A Study of Solving Hamiltonian Systems

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Abstract

The goal of this semester was to learn about the mathematics involved in studying a class of Hamiltonian systems. Specifically, we considered systems that describe lattice oscillators and, by the end of the semester, we understood a well-known proof of existence and uniqueness (of solutions) for a large class of such models.

Introduction: Motivation and General Background

The purpose of this research assistantship has been to study methods for solving certain Hamiltonian systems. This project began with some very basic ideas concerning solving differential equations and has progressed into an exploration of what it means to solve a Hamiltonian system. The main goal of this paper is to describe what has been studied over the course of the last semester, including such mathematical ideas as Lipschitz functions, Gronwall estimates, existence and uniqueness theorems for initial value problems, and time evolutions for certain anharmonic systems.

Theory

First, we begin by addressing two means that may be used to find solutions (or at least estimates) to certain first order differential equations. Specifically, we discuss Lipschitz functions and Gronwall estimates.

Lipschitz Functions

A vector function $\vec{f}(x,\vec{y}) = \begin{pmatrix} f_1(x,\vec{y}) \\ \vdots \\ f_n(x,\vec{y}) \end{pmatrix}$ where $\vec{y} = \begin{pmatrix} y_1(x) \\ \vdots \\ y_1(x) \end{pmatrix}$ satisfies a Lipschitz condition with respect to $\vec{y}$ in D (with Lipschitz constant L) if

$$\left|\vec{f}(x,\vec{y})-\vec{f}(x,\vec{y}_0)\right| \le L\left|\vec{y}-\vec{y}_0\right| \qquad \forall(x,\vec{y}),(x,\vec{y}_0)\in D\,. \tag{1}$$

It is also convenient to talk about local Lipschitz conditions: A vector function $\vec{f}(x,\vec{y})$ satisfies a local Lipschitz condition with respect to $\vec{y}$ in D if $\forall(x,\vec{y})\in D$ there exists a neighborhood $U:\left|x-x_0\right|<\delta,\left|\vec{y}-\vec{y}_0\right|<\delta$, where δ>0, such that $\vec{f}(x,\vec{y})$ satisfies a Lipschitz condition in $D\cap U$.

Lipschitz functions prove to be very helpful when discussing the existence of solutions for certain initial value problems. Thus, it is helpful to know specifically what types of functions satisfy a Lipschitz condition. Hence the following lemma:

Lemma (1):

(a) If D is convex and if $\vec{f}$ and all components of the Jacobian $\dfrac{\partial\vec{f}}{\partial\vec{y}}=\left(\dfrac{\partial f_v}{\partial y_\mu}\right)_{\mu,v=1}^{n}$ are continuous and bounded in D (μ,v = 1,…,n), then $\vec{f}$ satisfies a Lipschitz condition with respect to $\vec{y}$ in D.

(b) If D is a domain and if $\vec{f}$ and $\dfrac{\partial\vec{f}}{\partial\vec{y}}$ are continuous in D, then $\vec{f}$ satisfies a local Lipschitz condition with respect to $\vec{y}$ in D.

(c) If $\vec{f}\in C(D)$ satisfies a local Lipschitz condition with respect to $\vec{y}$ in D, then $\vec{f}$ satisfies a Lipschitz condition with respect to $\vec{y}$ on compact subsets of D.

Proof:

(a) We apply the mean value theorem to $f_v(x,\vec{y})$ and find

$$f_v(x,\vec{y})-f_v(x,\vec{y}_0)=\sum_{\mu=1}^{n}\frac{\partial f_v(x,\vec{y}^*)}{\partial y_\mu}(y_\mu-y_{0_\mu})\ , \tag{2}$$

where $(x,\vec{y}^*)$ is a point on the line segment between $(x,\vec{y})$ and $(x,\vec{y}_0)$. It follows, then, that there exists a constant $k\in\mathbb{R}$ such that

$$\left|f_v(x,\vec{y})-f_v(x,\vec{y}_0)\right|\le k\max_\mu\left|y_\mu-y_{0_\mu}\right|. \tag{3}$$

Therefore, $\vec{f}$ satisfies a Lipschitz condition with respect to the maximum norm $\left|\vec{a}\right|=\max_v\left|a_v\right|$.

(b) We know that a function $\vec{f} \in C(D)$ is always bounded on compact subsets of D, so the statement in (b) is a direct consequence of part (a).

(c) Proof by contradiction. We know if $K \subset D$ is compact and the statement in (c) is false (with respect to *K*), then there must exist sequences $(x_k, \vec{y}_k), (x_k, \vec{z}_k) \in K$ with

$$\left| \vec{f}(x_k, \vec{y}_k) - \vec{f}(x_k, \vec{z}_k) \right| \geq k \left| \vec{y}_k - \vec{z}_k \right| \quad \text{(k=1,2,...)} \tag{4}$$

Now K is compact, so we may assume that $(x_k, \vec{y}_k) \to (x_0, \vec{y}_0) \in K$. Also, because f is bounded in *K*, we have from (4) that $(x_k, z_k) \to (x_0, \vec{y}_0) \in K$. This produces a contradiction because, for large *k*, the points $(x_k, \vec{y}_k)$, $(x_k, \vec{z}_k)$ belong to a neighborhood around $(x_0, \vec{y}_0)$, with *f* satisfying a Lipschitz condition in $\vec{y}$.

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Thus, having understood what it means for a function to be Lipschitz, we finally develop the following theorem:

Existence and Uniqueness Theorem (1):

Let $\vec{f}(x, \vec{y})$ be continuous in a domain $D \subset \mathbb{R}^{n+1}$ and let $\vec{f}$ satisfy a local Lipschitz condition with respect to $\vec{y} \in D$. Then if $(\xi, \vec{\eta}) \in D$, then the initial value problem

$$\vec{y}' = \vec{f}(x, \vec{y}),\ \vec{y}(\xi) = \vec{\eta} \tag{5}$$

has exactly one solution. The solution can be extended to the left and right up to the boundary of D.

Gronwall Estimates

Following, we provide a generalized lemma (Gronwall's Lemma), along with its proof:

Lemma (2):

Let the real-valued function $\phi(t)$ be continuous in J = [0,a] and let

$$\phi(t) \leq \alpha + \int_0^t h(s)\phi(s)ds \quad \text{in J,} \tag{6}$$

where $a \in \mathbb{R}$ and $h(t)$ is continuous so that $h(t) \geq 0$. Then

$$\phi(t) \leq \alpha e^{H(t)} \qquad \text{with } H(t) = \int_0^t h(s)ds. \tag{7}$$

Proof:

Let $\varphi(t) = \alpha + \int_0^t h(s)\phi(s)ds$. Then $\varphi'(t) = h(t)\phi(t)$ and since $\phi(t) \le \varphi(t)$ (by assumption), we have $\varphi'(t) \le h(t)\varphi(t)$. Now, when $H(t) = \int_0^t h(s)ds$,

$$\left(e^{-H(t)}\varphi(t)\right)' = -h(t)e^{-H(t)}\varphi(t) + e^{-H(t)}\varphi'(t) \le -h(t)e^{-H(t)}\varphi(t) + h(t)e^{-H(t)}\varphi(t) = 0.$$

Hence, $e^{-H(t)}\varphi(t)$ is decreasing, i.e. $e^{-H(t)}\varphi(t) \le \varphi(0) = \alpha \Rightarrow \varphi(t) \le \alpha e^{H(t)}$.

Since $\phi(t) \le \varphi(t)$, we find $\phi(t) \le \alpha e^{H(t)}$.

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Fixed Point Theorem

A final consideration before addressing Hamiltonian systems involves a fixed point theorem for contractive mappings. Note, first of all, that a Banach space is defined as a complete normed vector space. In other words, a space is called Banach if it is a vector space V (over the real or complex numbers) with a norm ||·|| such that every Cauchy sequence (with respect to the metric d(x, y) = ||x − y||) in V has a limit in V. Then we have the following theorem:

Theorem (2): (A Contraction Principle)

Let D be a nonempty, closed set in a Banach space *B*, and let *T* be an operator, $T: D \to B$, that maps D onto itself ($T(D) \subset D$) such that *T* is a contraction, i.e. *T* satisfies a Lipschitz condition with constant q < 1. Then the equation $x = Tx$ has exactly one solution $x = x'$ in D.

Moreover, if a sequence (x_n) of "successive approximations" is formed, starting from an arbitrary element $x_0 \in D$ and setting

$$x_1 = Tx_0,\ x_2 = Tx_1,\ \ldots,\ x_{n+1} = Tx_n,\ \ldots, \tag{8}$$

then the sequence converges in the norm to x', and we have the estimate

$$\|x_n - x'\| \le \frac{1}{1-q}\|x_{n+1} - x_n\| \le \frac{q^n}{1-q}\|x_1 - x_0\| \tag{9}$$

Time Evolution

After reviewing these preliminary concepts (Lipschitz functions, Gronwall estimates, and the fixed point theorem), we now begin to use this information for solving (and in some cases, estimating solutions for) differential equations in order to look at time evolutions for certain Hamiltonian systems. In order to do so, we start by discussing Lanford's, Lebowitz's, and Lieb's journal article "Time Evolution of Infinite Anharmonic Systems." The purpose of their paper is to prove existence and uniqueness of a strong time evolution for a class of systems in arbitrary dimensions and a weaker time evolution for more general anharmonic systems. Following is a summary of their work regarding the existence of such solutions for a specific class of systems.

Looking at the lattice $\mathbb{Z}^{\nu}$, at each point $x \in \mathbb{Z}^{\nu}$ we have an oscillator with coordinate $q_x \in \mathbb{R}$ and momentum $p_x \in \mathbb{R}$. These variables are regarded as functions of time t, $\{q_x(t), p_x(t)\}$, and are represented by $\vec{q}(t)$ and $\vec{p}(t)$. They satisfy the infinite set of coupled differential equations:

$$\frac{dq_x(t)}{dt} = p_x(t) \quad \text{and} \quad \frac{dp_x(t)}{dt} = F_x = \frac{-\partial U_x(q_x(t))}{\partial q_x} + R_x(\vec{q}(t)) \ , \qquad (10)$$

where $U_x(q_x)$ is a self-energy term and R_i is the gradient of some interaction energy,

$$R_i = -\sum \frac{\partial V_j(\vec{q})}{\partial q_x} . \qquad (11)$$

We assume $U_x(q_x)$ dominates the motion of the particles when they are far from their equilibrium positions. More precisely:

a) $V_x(\vec{q})$ depends only on those q_y for which $|x-y| \le D$;
b) Each $U_y(q_y)$ and $V_y(\vec{q})$ is a twice continuously differentiable function;
c) $|q_y| \le C_1 U_y(q_y) + C_2$, where C_1 and C_2 are constants, $C_1, C_2 \ge 0$; and
d) There exist nonnegative bounded constants $A_{xy} < C$, $A_{xy} = 0$ for

$$|x-y| > D: \left| p_x R_x(\vec{q}) \right| \le \sum_y A_{xy} L_y . \qquad (12)$$

where

$$L_x(p_x, q_x) = \frac{1}{2} p_x^{\,2} + U_x(q_x) + k \ge 0, \text{ with k being a constant.} \qquad (13)$$

Denote by B_r the real Banach space of sequences $\xi = \{\xi_y\}$, $y \in \mathbb{Z}^{\nu}$ such that the norm

$$\|\xi\|_{\nu} = \sup_{y \in Z^{\nu}} \left\{ e^{-|y|_r} \left| \xi_y \right| \right\} \qquad (14)$$

is finite.

Now, we refer to the following lemma:

Lemma (3):

Let $\vec{q}(t), \vec{p}(t)$ be solutions of (10) and (11) defined for $0 \leq t \leq T$ with initial data

$$\vec{q}(0) : L(0) = \{L_x(0)\} \in B_r \text{ (where } L_x(t) = L_x(p_x(t), q_x(t))\text{).}$$

Then there exists a constant *a*, independent of $\vec{q}(0)$ but dependent on *r*, such that

$$\|L(t)\|_r \leq e^{at} \|L(0)\|_r . \tag{15}$$

It is important to note that Lemma 3 is a Gronwall type estimate adapted to a Hamiltonian framework. In this case, the on-site energies satisfy a Gronwall estimate. Using Lemma 3, the authors prove the following existence theorem:

Theorem (3):

Let $\vec{q}(0), \vec{p}(0)$ be such that *L(0)*, as defined in Lemma 3, belongs to B_r. Then there exists $a \in B_r$ such that a is a solution of (10) and (11) defined for all *t*.

Finally, it can be shown as an immediate consequence of Lemma 3 and Theorem 3 that $\vec{q}(t), \vec{p}(t)$ satisfy exponential upper bounds.

Conclusion

In order to understand how to begin finding a solution to a Hamiltonian system, we studied various mathematical concepts to gain a stronger background in the subject of finding solutions to differential equations. We first studied Lipschitz functions, including: what it means to be a Lipschitz function; the properties Lipschitz functions have; and how to use Lipschitz functions to solve initial value problems. We then looked at Gronwall estimates and how to use Gronwall's lemma to find solutions to differential equations. We also addressed a fixed point theorem for contractive mappings. We then used these ideas to begin studying time evolutions for certain general anharmonic systems.

Future Plans

At the start of this research experience, goals were set for learning more about solving differential equations, and more specifically the relation of these ideas to Hamiltonian systems. However, much of the semester was spent on building up a stable background in order to have the knowledge necessary to begin analyzing a specific system. Consequently, future plans include, first and foremost:

(a) progressing to the study of the proof of the existence theorem (Theorem 3) for a solution to (10) and (11); and

(b) looking at specific Hamiltonian systems relative to our subject and beginning a discussion of how, as well as what it means, to find a solution to these systems.

References

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2) Walter, W.: Ordinary Differential Equations. Graduate texts in mathematics; 182. New York, Springer-Verlag 1998.