MATHEMATICAL MODELING
A Comprehensive Introduction

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Preface

These materials are being developed with support from National Science Foundation Award no. 0126650 entitled *A Mathematical Modeling Program for Undergraduates in Science, Mathematics, Engineering and Technology.*

The objective of this project is the development of innovative educational materials that incorporate a novel educational approach and perspective to enhance the teaching and learning of mathematics for the purposes of knowledge discovery. The general undergraduate educated with these materials will possess a readily applicable toolbox of mathematical ideas for quantifying real world problems as well as problem solving skills, and possibly the most importantly, the ability to interpret results and further understanding.

Our pedagogical perspective consists of the observation that mathematical modeling is often taught backwards. An application of interest is presented and then appropriate mathematical tools are subsequently invoked. The beginner is left with the obvious concern. How does one decide which method to use on a new problem? Our proposed solution to this dilemma is to teach mathematics first and then show why a given mathematical methodology can be applied to the modeling problem. We will be successful if the student completes their modeling course based on these materials with a good sense of what makes various mathematical methods inherently different. Furthermore, students that are aware of the fundamental distinguishing characteristics of the array of methodologies should now be equipped to address this question of central importance in modeling, i.e., which method when!

This text is the first of two planned works to establish "proof of concept" of a new approach to teaching mathematical modeling. The scope of the text is the basic theory of modeling from a mathematical perspective. A second applications focussed text will build on the basic material of the first volume.

It is typical that students in a mathematical modeling class come from a wide variety of disciplines. In addition, their preparation and mathematical sophistication can vary as widely as their areas of interest. This heterogeneity makes the teaching and learning of mathematical modeling a significant challenge. One of the main student prototypes is a intelligent although possibly mathematically naive student that must learn mathematically modeling to make progress in an area of research. If a course or textbook does not provide the necessary information for these good students to bridge educational gaps students everyone suffers. Indeed, most textbooks fail to be accessible to such audiences.

With enhancing accessibility as our motivation, we propose to implement a simple pedagogical device to facilitate the use of the text by students of widely varying backgrounds. This device consists of graded levels of presentation denoted by (E) for elementary, (I) for intermediate and (A) for advanced.

- (E) Mathematical beginners will find much of interest in the elementary sections as well as foundation material for further study. The diligent student can use this self-contained treatment to pave the way to reading of more advanced sections. The basic properties of mathematical techniques will be presented with an emphasis on how methods lead to specific applications.

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- (I) Intermediate material builds on the elementary material and extends the students expertise. Often intermediate material will involve computer experiments to stimulate more theoretical discussions in the advanced material. A good understanding of intermediate material should permit a student to develop new applications of central mathematical ideas.

- (A) Advanced material will provide mathematically mature students with a solid theoretical foundation for the subject. Mastery of this subject matter should provide the student with the insight required to further develop mathematical models.

If a section is labeled as (E) then all its subsections are at the same level. If it is not labelled, then each individual subsection will be labelled for level of difficulty.

These texts will be pilot tested at Colorado State University during the course of development and will incorporate a fundamentally new approach to modeling through general mathematical principles rather than ad hoc lists of methods and techniques. These methods will be demonstrated within the context of on-going state-of-the-art interdisciplinary research projects. (Such an approach will have the added advantage of broadening students perspectives and appreciation for the nature of basic university research.) The basic aim of the materials is to present an innovative approach to inform and educate students about the power and importance of basic mathematics and mathematical modeling in the process of knowledge discovery.

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Mathematical Modeling

Mathematical modeling is becoming an increasingly important subject as computers expand our ability to translate mathematical equations and formulations into concrete conclusions concerning the world, both natural and artificial, that we live in.

1.1 EXAMPLES OF MODELING

Here we do a quick tour of several examples of the mathematical process. We present the models as finished results as opposed to attempting to develop the models.

1.1.1 Modeling with Difference Equations

Consider the situation in which a variable changes in discrete time steps. If the current value of the variable is a_n then the predicted value of the variable will be a_{n+1}. A mathematical model for the evolution of the (still unspecified) quantity a_n could take the form

$$a_{n+1} = \alpha a_n + \beta$$

In words, the new value is a scalar multiple of the old value offset by some constant β. This model is common, e.g., it is used for modeling bank loans. One might amend the model to make the dependence depend on more terms and to include the possibility that every iteration the offset can change, thus,

$$a_{n+1} = \alpha_1 a_n + \alpha_2 a_n^2 + \beta_n$$

This could correpsond to, for example, a population model where the the migration levels change every time step. In some instances, it is clear that information required to predict a new value goes back further than the current value, e.g.,

$$a_{n+1} = a_n + a_{n-1}$$

Note now that two initial values are required to evolve this model. Finally, it may be that the form of the difference equations are unknown and the model must be written

$$a_{n+1} = f(a_n, a_{n-1}, a_{n-M-1})$$

Determining the nature of f and the step M is at the heart of model formulation with difference equations. Often observed data can be employed to assist in this effort.

1.1.2 Modeling with Ordinary Differential Equations

Although modeling with ordinary differential equations shares many of the ideas of modeling with the difference equations discussed above, there are many fundamen-

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tal differences. At the center of these differences is the assumption that time is a
continuous variable.

One of the simplest differential equations is also an extremely important
model, i.e.,

$$\frac{dx}{dt} = \alpha x$$

In words, the rate of change of the quantity x depends on the amount of the
quantity. If $\alpha > 0$ then we have exponential growth. If $\alpha < 0$ the situation is
exponetial decay. Of course additional terms can be added that fundamentally
alter the evolution of $x(t)$. For example

$$\frac{dx}{dt} = \alpha_1 x + \alpha_2 x^2$$

The model formulation again requires the development of the appropriate right-
hand side.

In the above model the value x on the right hand side is implicitly assumed to
be evaluated at the time t. It may be that there is evidence that the instantaneous
rate of change at time t is actually a function of a previous time, i.e.,

$$\frac{dx}{dt} = f(x(t)) + g(x(t - \tau))$$

This is referred to as a delay differential equation.

1.1.3   Modeling with Partial Differential Equation

In the previous sections on modeling the behaviour of a variable as a function of
time we assumed that there was only one independent variable. Many situations
arise in practice where the number of independent variables is larger than two. For
spatio-temporal models we might have time and space (hence the name!), e.g.,

$$\frac{\partial f}{\partial t} = \alpha \frac{\partial^2 f}{\partial x^2}$$

or

$$\frac{\partial^2 f}{\partial t^2} = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$$

1.1.4   Optimization

In many modeling problems the goal is to compute the "best" solution. This may
correspond to maximizing profit in a company, or minimizing loss in a conflict. It
is no surprise that optimization techniques take a central seat in the mathematical
modeling literature.

Now one may allow $x \in \mathbb{R}^n$ and require that

$$x^* = \arg\min f(x)$$

The quantity $f(x)$ is referred to as the *objective function* while the vector x con-
sists of decision variables. Because x sits in $\mathbb{R}^n$ the problem is referred to as
unconstrained.

Alternatively, one might require that the solution x have all positive components. If we refer to this set as S then the optimization problem is constrained

$$x^* = \arg\min_{x \in S} f(x)$$

If the objective function as well as the equations that define the constraint set are linear, than the optimization problem is called a *linear programming problem*. Otherwise, the problem is referred to as a nonlinear programming problem. As we shall see, solution methods for linear and nonlinear programming problems are very different.

1.1.5   Modeling with Simulations

Many problems may afford a mathematical formulation yet be analytically intractable. In these situations a computer can implement the mathematics literally and repetitively often times to extreme advantage.

Simulating Games.

• What is the probability that you can win a game of solitaire?

• What is the best strategy for playing blackjack?

• Given a baseball team consisting of certain players, in what order should they hit?

On the other hand, computer simulations can be employed to model evolution equations. Applications in the realm of fluid dynamics and weather prediction are well established. A striking new example of such simulation modeling is attempting to model electrical activity in the brain.

1.1.6   Function Fitting: Data Modeling

Often data is available from a process to assist in the modeling. How can functions be computed that reflect the relationships between variables in the data. Produce a model

$$y = f(x; w)$$

and using the set of input output pairs compute the parameters w. In some cases the form of f may be guessed. In other cases a model free approach can be used.

1.2   THE MODELING PROCESS

The goal in all modeling problems is *added value*. Something novel must be learned from the modeling process or one has completed an exercise in futility, or mathematical wheel spinning, depending on your perspective. There are many obvious questions the answers to which have inherent added value. For example:

• Should a stock be bought or sold?

• Is the earth becoming warmer?

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- Does creating a law have a positive or negative societal effect?

- What is the most valuable property in monopoly?

Clearly this is a very small start to an extremely long list.

1.2.1 An Algorithm for Modeling?

The modeling process has a sequence of common steps that serve as an abstraction for the modeler:

- Identify the problem and questions.

- Identify the relevant variables in a problem.

- Simplify until tractable.

- Relate these variables mathematically.

- Solve.

- Does the solution provide added value?

- Tweak model and compare solutions.

1.3 THE DELICATE SCIENCE OF ERRORS

If one had either infinite time or infinite computing power error analysis would presumably be a derelict activity: all models would be absolutely accurate. Obviously, in reality, this is not the case and a well-accepted *modus operandi* in modeling is committing admissible errors. Of course, in practice, the science is more *ad hoc*. If terms in an equation introduce computational difficulties the immediate question arises as to what would happen if those terms are ignored? In theory we would rather keep them but in practice we can't afford to. Thus the delicate science of modeling concerns retaining just enough features to make the model useful but not so many as too make it more expensive to compute than necessary to get out the desirable information.

We illustrate this concept by examining the seemingly innocuous junior high school problem

$$\epsilon x^2 + x + 1 = 0$$

Of course we can solve this problem exactly using the quadratic formula[1]

$$x = -\frac{1}{2\epsilon} \pm \frac{\sqrt{1 - 4\epsilon}}{2\epsilon} \tag{1.1}$$

For a moment, let us assume that the quadratic term were actually an unknown term, e.g.,

$$\epsilon f(x) + x + 1 = 0$$

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[1] If you don't recall this, then the famous Science Fiction write Robert Heilein suggested you not be allowed to vote.

and that actually computing f might be rather expensive. We might argue that if ϵ were very small that this term could safely be ignored. Now let us return to the simple case of $f(x) = x^2$. If ϵ is taken as zero then clearly it follows that

$$x = -1$$

is the unique solution. However, we know from our quadratic equation however that if $\epsilon = 0.0000001$ (any non-zero number would do), then there are two solutions rather than one. So we have actually lost a potentially important solution by ignoring what appeared to be a small quantity. In addition, we may also have introduced inaccuracies into the obtained solution and this issue must be explored.

In essence we are concerned with how quickly the solution changes about the point $\epsilon = 0$. A quick graph of Equation (1.1) reveals that the solution changes rather quickly.

To see how this solution changes as a function of ϵ consider the series expansion

$$x = a_0 + a_1\epsilon + a_2\epsilon^2 + a_3\epsilon^3 + \dots$$

Substituting this expansion into the original quadratic results in the new equation

$$a_0 + 1 + (a_0^2 + a_1)\epsilon + (2a_0a_1 + a_2)\epsilon^2 + \dots = 0$$

Setting the coefficients of the different powers of ϵ to zero gives the series solution for x as

$$x = -1 - \epsilon - 2\epsilon^2 + \dots \tag{1.2}$$

So if $\epsilon \approx 0.01$ we can conclude the error is on the order of 1% and the error will grow quickly with ϵ.

This problem is explored further in the exercises and function iteration is introduced to track down the 2nd solution in the quadratic equation. For further discussion of these ideas see [4].

1.4   PURPOSE OF THIS COURSE

The primary goal of this course is to assist the student to develop the skills necessary to effectively employ the ideas of mathematics to solve problems. At the simplest level we seek to promote an understanding of why mathematics is useful as a language for characterizing the interaction and relationships among quantifiable concepts, or in mathematical terms, variables. Throughout the text we emphasize the notion of *added value* and why it is the driving force behind modeling. For a given mathematical model to be deemed a success something must be learned that was not obvious without the modeling procedure. Very often added value comes in the form of a prediction. In the absence of added value the modeling procedure becomes an exercise not unrelated to digging a ditch simply to fill it back up again.

The emphasis in this course is on learning why certain mathematical concepts are useful for modeling. We proceed *from mathematics to models* rather than the popular reverse approach and downplay interdisciplinary expertise required in many specific contexts. We firmly believe that by focusing on mathematical concepts the ability to transfer knowledge from one setting to another will be significantly enhanced. Hence, we emphasize the efficacy of certain mathematics for constructing models.

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PROBLEMS

1.1. Name three problems that might be modeled mathematically. Why do you think mathematics may provide a key to each solution. What is the added value in each case?

1.2. Consider the differential equation

$$\frac{dx}{dt} = x$$

Translate this model to a difference equation. Compare the solutions and discuss.

1.3. Consider the equation

$$x^2 + \epsilon x - 1 = 0$$

for small ϵ. How does ignoring the middle term ϵx change your solution? Is this a serious omission?

1.4. Using a Taylor series expansion express the solution to the quadratic equation in Equation 1.1 as a series. Include terms up to cubic order.

1.5. Find the cubic term in the expansion in Equation (1.2).

1.6. One approach to determining zeros of a general function, i.e., computing roots to $f(x) = 0$, is to rewrite the problem as $f(x) = x - g(x)$ and to employ the iteration $x_{n+1} = g(x_n)$.

(a) If we take

$$g(x) = -\frac{1}{x}$$

show that the iteration can be written

$$x_{n+1} = -\frac{1}{\epsilon}(1 + \frac{1}{x_n})$$

(b) Let $x_0 = -1/\epsilon$ and compute x_1. By considering the Taylor series of the solution of the quadratic equation argue that this is a two term approximation to the *missing* solution.

(c) Compute x_2.

1.7. (a) Substitute $x = y/\varepsilon$ into the equation

$$\varepsilon x^2 + x + 1 = 0 \tag{1.3}$$

and multiply the resulting equation for y by ε. Show that this leads to

$$y^2 + y + \varepsilon = 0. \tag{1.4}$$

When $\varepsilon = 0$, the equation (1.4) has two solutions: $y = 0$ and $y = -1$. This suggests that (1.4) allows us to compute both solutions of (1.3) through a perturbation analysis.

(b) Reproduce the solution to (1.3) given by Eq. (1.2) by computing a solution of the form

$$y = b_1\varepsilon + b_2\varepsilon^2 + b_3\varepsilon^3 + \dots$$

for (1.4).

(c) Proceed similarly using the form

$$y = -1 + c_1\varepsilon + c_2\varepsilon^2 + \dots$$

to find the expansion of the missing solution to (1.3).