Fundamentals of Modeling Part 2

Course: Complex Systems Modeling

Robert Flassig

Brandenburg University of Applied Sciences

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Outline

Approaches to Scientific Model Building

There are two major families of modeling approaches in science and engineering:

- **Descriptive Modeling**
- **Rule-Based Modeling**

Descriptive Modeling

In descriptive modeling, researchers aim to specify the actual state of a system at a given time. Examples include:

- Taking a picture
- Creating a miniature
- Writing a biography

This can also be done using quantitative methods like:

- Regression analysis
- Pattern recognition

Goal: Capture "What the system looks like."

Rule-Based Modeling

In rule-based modeling, researchers define dynamical rules to explain system behavior. Examples include:

- Dynamical equations
- Theories
- First principles

This approach helps predict future states and can be quantitative or conceptual (e.g., Darwin's evolutionary theory).
Goal: Capture "How the system will behave."

Cycle of Descriptive and Rule-Based Modeling

Newton's law of motion is an example of rule-based modeling, making sense of observational information and predicting planetary movement.

Descriptive modeling accumulates descriptions, while rule-based modeling explains them. These two approaches form a cycle in scientific modeling, taking turns in driving discoveries.

Focus on Rule-Based Modeling

This course focuses on rule-based modeling, particularly for complex systems. Rule-based models help:

- Understand emergence
- Study self-organization

This is done through computer simulation and mathematical analysis at microscopic scales.

Typical Rule-Based Modeling Cycle

The typical steps of rule-based modeling include:

1. Observe the system of interest.
2. Reflect on possible rules causing the observed characteristics.
3. Derive predictions and compare with reality.
4. Modify the rules and repeat the cycle.

Termination is based on the modeler's satisfaction or resource limitations.

Challenges in Rule-Based Modeling

Among the four steps, reflecting on possible rules is particularly challenging because:

- It relies heavily on the modeler's personal knowledge and experience.
- It is deeply connected to how one perceives the world, making it a difficult process to teach or learn.

Examples

Here are some examples...

Examples of Descriptive vs. Rule-Based Models

Descriptive (What it looks like)

- Regression of temperature vs. CO2
- Population data fitting
- Image-based pattern recognition
- Empirical load forecasting

Rule-Based (How it behaves)

- Pendulum dynamics
- Lotka–Volterra predator–prey
- Heat diffusion
- Sierpiński carpet (geometric rule)

Upcoming: explore these models interactively in the Jupyter notebook.
But first, let's dig into key considerations for modelers

Modeling Complex Systems: Key Considerations

- **Key Questions:** What are the main questions to address in the system?
- **Scale of Description:** At what scale should the system's behaviors be described?
    - Define the "microscopic" components and their dynamics.
- **System Structure:** How is the system organized?
    - Identify components and their interactions.

Modeling Complex Systems: Dynamics and Changes

- **Possible States:** What dynamic states can each component exhibit?
- **Temporal Changes:** How does the system evolve over time?
  - Define rules for state changes due to interactions.
  - Determine how interactions between components change over time.

From Examples to Model Refinement

Goal: Connect real-world phenomena to the process of building and refining models.

Examples:

- **Egg boiling time:** Predict yolk softness based on time and temperature. Compare a descriptive fit (empirical cooking chart) to a rule-based model (heat diffusion in a sphere).
- **Traffic flow:** Each driver follows local rules (distance, braking, reaction time) — yet global patterns such as stop-and-go waves emerge.
- **Population dynamics:** Simple birth–death or predator–prey rules lead to rich collective behavior (equilibrium, oscillation, collapse).

Exercise – Refining Your Model:

Example Solutions (1/3): Descriptive vs. Rule-Based Models

Egg Boiling Time

- **Descriptive model:** Empirical relation between cooking time t, water temperature T_w, and yolk softness S:

$$S = a - b\, e^{-c\, t(T_w - 100)}.$$

  Captures observed outcomes without physical reasoning.

- **Rule-based model:** Transient heat diffusion inside a spherical egg:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T, \qquad T(R,t) = T_w,\ \ T(0,0) = T_0.$$

  The egg is "soft" when the yolk center reaches $T(0,t) = T_y$.

Interpretation: Descriptive models fit data; rule-based models explain underlying heat transport.

Example Solutions (2/3): Descriptive vs. Rule-Based Models

Traffic Flow

- **Descriptive model:** Empirical *fundamental diagram* relating density ρ and mean speed $v(\rho)$:

$$q(\rho) = \rho\, v(\rho), \quad v(\rho) \approx v_{\max}\left(1 - \frac{\rho}{\rho_{\max}}\right).$$

  Derived from aggregated traffic data.

- **Rule-based model:** Microscopic car-following dynamics for vehicle i:

$$\frac{dv_i}{dt} = a\left(1 - \frac{v_i}{v_0}\right) - b\left(\frac{s^*(v_i, \Delta v_i)}{s_i}\right)^2,$$

  where each driver adjusts acceleration based on distance and speed difference.

Interpretation: Local driving rules create global phenomena such as stop-and-go waves.

Example Solutions (3/3): Descriptive vs. Rule-Based Models

Population Dynamics

- **Descriptive model:** Logistic growth fitted to measured population data:

$$N(t) = \frac{K}{1 + e^{-r(t-t_0)}}.$$

  Describes saturation but not interaction mechanisms.

- **Rule-based model:** Lotka–Volterra predator–prey system:

$$\frac{dx}{dt} = \alpha x - \beta xy, \qquad \frac{dy}{dt} = \delta xy - \gamma y.$$

  Captures feedback between resource and consumer populations.

Takeaway

- Descriptive $\Rightarrow$ summarizes observed behavior (*what is*).
- Rule-based $\Rightarrow$ encodes mechanisms (*how it changes*).
- Model refinement connects both: fit parameters $\leftrightarrow$ test rules.