Some Techniques in Deterministic Modeling for Mathematical Biology

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Introduction

This project was initiated from a study on mathematical biology, which used the methods of nondimensionalization and regular perturbation theory. Last semester we studied biochemical modeling, which uses the aforementioned techniques in order to solve difficult bio-chemical approximations.

Our presentation, however, uses a physics model to describe how these techniques can be applied.
Objective:
To form a differential equation to model the motion of a simple pendulum.
Pendulum Motion Model

What we know

L = Length of Weightless Rod
p = Fixed Point of Suspension

A “bob” of mass m

F₁ = tension in the Rod
F₂ = mg where g is gravity

s = distance from the “bob” to the bottom of the arc

θ = θ(t) = Angle of Rod relative to plane perpendicular to earth

θ(0) = a
θ′(0) = 0
Find the Tangential Acceleration

Any Force on an arc can be broken down into the sum of a tangential and normal force.

\[ \sin(\theta) = \frac{F_{2T}}{F_2} \]

\[ \sin(\theta) = \frac{F_{2T}}{mg} \]

\[ F_{2T} = mg \sin(\theta) \]
Pendulum Motion Model

Find Acceleration of change in the ArcLength

Use the Arc Angle Formula

\[ S = L \theta \]
\[ \frac{dS}{dt} = L \frac{d\theta}{dt} \]
\[ \frac{d^2S}{dt^2} = L \frac{d^2\theta}{dt^2} \]

So in this case, the acceleration of change in traversed arc length is

\[ = -L \frac{d^2\theta}{dt^2} \]
Pendulum Motion Model

If you magnify an arc many times it begins to look flat. For this reason we can set the tangential force equal to the force derived from using the acceleration of decrease in arc length.

Therefore:

\[ F_{2T} = mg \sin(\theta) = -mL \frac{d^2\theta}{dt^2} \]
Pendulum Motion Model

A differential equation can now be formed.

\[ mg \sin(\theta) = -mL \frac{d^2\theta}{dt^2} \]

\[ g \sin(\theta) = -L \frac{d^2\theta}{dt^2} \]

\[ L \frac{d^2\theta}{dt^2} + g \sin(\theta) = 0 \]

\[ \frac{d^2\theta}{dt^2} + \frac{g}{L} \sin(\theta) = 0 \]

Let \( \omega^2 = \frac{g}{L} \) and * denote a variable with dimension.

\[ \frac{d^2\theta^*}{dt^*^2} + \omega^2 \sin(\theta^*) = 0 \]

(a non-linear differential equation)
Nondimensionalization is a technique of dimensional analysis that creates dimensionless variables, which allows differential equations to be stated in a dimensionless form. This is useful to scientists and engineers because it simplifies complex equations and puts the problem in a form amenable to the techniques of perturbation theory.
The differential equation of our Pendulum Model is:

\[ \frac{d^2 \theta^*}{dt^*^2} + \omega^2 \sin(\theta^*) = 0 \]

First list variables and parameters with their dimensions

<table>
<thead>
<tr>
<th>Variable</th>
<th>Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta^* )</td>
<td>L (length)</td>
</tr>
<tr>
<td>( t^* )</td>
<td>T (time)</td>
</tr>
<tr>
<td>( \omega )</td>
<td>T^{-1}</td>
</tr>
<tr>
<td>( a )</td>
<td>L</td>
</tr>
</tbody>
</table>

Conditions: \( \theta^*(0) = a \) and \( \frac{d \theta^*}{dt^*}(0) = 0 \)
Next for each variable \( v^* \), let \( p^* \) (known as the intrinsic reference quantity) be some combination of the parameters that have the same dimension as \( v^* \). The new dimensionless variable, \( v \) is defined as

\[
v := \frac{v^*}{p^*}
\]

Our new dimensionless variables are now:

\[
\theta := \frac{\theta^*}{a} \left( \frac{L}{L} \right) \quad t := t^* \omega \left( \frac{TT^{-1}}{TT^{-1}} \right)
\]

With new conditions: \( \theta(0) = 1 \) and \( \frac{d\theta}{dt}(0) = 0 \)
Now rewrite the dimensional variable $\theta^*$ in terms of the parameter and the dimensionless variable, leaving the dimensionless variable $t$. 

\[ \theta^* = a \theta \]
\[ t = \omega t^* \]

Next we will change our dimensional differential equation to a dimensionless equation by substitutions.
Next find the derivative of $\theta^*$. 

$$\frac{d\theta^*}{dt^*} = a \frac{d\theta}{dt^*}$$

By the chain rule:

$$a \frac{d\theta}{dt^*} = a \frac{d\theta}{dt} \frac{dt}{dt^*}$$

Now with substitution:

$$a \frac{d\theta}{dt} \frac{dt}{dt^*} = a \omega \frac{d\theta}{dt}$$

$$\frac{d\theta^*}{dt^*} = a \omega \frac{d\theta}{dt}$$
Next find the 2nd derivative of $\theta^*$. 
\[
\frac{d^2 \theta^*}{dt^*^2} = \frac{d}{dt^*} \left( a\omega \frac{d\theta}{dt} \right) = a\omega \frac{d}{dt^*} \left( \frac{d\theta}{dt} \right)
\]

Rewrite as:
\[
a\omega \frac{d\left( \frac{d\theta}{dt} \right)}{dt^*}
\]

By the chain rule:
\[
a\omega \frac{d\left( \frac{d\theta}{dt} \right)}{dt^*} = a\omega \frac{d\left( \frac{d\theta}{dt} \right)}{dt} \frac{dt}{dt^*}
\]
Now with substitution:

\[ a \omega \frac{d\left(\frac{d \theta}{dt}\right)}{dt} \frac{dt}{dt^*} = a \omega^2 \frac{d^2 \theta}{dt^2} \]

\[ \frac{d^2 \theta^*}{dt^{*2}} = a \omega^2 \frac{d^2 \theta}{dt^2} \]
Finally we can rewrite our original model:

\[ \frac{d^2 \theta^*}{dt^*^2} + \omega^2 \sin(\theta^*) = 0 \]

Substituting in:

\[ \frac{d^2 \theta^*}{dt^*^2} = a \omega^2 \frac{d^2 \theta}{dt^2} \]

We get the new dimensionless model:

\[ \frac{d^2 \theta}{dt^2} + a^{-1} \sin(a \theta) = 0 \]

With initial conditions: \( \theta(0) = 1 \) and \( \frac{d \theta}{dt}(0) = 0 \)
The Series Method of Regular Perturbation Calculations


- 5 step process
Assumptions

The dependent variable can be expressed in a series of the small parameter.

\[ \theta = \theta(t, a) = \sum_{i=0}^{\infty} \theta_i(t) a^i \]

Thus,

\[ \frac{d\theta}{dt} = \sum_{i=0}^{\infty} \theta'_i(t) a^i \]

\[ \frac{d^2\theta}{dt^2} = \sum_{i=0}^{\infty} \theta''_i(t) a^i \]
Step A:

Substitute the power series into the differential equation.

Recall: The pendulum model differential equation.

\[ \frac{d^2 \theta}{dt^2} + a^{-1} \sin(a \theta) = 0 \]

Substituting:

\[ \sum_{i=1}^{\infty} \theta_i''(t)a^i + a^{-1} \sin[a \sum_{i=1}^{\infty} \theta_i(t)a^i] = 0 \]
Step B:

Expand all quantities so that each term is written as a power series in $a$.

Recall:  \[ \sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \ldots \]

\[
\sum_{i=1}^{\infty} \theta_i''(t)a^i + a^{-1}\left\{ \left[ a \sum_{i=0}^{\infty} \theta_i(t)a^i \right]^3 - \frac{\left[ a \sum_{i=0}^{\infty} \theta_i(t)a^i \right]^5}{3!} + \frac{\left[ a \sum_{i=0}^{\infty} \theta_i(t)a^i \right]^7}{5!} \right\} = 0
\]
Step B (Continued):

(Note: We are using only powers of a no greater than 2)

The equation from the previous page simplifies into the following:

\[ \theta''(t) + \theta'_1(t)a + \theta'_2(t)a^2 + \left[ \theta_o(t) + \theta_1(t)a + \theta_2(t)a^2 \right] - \frac{1}{6} \theta_o^3 a^2 + O(a^3) = 0 \]
Step C:

Collect all terms in the equation and equate to zero the successive coefficients in the series.

\[
[\theta''_o(t) + \theta'_o(t)] + a[\theta''_1(t) + \theta'_1(t)] + a^2[\theta''_2(t) + \theta'_2(t) - \frac{1}{6} \theta^3_o] + O(a^3) = 0
\]

3 Differential Equations:

\[
\theta''_o + \theta'_o = 0
\]

\[
\theta''_1 + \theta'_1 = 0
\]

\[
\theta''_2 + \theta'_2 - \frac{1}{6} \theta^3_o = 0
\]
Step C (Continued):

Remark: The original non-linear differential equation has been replaced by a sequence of linear differential equations. This is a characteristic feature of perturbation methods.
Step D:

Substitute the power series into the original initial (or boundary) conditions, expand and equate the coefficients to zero and obtain a set of new initial (or boundary) conditions to supplement the sequence of differential equations obtained in Step C.

\[
\theta(t, a) = \sum_{i=0}^{\infty} \theta_i(t) a^i
\]

\[
\frac{d\theta}{dt} = \sum_{i=0}^{\infty} \theta_i'(t) a^i
\]
Step D (Continued):

We will now plug in our initial conditions and as a result we get (a) and (b)

Initial conditions: \( \theta(0) = 1 \) and \( \theta'(0) = 0 \)

(a) \[ \theta(0, a) = \sum_{i=0}^{\infty} \theta_i(0)a^i = 1 \]

(b) \[ \theta'(0, a) = \sum_{i=0}^{\infty} \theta'_i(0)a^i = 0 \]
Step D (Continued):

We will now expand and equate the coefficients to zero and obtain a set of new initial or boundary conditions.

(a) \[ \theta_0(0) - 1 + \sum_{i=1}^{\infty} \theta_i(0) a^i = 0 \]

so, \( \theta_0(0) - 1 = 0, \quad (\theta_0(0) = 1) \)

\[ \therefore \theta_i(0) = 0 \quad \forall \ i \geq 1 \]
Step D (Continued):

(b) \[ \theta'(0, a) = \sum_{i=0}^{\infty} \theta'_i(0)a^i = 0 \]

so, \[ \theta'_i(0) = 0 \quad \forall \quad i \]
Step D (Continued):

We will now supplement the sequence of differential equations obtained in Step C with our new boundary conditions found in (a) and (b).

\[
\begin{align*}
\theta''_0 + \theta_0 &= 0, & \quad \theta_0(0) = 1, \quad \theta'_0(0) = 0 \\
\theta''_1 + \theta_1 &= 0, & \quad \theta_1(0) = 0, \quad \theta'_1(0) = 0 \\
\theta''_2 + \theta_2 - \frac{1}{6} \theta^3_0 &= 0, & \quad \theta_2(0) = 0, \quad \theta'_2(0) = 0, \quad \theta_0(0) = 1
\end{align*}
\]
Step E:

Solve the linear differential equations in sequence.

1) \( \theta''_o + \theta'_o = 0 \)

2) \( \theta''_1 + \theta'_1 = 0 \)

3) \( \theta''_2 + \theta'_2 - \frac{1}{6} \theta^3_o = 0 \)
Step E (Continued):

Solving 1)

\[ \theta_0'' + \theta_0 = 0 \text{ where } \theta_0(0) = 1, \quad \theta_0'(0) = 0 \]

\[ \theta_0(t) = A \cos(t) + B \sin(t) \]

\[ A = 1, \quad B = 0 \]

\[ \therefore \theta_0(t) = \cos(t) \]
Step E (Continued):

Solving 2)

\[ \theta_1'' + \theta_1 = 0 \text{ where } \theta_1(0) = 0, \theta_1'(0) = 1 \]

\[ \therefore \theta_1(t) = 0 \]
Step E (Continued):

Solving 3)

\[ \theta_2'' + \theta_2 - \frac{1}{6} \theta_0^3 = 0 \quad \text{where} \quad \theta_2 = 0, \quad \theta_2'(0) = 0 \]

\[ = \theta_2'' + \theta_2 - \frac{1}{6} \cos^3(t) = 0 \]

\[ = \theta_2'' + \theta_2 = \frac{1}{6} \cos^3(t) \]
Step E (Continued):

This non-homogeneous differential equation can be solved using the method of “undetermined coefficients,” which gives the following result:

$$\theta_2(t) = \frac{1}{192}\cos(t) - \frac{1}{192}\cos(3t) + \frac{1}{16}t\sin(t)$$
Finally, an approximation:

By expanding the power series of  \( \theta = \theta(t, a) = \sum_{i=0}^{\infty} \theta_i(t) a^i \)

to powers of \( a \) no greater than 2, we achieve the following:

\[
\theta = \theta(t, a) \approx \cos(t) + a^2 \left[ \frac{1}{192} \cos(t) - \frac{1}{192} \cos(3t) + \frac{1}{16} t \sin(t) \right]
\]
Conclusion

Nondimensionalization and Perturbation methods are effective ways of approximating solutions to differential equations. In the study of enzyme kinetics (physical chemistry), chemical reactions are modeled by non-linear differential equations. Their solutions are approximated by the Quasi-Steady-State Approximation and Equilibrium Approximation, which utilize the methods of nondimensionalization and perturbation that were demonstrated earlier.
Bibliography

• Mathematics Applied to Deterministic Problems in the Natural Sciences by Lin and Segal, SIAM 1988
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