Computational Modeling by Case Study

Computational Modeling by Case Study:

All Models Are Uncertain

By

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PREFACE

Sometime in 2014, Zach first came to Gianluca as a Ph.D. candidate looking for an advisor. In that conversation, Gianluca said something that would drive Zach's professional interests for the next decade—engineers use quantitative models to make important decisions, but they almost never quantify *uncertainty*. This book collects much of the conceptual and computational developments we have made in our technical research on uncertainty quantification since that first conversation. It's the book Zach wishes he had when he started in this research area.

There are many excellent texts that describe *how* to quantify uncertainty and we cite many of them throughout this book. However, we felt that there was no book that sufficiently connected the *how* to the *why*. This book takes a different approach to uncertainty quantification than existing texts: Our focus is not on mathematical derivations (not just *how*), but rather on drawing connections (*why* quantify uncertainty). We use computer programming tools to give you examples you can quickly adapt to your own problems.

This book would not have happened without the help of several colleagues. Art Owen and Ron Kenett conducted a technical review of this manuscript, which substantially improved the accuracy and presentation of the material. We are grateful for them lending their deep statistical expertise to this project. (All errors are, of course, our own.)

Mike Baiocchi and Abe Levitan contributed many helpful ideas when Zach was developing the cause / source framework that appears in Chapter 6. Zach's former student Alana Huitric drew the "manufacturing diagram" that appears in Chapter 6. Dave Sharp advised the original work on the Hanford case study

(Section 10.1) and served as a mentor to Zach in the early days of his Ph.D. training. Andrew Ziccarelli reviewed the LRFD case study, providing his expertise as a Structural Engineer (Section 10.3). Mark Benjamin generated the turbulence dataset (Appendix A.2). Finally, Suzanne Olivier copyedited the manuscript and provided the photo of the Ivanpah Solar Power Facility used in Section 10.4. We are grateful to all of you for helping make this book happen!

- Zach del Rosario, Olin College
- Gianluca Iaccarino, Stanford University

Orienting

CHAPTER

ONE

ORIENTING

1.1 What Is a Model?

This book is about models, but what is a model? For our purposes, a **model** is a representation of something in the real world. As a model is only a representation, it is necessarily a *simplification* of the real world thing it represents. This leads to many limitations associated with the model, a fact captured in this famous quote:

> All models are wrong, but some are useful.
>
> ---George E.P. Box

This quote is the inspiration for this book's title: If all models are wrong, then all models are definitely uncertain. Box's adage is profound, but often misunderstood. While quantitative tools in science and engineering are often treated as a source of truth, *all* mathematics applied to describe the physical world are *only* models. Taking Box seriously means that we must directly confront the uncertainties in our models.

Conversations with a Model: What Is a Model?

To provide some additional perspective throughout this book, we've included some "conversations with a model"—lightly-edited conversations with a large-language model (LLM)-based chatbot.

Gianluca: "What is a model?"

Bot: "A model is a simplified representation of a system or process, often used to make predictions or understand the underlying mechanics of the system.

Models can take many forms, such as mathematical equations, computer simulations, or physical prototypes. They are often used in fields such as science, engineering, and economics to better understand complex systems and make informed decisions."

Gianluca: "Give me a couple of examples."

Bot: "Sure, here are a few examples of different types of models:

- In weather forecasting, meteorologists use mathematical models to simulate the Earth's atmosphere and predict future weather patterns.
- In finance, economists use economic models to predict changes in interest rates and the stock market.
- In engineering, a physical model of a car is often built to test its aerodynamics and fuel efficiency.
- In machine learning, a model is a set of algorithms that take in data, learn from it, and make predictions or classifications.
- In biology, researchers use models of cells and organisms to study their functions and interactions with other living things.
- In physics, theoretical models are used to explain the behavior of subatomic particles and the behavior of the universe as a whole."

This book aims to give you both *tools* and *understanding* to handle the uncertainty in models. The tools will come in the form of a **grammar of model analysis**, implemented in the Python package Grama. Understanding comes in many forms, including domain-specific knowledge and more general modeling ideas. In this book, we synthesize ideas across disciplines to learn how to handle uncertainty in physical models. We will focus less on mathematical details and more on integrating ideas into a practical perspective.

Conversations with a Model: A Philosopher's Take on Uncertainty

Zach: "Socrates, what is uncertainty?"

Bot: "Uncertainty is a natural aspect of the human condition. We can never truly know everything, and there will always be gaps in our understanding. However, this does not mean that we cannot strive for knowledge and understanding. I believe that the pursuit of knowledge is a lifelong endeavor and that the more we question and reflect on our beliefs, the more certain we can become in our understanding of the world. Through my method of questioning (the Socratic method) I would encourage individuals to question their own beliefs and to seek out the truth through critical thinking and self-reflection. In this way, we can move closer to certainty and understanding, even if we will never reach a state of complete understanding."

This first part of the book—Orienting—provides a high-level overview of both components: tools in the form of Grama, and understanding in the form of mindset.

1.2 Intended Audience

This book is intended for students of science and engineering who are focused on mathematical and computational analysis. We have designed the book accordingly:

- **Students**
  - This book is intended for early graduate students and advanced undergraduates in a scientific or engineering discipline. It is intended primarily as a volume for learning but may serve secondarily as a reference volume.
- **Scientists and engineers**
  - We assume that you know how to carry out a mathematical analysis of physical systems but do not yet know how to quantify uncertainties in those systems.
- **Those focused on analysis rather than experimentation**
  - This book is written from the perspective of computational science. While we will discuss some considerations of experimentation (particularly as it pertains to data), our focus is on computational modeling and analysis.

1.3 Required Skills

We are expecting that you have a few basic skills. To get the most out of this book, you should have:

- Basic proficiency with the Python computing language. You should be familiar with basic datatypes (strings, lists, dictionaries, objects, and methods), control flow (loops), comments, and functions.
  - This book uses the `py-grama` software package to minimize your required coding knowledge. You should be able to use this book if you have taken a first course in Python or have a few months of experience with the language.
- Fundamental understanding of probability, and possibly some knowledge of statistics. You should know what a (continuous) random variable is, and how mathematical objects such as distributions and densities relate to random variables.
  - This book makes *thorough* use of probability. We assume a fundamental knowledge of probability, so this should not be your introduction to probability theory.
  - This book also uses some ideas from statistics. We will use ideas such as estimation and statistical intervals but will provide a gentle introduction to these concepts and will explain them in context.
  - This book is about applying probability and statistics to science and engineering topics, so if you have taken a first course in probability, this book will enable you to put those skills to productive use!
- Fundamental understanding of mechanical physics. You should be familiar with calculus, Newton's laws of motion, and differential equations.
  - This book is organized around case studies: detailed investigations of particular topics. To follow these case studies, you will need some basic background knowledge. However, we will introduce more domain-specific concepts when necessary.
- Domain-specific knowledge from your discipline.
  - You should have the skills to build and implement domain-specific

physical models. Your models should be able to map between known input quantities to predict output quantities.

- This book is intended to inspire you with ideas on how to use uncertainty quantification techniques in practice and to enable you to put those ideas into practice quickly using the `py-grama` programming package. This book will give you new ideas on how to solve problems… and new kinds of problems to solve!

1.4 Where to Start / How to Use This Book

This book is divided into three parts (plus appendices):

1. Orienting: High-level ideas for reasoning about uncertainty in models
2. Developing: More detailed ideas for building models and quantifying uncertainty
3. Answering: Case studies applying the aforementioned ideas to complex problems
4. Appendices: Supplemental materials

You can certainly read this book from cover to cover! However, we recommend the following reading strategy.

- Read Part 1: Orienting in full.
- Skim the case studies in Part 3: Answering to find topics that interest you. Pick one to study further.
- Each case study has a list of “dependency” chapters from Part 2: Developing. Read the appropriate Part 2 chapters to help understand each chosen case study.

Exercise 1.4.1: Ideas.

To get the most out of this book, you should copy the code examples into your own coding environment and try adapting them. Throughout the book we will mark these exercise ideas with similar “Exercise” blocks.

CHAPTER TWO

CURIOSITY AND SKEPTICISM: A HEALTHY MINDSET

This chapter is focused on helping you develop a healthy **mindset**, or mental attitude, for scientific investigation. This mindset is composed of two opposing *modes* of operation: curiosity and skepticism.

Learning Objectives In this chapter, you will learn:

- the dual modes of curiosity and skepticism[1]

Running Example: Detective Enola

This book is full of examples of curiosity and skepticism in action. But before we introduce any of the detailed scientific case studies, let's use the scenario of a detective story for this chapter: The owner of a large fortune has just been found in her manor with a knife in her back, and Detective Enola Knox suspects a family member is responsible. As we'll see below, the protagonist of a murder mystery exemplifies the dual modes of curiosity and skepticism.

---

[1] We are grateful to Bill Behrman, who first introduced Zach to the idea of curiosity and skepticism as modes of operation. These dispositions are also discussed by Wild and Pfannkuch [1999].

2.1 Using a Scientific Mindset Rather Than Following a Procedure

Curiosity and skepticism are not a fixed procedure, but rather two modes of a mindset. The subjects of the following sections are not a checklist to go through sequentially, but rather a set of "moves" or approaches we can employ during the scientific investigative process.

An analogy: The U.S. legal system is based on the idea that truth can be found by pitting two rational opposing forces against each other. Through the defense and prosecution teams working against each other, presenting evidence, and finding holes in each other's arguments, society can come closer to the truth and hence justice.

The back-and-forth between curiosity and skepticism is similar: two modes we should switch between during scientific investigations. By acting out of curiosity, we can ask questions and pose tentative answers. By engaging in skepticism, we can identify flaws and improve our analysis. In practice, we should move between the two modes iteratively throughout an investigative process, as this will improve our analysis and uncover flaws (**Figure 2.1.1**). Let's look at these two modes in greater detail.

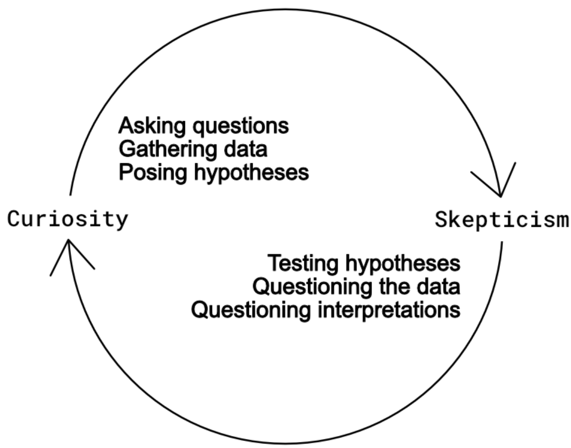

Figure 2.1.1: The dual modes of curiosity and skepticism, with some of their associated "moves."

2.2 Curiosity

The mode of **curiosity** is characterized by openness: to exploration, to new questions, to other approaches, and to possible answers. Some of the "moves" in the curious mode are (1) asking questions, (2) gathering data, and (3) posing hypotheses.

2.2.1 Asking questions

The very notion of curiosity is closely associated with asking questions: We describe a child as "curious" if they tend to ask a lot of questions. Most scientific investigations start with some sort of overarching question that kicks off a research effort—we will call this a **modeling question**. However, the process of asking questions doesn't stop there. The process of scientific inquiry tends to involve posing new questions in an iterative manner.

Running Example: Detective Knox.

In a murder mystery, a detective will generally have one overarching question: "Whodunit?" But to answer this driving question, Detective Knox will have to pose and answer a variety of subordinate questions: Who are the suspects? What facts do I know? Why is the eldest son being cagey? These questions can help the detective decide what data to gather next.

2.2.2 Gathering data

Questions are useful in part because they focus our efforts. One of the main ways we make progress in answering our questions is to gather data.

In scientific modeling, we can gather both experimental data (from a physical experiment) and simulated data (from a simulation of a model). Experimental data requires running a physical experiment. Experiments require time and hardware but come directly from reality. Lightweight computational models can be run far more quickly to suggest possible trends, which can help to plan physical experiments.

Note that we can gather data in a curious exploratory way or in a more skeptical testing fashion. The data collection we plan in the curious mode tends to be more *ad hoc*. Perhaps we plan out a quick pilot study or obtain some archival data that is only somewhat associated with our question. The point of gathering data in the curious mode is not to be comprehensively formal; rather, it is to move quickly and refine our questions so we can move toward the greater clarity of a formal hypothesis.

Running Example: Detective Knox.

Even before Detective Knox formulates an answer to any of her initial questions, she will try a variety of "moves" to gather data for her investigation. She might try dusting for prints at the scene of the crime, interviewing eyewitnesses to search for plausible motives, or sending the murder weapon out to the lab for a forensic test. In addition, the coroner's examination of the victim's body provides Detective Knox with a time of death, information about blunt trauma to the victim's face, and a knife wound as the cause of death, all of which narrow the set of possible suspects—hence the possible hypotheses.

2.2.3 Posing hypotheses

The primary output of the curious mode is a **testable hypothesis**—an assertion about the world that we can assess. This is a synthesis of the available data and initial questions, one which ideally addresses our original modeling question. Through this synthesis, we may change our modeling question to align with a testable hypothesis. Arriving at a hypothesis is often the inflection point to move from the curious mode to the skeptical mode.

Posing a hypothesis requires interpreting the data. This is where domain-specific knowledge of the problem is essential: Only a specialist in your field can interpret the data in terms of your discipline's accepted conventions. However, regardless of one's discipline, there is one criterion that all hypotheses *must* meet—a scientific hypothesis must be testable.

As Popper [2005] wrote on the philosophy of science, a scientific hypothesis should be specific enough to be *falsifiable*; that is, able to be shown to be false. Falsifiability is a reasonable criterion for determining what is a testable hypothesis. If a hypothesis is too flexible or too vague to be testable, this is a sign that the hypothesis needs refinement. Usually, a falsifiable hypothesis makes predictions about what would happen under a certain experimental setting; in this case, the hypothesis would be falsified if the prediction failed to hold.

Running Example: Detective Knox.

Detective Knox wants to know "whodunit," so her hypothesis should include a suspect, motive, and opportunity. She suspects the eldest son is responsible, as the household staff intimated that he is greedy and impatient to inherit. She makes sure to incorporate all the data she has gathered in formulating her hypothesis; she thinks the son stabbed his mother in the back with a knife around the time of death, causing her to fall forward onto her face.

2.3 Skepticism

The mode of **skepticism** is characterized by rejection: rejecting hypotheses, finding flaws in the data and methods, and even probing the importance of questions. Some of the "moves" in the skeptical mode include (1) testing hypotheses, (2) questioning the data, and (3) questioning the interpretation. Let's look at each of these in turn.

2.3.1 Testing hypotheses

Once we have posed a hypothesis, it needs to be subjected to testing. As noted under Posing hypotheses just before, any scientific hypothesis must be testable, usually by being falsifiable. However, you might not recognize your hypothesis as untestable until you switch over to the skeptical mode.

Remember, a skeptic would not use a "friendly" test. Try to formulate a strenuous test of your hypothesis. What would a worst-case scenario look like for your hypothesis? What would be a convincing argument, even to your toughest critic?

We'll see more about this in Section 8.2, but as a preview, you should use data that are independent of your exploratory data to test a hypothesis. In the parlance of machine learning, testing a model on the same data that was used to train it is an optimistic (and even foolish!) way to assess a model [James *et al.*, 2013]. If your hypothesis is true, then your findings should hold for an independently gathered dataset.

Running Example: Detective Knox.

Detective Knox is confident in her hypothesis, so she accuses the son. However, he denies the accusation and produces a compelling alibi: He was with the butler during the victim's time of death, and the butler is beyond reproach. Clearly, something about Detective Knox's hypothesis does not hold up.

If your hypothesis does *not* hold, then you need to reexamine your reasoning. This includes both your data and your interpretation of the facts.

2.3.2 Questioning the data

Sometimes the data themselves are in error, either in the values recorded or in the context of the data. Simulations can be misconfigured or unconverged, which will lead to errors in the data values. Experiments can have confounding (aka *lurking*) variables, which will lead to an incorrect understanding of the data context. When your hypothesis does not hold, you must hunt down and eliminate these kinds of issues.

Conversations with a Model: Confounding Variables

Gianluca: "What is a confounding variable?"

Bot: "A confounding variable is an extraneous variable that affects the relationship between the independent variable and the dependent variable in a study. Confounding variables can make it difficult to determine the true relationship between the variables of interest.

For example, imagine a study that seeks to examine the relationship between coffee consumption and heart disease. However, if the study participants who drink more coffee also tend to smoke cigarettes more frequently, it may be difficult to determine whether the observed relationship between coffee consumption and heart disease is due to the coffee or the smoking. In this case, smoking would be considered a confounding variable."

As we will see in Chapter 6, uncertainty can be either real or erroneous, with respect to a target quantity. *Real uncertainty* affects the quantity we aim to study, while *erroneous uncertainty* affects only our measurement. Determining whether the uncertainty we see is due to real or erroneous sources helps us narrow our search to either before or after the phenomenon of interest. If there is an explanation for erroneous uncertainty, then our measurement is subject to a mistake that we can eliminate. Collecting new data while eliminating such sources of erroneous uncertainty will help us more accurately understand the object of our scientific study.

Running Example: Detective Knox.

Detective Knox thinks there may be something fishy about the reported time of death, so she has a longer conversation with the coroner. A closer inspection of the victim's body confirms the time of death, so the data do not seem to be in error….

2.3.3 Questioning interpretations

Sometimes it's not the data that are in error, but rather our interpretation. This can mean we made an error in our reasoning, or that we were missing some key facts about the scenario at hand.

If we see unexpected variation in our measurements that seems to arise from some consistent phenomena, we might find that a previously unknown phenomenon can explain this behavior[2]. Such anomalous variability can lead to a scientific discovery. However, a *lack* of variability can also lead to scientific advancement.

Before Einstein formulated his theory of relativity in the early 1900s, all waves had been observed to travel within some medium. Hence, scientists at the time believed that light, exhibiting wavelike properties, must travel within a medium called the *luminiferous aether*. Scientists such as Albert Michelson carried out experiments to detect the "aether wind" due to the motion of Earth through this "aether" but failed to detect any change in the speed of light. Einstein's contribution overturned this understanding of physics, and

[2] We will see an example of *lurking variables* and the techniques used to detect them in Section 9.2.

our modern understanding is that light travels through a vacuum at a speed constant to all observers.

Running Example: Detective Knox.

In conversation with the coroner, Detective Knox realizes that the knife wound and face trauma could have occurred at different times. If the victim were killed at one time and her body clumsily moved later, this could account for both wounds. Upon further investigation, she finds a cunning mechanism hidden in the victim's chair: The mother died by a deadly trap while the son was with the butler, and the son returned later to rearrange the scene to make it appear to be a much simpler murder. By employing both curiosity and skepticism, Detective Knox solved the case.

2.4 Using the Mindset to Reduce Uncertainty

This book is focused on modeling in the presence of *uncertainty*. Using a mindset that switches between curiosity and skepticism will help you reduce uncertainty to a tolerable level: Curiosity will help you learn new things, while skepticism will help you arrive at sound conclusions. Iterating between these modes until the uncertainty is tolerable will help you reach an answer to your modeling questions.

2.5 Practicing the Mindset

These ideas about curiosity and skepticism are important, but if they remain only ideas they are just theoretical. You need to go beyond simply knowing about these ideas and start using them in your own scientific practice. However, this is easier said than done!

To help you make use of the curious and skeptical modes, the case studies in this book are written to emphasize these modes. With a bit of imagination, you can generalize these sorts of insights to your own context. While reading this book, think about ways the same kinds of observations or issues could show up in your scientific investigations. Better yet, try practicing some of the techniques suggested in this book on your own problems!

CHAPTER

THREE

THE MODELING PROCESS

This chapter introduces a general *modeling process*. Much of the real work of modeling does not involve manipulating equations or running simulations but rather focuses on broader critical inquiry. The modeling process presented here is focused on posing and answering scientific questions within a chosen context.

Learning Objectives In this chapter, you will learn:

- the importance of a question to guide modeling
- model fundamentals: the system boundary and quantities of interest (QOI)
- key steps to modeling: gathering information and building and assessing the model

3.1 Start with a Modeling Question

Scientific modeling is done to answer some form of question, which we will call a **modeling question**. Some examples of modeling questions include "How can we make this bridge design safe?" "What will the global mean temperature be in the year 2100?" "Do we need this assumption to explain this observed phenomenon?"

To help steer modeling, we need to first understand what sort of question we are asking. The framework in **Figure 3.1.1** categorizes such questions based on the *kind of action* we will take and the *degree of specificity* in our question.

We list four examples on these axes, which will be described in detail later in the chapter.

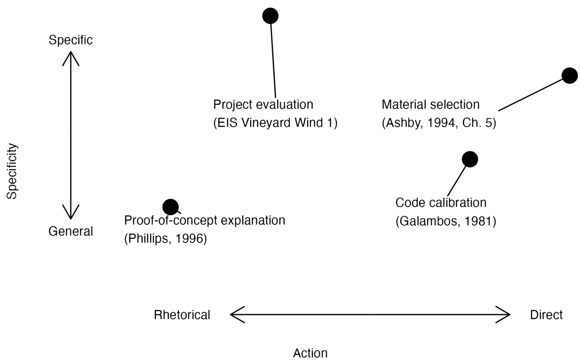

Figure 3.1.1: The four modeling examples in this chapter, plotted on two axes. The *specificity* axis refers to the specificity (or generality) of the modeled scenario. The *action* axis refers to how directly the modeling work will influence a decision.

3.1.1 Action: Rhetorical or Direct

The **action axis** (Figure 3.1.1) ranges from direct to rhetorical. **Direct action** implies the modeler (or modeling team) will take action on their own. For instance, engineers use models to inform their design work—their modeling work will directly influence their actions. Note that *truly* direct action is rare in practice; most organizations diffuse decision power to some degree. However, direct action is a useful contrast to *rhetorical action*.

Rhetorical action refers to the modeler's efforts to influence others' actions. The modeler will not be taking direct action based on the model's results. This is often done in research, where a researcher publishes a paper explaining a specific phenomenon with the intent of inspiring other researchers to build on their ideas. This is also done in the policy space, where modelers predict the potential outcomes for different policy choices to inform and influence decision-makers. While it is always important to be effective when communicating the results of a study, such communication is even more crucial when one's goals are rhetorical.