamiltonian Mechanics）。

  A classical physical system is described by a set of canonical coordinates (正则坐标) $r = (q, p)$. The time evolution of the system is uniquely defined by Hamilton's equations

  $$\frac{dq}{dt} = \frac{\partial \mathscr{H}}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial \mathscr{H}}{\partial q},$$

  where $\mathscr{H} = \mathscr{H}(q, p, t)$ is the Hamiltonian, which often corresponds to the total energy of the system. For a closed system, it is the sum of the kinetic and potential energy in the system.

  这里，我们不去推导或者验证哈密顿方程。但是我们会在接受了这个模型构成的基础上继续做一些数学上的演绎推导。

  For example,

  $$\mathscr{H} = T + V, \quad T = \frac{p^2}{2m}, \quad V = V(q).$$

  Then, we get

  $$\frac{dq}{dt} = \frac{p}{m}, \quad \frac{dp}{dt} = -\nabla V(q) =: F(q).$$

  Finally, if we have a distribution $f(q, p, t)$ of those classical particles, then we have

  $$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{dq}{dt} \cdot \frac{\partial f}{\partial q} + \frac{dp}{dt} \cdot \frac{\partial f}{\partial p}.$$

  Since the phase space velocity has zero divergence, and probability is conserved, the convective derivative of the distribution function is zero, namely $\frac{df}{dt} = 0$.

  To be more specific, we write the phase space velocity in the conservation law form

  $$\frac{\partial f}{\partial t} + \frac{\partial}{\partial q}(f\dot{q}) + \frac{\partial}{\partial p}(f\dot{p}) = 0.$$

  By direct calculation, we know

  $$\frac{\partial}{\partial q}(\dot{q}) + \frac{\partial}{\partial p}(\dot{p}) = \frac{\partial}{\partial q}(\frac{p}{m}) + \frac{\partial}{\partial p}(-\nabla V(q)) = 0.$$

  Thus, we have

  $$\frac{\partial f}{\partial t} + \frac{p}{m} \cdot \frac{\partial f}{\partial q} + F(q) \cdot \frac{\partial f}{\partial p} = 0,$$

  which is the collisionless Boltzmann equation (Vlasov equation). This is called Liouville's theorem (刘维尔定理).

- 薛定谔方程（ Schrödinger equation）。

  在量子力学的领域，我们还是需要位置和动量这两个变量还是我们表示一个量子态的常用方法（虽然，也存在很多其他的方法），但是由于所谓的测不准原理等原因，在量子学的基本假设下，我们把位置和动量部分的或者全部的看成了算子。这里我们不讲解具体的原因，但是我们下面演算一下一些这种数学模型的几个简单推论。

  In quantum mechanics (量子力学), the quantum Hamiltonian is given by

  $$\hat{H} = \hat{T} + \hat{V}, \quad \hat{T} = \frac{\hat{k}^2}{2m}, \quad \hat{V} = V(\hat{x}),$$

  where $\hat{x}$ and $\hat{k}$ are the position operator and the momentum operator respectively.

In the position-space, we formally have $\hat{k} = -i\hbar\nabla$, and the Hamiltonian is represented as

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(x).$$

Here $V(x)$ is real-valued as in the classical case. 也就是说在位置空间（或者叫位置表象下），位置x可以理解成自变量，但是动量算符就变成了一个微分算子。

The eigenvalues of $\hat{H}$ are interpreted as energy, which are determined by the time-independent Schrödinger equation

$$\hat{H}\psi_k(x) = E_k\psi_k(x).$$

有趣的是，虽然$\psi_k(x)$可以是复数值的，但是E_k都是实数值的。其背后的原因是，这里的$\hat{H}$是一个自伴算子，可以被理解成一个Hermitian matrix（埃尔米特矩阵）的无限维推广。大家会在泛函分析等课程中系统学习算子的谱理论，我们在这学期只会零散的接触到一些自伴算子的应用和形式演算（也就是说，大家不用关心严格的定义和证明）。

If a quantum state in the position-space is represented by the position space wave function $u(x,t)$, its time evolution is governed by the time dependent Schrödinger equation

$$i\hbar u_t = \hat{H}u.$$

The wave function is complex valued, and one can show that

$$\frac{d}{dt}\int |u(x,t)|^2 dx = 0.$$

Therefore, $\rho(x,t) = |u(x,t)|^2$ is interpreted as the position density function, which is measurable in experiments. 可观测这件事是一个题外话了，大家不必深究。

- 在固体物理（solid state physics）、电磁学（electromagnetism）、统计力学（statistical mechanics）等学科中也有很多有趣的数学模型。

需要注意的是，对于同样的对象，数学模型也不同，其原因往往是时间空间尺度（scale）的不同。然而更有挑战性的往往是，一个问题中，有多个不同的尺度。这样的问题往往是不错的科研问题。

另外，希望同学们这学期学习过程中能够思考一个问题：数学家和科学家、工程师相比，有什么相同和不同呢？

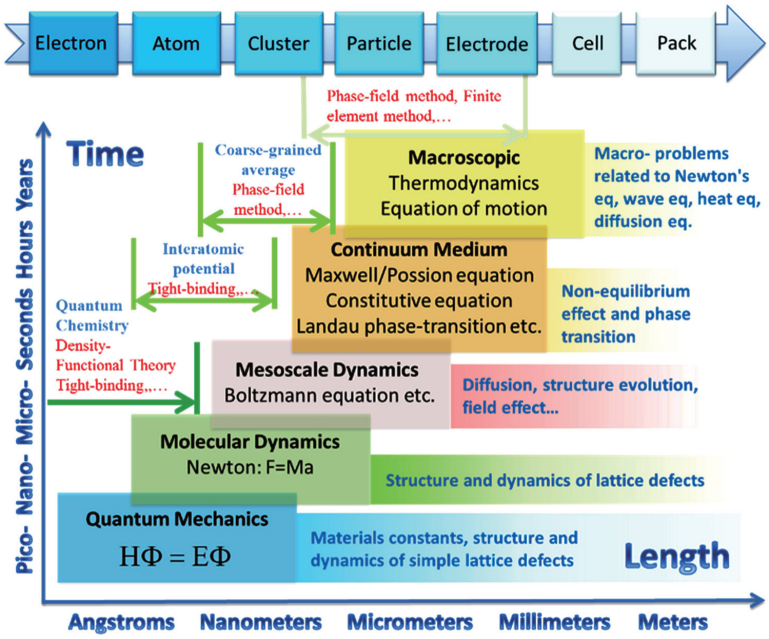


图 1: Chinese Physics B , 2016, 25(1): 018212