Scientific Modeling: a multilevel feedback process

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Abstract

Model construction is one of the key scientific activities. In distinction to the majority of the previous machine discovery systems, model formation applies in theory-rich context. Our long term goal is automation of model construction. This paper reports on exploratory work towards that goal. We start from the distinction between models and theories, which is critical to the presented approach. We also distinguish between modeling and two scientific activities, which are different but which support modeling: construction of operational definitions and experimentation. Then we present the basic steps of scientific model construction, outlining data structures and an algorithm which, using a number of feedback loops, incrementally develops a model of a natural phenomenon. A walk through example is used to present the algorithm: motion of a cylinder that rolls downwards on an inclined plane.

Modeling: a walk-through example

Scientific modeling aims at detailed understanding of concrete classes of physical structures or processes. On one end of the spectrum, modeling is construction of empirical equations from data about the modeled situation. Automated discovery systems such as BACON (Langley Simon, Bradshaw and Zytkow, 1987) and FAHRENHEIT (Zytkow, 1996) generate such models by making experiments and by induction of equations from data. But models can be constructed in theory-rich situations, using the appropriate pieces of theoretical knowledge and conducting experiments in order to verify the theoretical explanation. In this paper we analyze the main steps of theory-based model construction on a walk-through example. It is based on a famous experiment of Galileo. We describe work in progress, far from being complete.

Galileo's experiment

Galileo investigated the motion of objects rolling down an inclined plane. A ball, released at height h on the inclined plane, depicted in Figure 1a, rolled down and finally reached the bottom of the inclined plane above the point marked as Q. Galileo was not able to measure the accurate time at which the ball reached the bottom, but he could indirectly measure the final velocity. He attached a "jumping board" to the bottom of the inclined plane. Reaching the bottom, the ball assumed horizontal velocity at the jumping board and then fell through the air to hit the floor at point P. Galileo measured the distance PQ and used this distance to calculate the velocity of the ball at the bottom of the slope. After a sequence of experiments in which he varied the height h from which the ball started to roll, he derived an empirical equation for velocity v at the bottom of the inclined plane:

$$v = \sqrt{ah}\ , \qquad a = constant \tag{1}$$

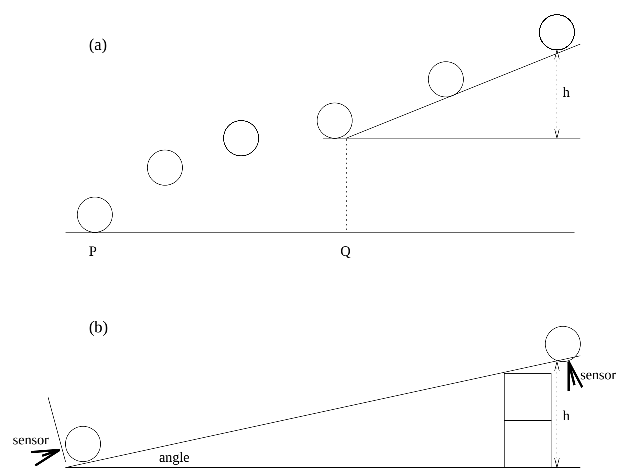

Figure 1: Motion on the inclined plane. (a) Galileo's experiment. A ball is rolling down the inclined plane. The experimenter controls height h. When the ball reaches the bottom of the ramp directly above point Q, it assumes horizontal direction and falls to the floor at point P. The distance PQ is proportional to velocity. (b) Our experiment. A cylinder is rolling down. It covers a fixed distance between a sensor at the top of the ramp and a sensor installed at the bottom. Different cylinders and different angles have been used for data collection.

Modeling the motion on inclined plane

In this paper we use the knowledge of mechanics as well as data that come from a robotic version of Galileo experiment to develop a model of motion on the inclined plane. We do not pay attention to cognitive modeling and historical accuracy. We focus on the main steps of modeling and on empirical accuracy of a model.

To make it easier to trace the modeling process, let us briefly describe some of the main steps that we will later examine in detail. As a body of mass m rolls down, its kinetic energy grows from zero to $mv^2/2$, where v is the final velocity. At the same time, its potential energy decreases from gmh to zero, where g is Earth acceleration. Both energy terms can be used jointly in the law of energy conservation to produce the equation $mv^2/2 - mgh = 0$. Solved for v, this equation is transformed into

$$v = \sqrt{2gh} \tag{2}$$

Velocity can be predicted from equation (2). The model can be verified by comparing the predicted values against the measured velocity values.

In this paper we will expand this brief description, analyzing details of many steps with an eye on automation of modeling.

Modeling: a major scientific activity

We can divide scientific activities into discovery of basic theories, discovery of structure, construction of operational definitions, construction of experiments, and model construction. In machine discovery, they have been treated in isolation, but in real science each requires the support of others. In this paper, while we focus on model construction, we must take those other activities and their results into account.

Models and theories are developed in response to opposite tasks.

Theory is a product of analysis. It describes simple elements of nature, their states and their interaction viewed from a particular singular perspective of gravity, electromagnetism, and the like. In our example, theory includes (1) terms that describe two types of energy: potential and kinetic, (2) the principle of energy summation: energy of a state is the total of individual energy terms (the summation applies separately to the initial state and the final state), and (3) the principle of energy conservation from state to state. Each form of energy describes a simple aspect of physical states, characterized by a single property of individual bodies, such as height, velocity or temperature.

Model is a product of synthesis and describes a complex structure and interactions between elements of that structure. In the majority of situations, several theories and many interactions must be used to build an adequate model. While physicists are interested in elementary objects and interactions, and look for particularly simple situations, researchers in other domains are occupied with complex objects. Analytical chemists work on chemical samples, geologists investigate the structure of Earth, biologists study organisms. They investigate complex structures which can be understood through their models. In the field of automated scientific discovery, early attempts at computational theory of model construction include Sleeman, Stacey, Edwards, & Gray (1989) and Gordon, Sleeman, and Edwards (1995).

Empirical data

Model predictions must be verified against empirical data, collected by observation or experiment. It is rare that model construction is successful at the first attempt. Mismatch between model predictions and empirical data can be detected and analyzed in search for model improvements that would reduced the mismatch.

For the sake of model verification we used empirical data generated in a robotic experiment (Huang and Zytkow, 1996). In our experiment we used the inclined plane, but precise time measurement turned out easier for us than measurements of velocity. Two touch sensors, that signal the beginning and the end of the process have been placed at fixed points at the top and bottom of the inclined plane at distance D (cf. Figure 1b) and attached to the parallel port of a PC. The equivalent of Galileo's equation (2) expressed in terms of time t, angle α and Earth acceleration g is

$$t = \sqrt{\frac{2D}{gsin(\alpha)}} \tag{3}$$

Instead of a ball, we used nine cylinders of equal external radius, with holes of different radius drilled symmetrically through the axis of each cylinder. Since the fixed locations of touch sensors determined the scope of motion, instead of various locations on the fixed board that Galileo used as his initial states, we varied the angle of the inclined plane. Altogether we used five angles.

Experiment design and experimentation strategies have been the focus of earlier work on automation of scientific discovery, such as Langley, Simon, Bradshaw and Zytkow (1987), Kulkarni and Simon (1987), Nordhausen and Langley (1993), Rajamoney (1993) and Zytkow (1996).

Galileo's operational definition

Consider the way in which Galileo measured the velocity reached by the ball at the bottom of the inclined plane. A jumping board mounted at the bottom of the plane changed the direction of motion to horizontal, without affecting the velocity. Galileo decomposed the parabolic motion in the air into free vertical fall and horizontal motion with constant speed. Since he knew that all bodies fall the same vertical distance in the same time, he could infer that the horizontal distance covered before reaching the floor at point P is proportional to the velocity at the bottom of the inclined plane.

This is an example of an operational definition of velocity and at the same time an example of model application. Galileo used an earlier confirmed model of motion between the end of the inclined plane above Q and P. The model combined free vertical fall with uniform horizontal motion, for which he already knew the theories sufficient for computing the velocity needed in his inclined plane experiment. The model yields the computation of velocity, as proportional to the distance PQ.

Operational definitions have been studied by physicists and philosophers of science (Bridgman, 1927; Carnap, 1936). Research on automation of scientific discovery includes attempts at operational definitions such as Kulkarni and Simon (1987), Zytkow, Zhu and Zembowicz (1992).

Our operational definition for time measurement

In our experiment, two touch sensors have been attached to the inclined plane and their wires connected to different pins at the PC's printer port. Sensor signals triggered the time measurement process, providing it with the initial and the final event. Time measurement proceeds by counting fixed time units between two events.

When the cylinder starts to roll, the top sensor is released, creating an interrupt at the printer port, and causing the timer to start up. When the cylinder engages the bottom sensor, the difference in time is measured and recorded:

```
If interrupt-1 then read time-1
if interrupt-2 then read time-2
time := time-2 - time-1
```

After our system made a sequence of experiments, we realized that the PC system clock can only be read from a running program very inaccurately, at 18.2 readings per second. This means that one readable clock tick is about 0.055 seconds. Since the cylinders take between 1.6 and 0.5 seconds to roll from the top to the bottom, the inaccuracy of time reading leads to large error at the order of 10%.

Could we find a more precise time measurement process on the computer? Our immediate choice has been a loop which counts the number of repetitions of a simple constant computation. This works fine on a PC, because it runs a single process. At a time-sharing workstation it would introduce a considerable error.

```
If interrupt-1 then start loop
if interrupt-2 then terminate loop
return the number of cycles
```

The number of cycles c gives the time measurement. We could use time c to derive empirical equations, but since we wanted to compare empirical and theoretical equations, we calibrated in seconds time measured by c. Calibration is a discovery process, too, simple only when it returns a desired constant.

To calibrate the loop, we run it for many seconds, triggering it by releasing the top touch sensors and then depressing the bottom sensor at the inclined plane. The second process has been system clock between the same two events. Sample data obtained in five experiments out of thirty are shown in Table 1:

Table 1. Sample data taken for the timer calibration and calibration results

Time in seconds	Number of Cycles	Average for one cycle
32.42	14426343	2.247e-06
41.04	18244828	2.250e-06
69.23	30784135	2.249e-06
99.45	44237041	2.248e-06
138.90	61806238	2.247e-06

Mean from 30 experiments: 2.2487e-06
Standard deviation: 0.0018e-06

The calibration procedure reads the PC clock, but now the error of clock reading averages over the period of many seconds, so that calibration can be very accurate. The results show that error has been reduced 40 times. Standard deviation (0.5 error) for the loop has been 0.0007 second, while for direct reading of the PC clock it was 0.028 second.

Model construction: a multi-layer task

The construction of each model is oriented on a concrete goal, such as the explanation of an interesting phenomenon. A successful model uses enough of the modeled structure to provide an adequate explanation of the phenomenon, but is simple enough to ensure mathematical representation and solvability, so that empirical predictions can be reached. Given an object (phenomenon, process, structure) O, we distinguish the following modeling steps:

a. make a listing of objects, properties and processes present in O; decide which empirical parameters P of O we want to explain and which we can measure in O; a modeling task depends on how much of the modeled objects we want to represent in the model;

b. create a model-diagram that captures interaction and structure of objects, properties, and processes recognized in O;

c. construct a model-formalism that consists of equations corresponding to the model-diagram;

d. simplify and augment the equations until solvable; use the right number of equations needed to eliminate non-measurable terms. Solve the equations for parameters P;

e. verify the solution against empirical data for P measured for O. Empirical data can take on the form of an empirical equation generated from raw data. In that case, compare empirical equation with model equation. For instance, Kepler Laws have been derived as empirical equations. They can be used to verify Newtonian model of planet motion around the Sun.

A walk-through example in details

We will analyze the details of modeling the motion on the inclined plane and draw a number of general conclusions about modeling.

Modeling task

Only one object changes its properties: the body that rolls down the inclined plane; it undergoes several processes in which body location and velocity change. We want to explain the velocity and time at which the body reaches the bottom of the plane. As two alternatives, we can measure either velocity or time.

Intro-1: brief description of the situation. *Inclined plane: the object under study is a ball.* The behavior is motion from the top to the bottom of the plane. This is a change of state: Change of h and change of v.

Create model-diagram

Model-diagram consists of the initial state (state-1: body located on the top of the inclined plane, zero velocity), and the final state (state-2: body location at the bottom of the inclined plane, positive velocity). Both states are connected by process links for each property whose value is being changed. Each process consists in change of one parameter.

```
state-1                 state-2

h1=h -------------------> h2=0

v1=0 -------------------> v2=v
```

In general, model-diagram includes:

- objects
- properties of each objects
- processes (one per each object and per each varied property)

For each object included in the model, model-diagram represents all the processes this object is involved in.

Principle 1: consider one process per each object involved and each parameter that changes its value

Work on qualitative process theory provides a number of alternatives to our model-diagram (Forbus, 1984; Rajamoney, 1993).

Add model-formalism

Principle 2: for each process and the parameter varied in that process, consider a conserved quantity (quantities) that include that parameter.

Examples of such quantities for velocity are momentum and kinetic energy. Example of such quantity for height is potential energy. Each conserved quantity q is represented by a schema:

```
q(state-1) = q(state-2)
```

The only schema that applies to both the change of h and v is the principle of energy conservation.

The known terms available in a model determine the schemas to be considered. For each schema under consideration, we try to add to the model all other variables that occur in that schema. Before we do that, we must consider whether they can be measured. If sufficient variables are available, other variables may be removed from consideration.

In the case of the inclined plane:

- Energy term that describes the change of h is mgh.
- Energy term that describes the change of v is $mv^2/2$.
- Both terms are substituted into the energy conservation schema. The result is: $mv^2/2 - mgh = 0$

In general, model-formalism must include a sufficient number of equations to eliminate all variables that are be measured.

Infer observable predictions

The equation of energy conservation can be solved for velocity, producing the solution in the form

$$v = \sqrt{2gh} \qquad (2)$$

The equation solving mechanism can solve that equation for time when model-formalism is augmented by an equation which links the velocity and distance with time.

In general, it is practical to require that the equation solving mechanism solves the equation(s) for variables which are measured in the final state. Equation solving can be treated as one of the subtasks in the category of equation transformation (Zytkow, 1990).

Confront predictions with measurements

The verification of the solved equation against empirical data demonstrates inadequacy of the Galileo model represented by equation (2) and by predictions of time computed from (2). Those predictions are shown in column 6 of Table 2. According to the model, the time should be constant for different cylinders represented as different masses in column 2 of Table 2, whereas the measurements (column 3) show different time for different cylinders.

Table 2. Comparison of data and predictions of theoretical models.

Angle	Mass	Robot data	Stand. error	Theoret predict	Galileo theory
1	2	3	4	5	6
3.37	56.46	1.657	0.024	1.600	1.164
3.37	100.08	1.685	0.014	1.563	1.164
3.37	141.10	1.586	0.008	1.528	1.164
3.37	176.63	1.551	0.009	1.497	1.164
3.37	203.77	1.528	0.011	1.472	1.164
3.37	224.93	1.520	0.007	1.453	1.164
3.37	239.26	1.507	0.008	1.440	1.164
3.37	251.28	1.508	0.014	1.429	1.164
3.37	254.35	1.483	0.009	1.426	1.164
8.25	56.46	1.004	0.008	1.024	0.745
8.25	100.08	1.002	0.008	1.001	0.745
8.25	141.10	0.981	0.007	0.978	0.745
8.25	176.63	0.948	0.003	0.958	0.745
8.25	203.77	0.955	0.009	0.942	0.745
8.25	224.93	0.950	0.007	0.930	0.745
8.25	239.26	0.935	0.008	0.922	0.745
8.25	251.28	0.927	0.011	0.914	0.745
8.25	254.35	0.910	0.008	0.913	0.745
12.95	56.46	0.809	0.004	0.820	0.596
12.95	100.08	0.815	0.007	0.801	0.596
12.95	141.10	0.780	0.011	0.783	0.596
12.95	176.63	0.771	0.008	0.767	0.596
12.95	203.77	0.737	0.006	0.754	0.596
12.95	224.93	0.723	0.011	0.744	0.596
12.95	239.26	0.708	0.009	0.737	0.596
12.95	251.28	0.703	0.010	0.732	0.596
12.95	254.35	0.702	0.008	0.730	0.596
17.53	56.46	0.709	0.003	0.707	0.514
17.53	100.08	0.685	0.010	0.691	0.514
17.53	141.10	0.662	0.008	0.675	0.514
17.53	176.63	0.641	0.005	0.661	0.514
17.53	203.77	0.619	0.007	0.650	0.514
17.53	224.93	0.613	0.007	0.642	0.514
17.53	239.26	0.608	0.006	0.636	0.514
17.53	251.28	0.606	0.009	0.631	0.514
17.53	254.35	0.604	0.010	0.630	0.514
21.82	56.46	0.615	0.007	0.636	0.463
21.82	100.08	0.604	0.007	0.622	0.463
21.82	141.10	0.587	0.006	0.608	0.463
21.82	176.63	0.567	0.007	0.595	0.463
21.82	203.77	0.552	0.006	0.586	0.463
21.82	224.93	0.547	0.006	0.578	0.463
21.82	239.26	0.546	0.009	0.573	0.463
21.82	251.28	0.551	0.008	0.568	0.463
21.82	254.35	0.536	0.007	0.567	0.463

Since the predictions are clearly wrong, the model must be improved. What went wrong? A more incisive observation of the cylinders reveals that they rotate as they roll. Thus, we add the change of angular velocity as an extra process.

A new model-diagram is augmented by angular velocity included both in the initial state (state-1: body located on the top of the inclined plane, zero velocity, zero angular velocity), and in the final state (state-2: body location at the bottom of the inclined plane, positive velocity, positive angular velocity). Both states are connected by process links for each property whose value is being changed:

```
state-1                    state-2

h1=h -------------------> h2=0

v1=0 -------------------> v2=v

w1=0 -------------------> w2=w
```

Now, model-formalism yields an equation

$$t = \sqrt{\frac{D(4M-m)}{sin(\alpha)gM}} \qquad (4)$$

where D is the distance rolled by the cylinder, M is mass of a solid cylinder of the same diameter as the given cylinder (mass m), and g is Earth acceleration.

Actually, to match the experiments, we should use equation 5 that takes into account distance d that the cylinder covered before the top sensor was released

$$time = \sqrt{\frac{D(4M-m)}{sin(\alpha)gM}} - \sqrt{\frac{d(4M-m)}{sin(\alpha)gM}} \qquad (5)$$

In our experiment $D = 50.2cm$ and $d = 0.7cm$. We used $g = 980.03cm/s^2$ provided by physicists in our building.

Equation (5) is a far better fit that equation (2). It can be seen in column 5 of Table 2, which represents predictions derived from (5).

Even though the resultant model is more adequate, but a fine comparison against empirical data demonstrates two areas of misfit that call for further model refinements: for the smallest and the largest angle.

According to our background knowledge, those small inadequacies seem to be caused by static friction (for small angles) and by rotation that may be not complete at large angles. The directions of mismatch confirm these conjectures.

Further model improvements must take into account properties such as static and dynamic friction.

In our example, we merely add a known variable (angular velocity) to the model. Other work on automation of scientific discovery proposed various reasons for postulating new variables (Langley et al, 1987; Kocabas, 1991; Valdes-Perez, 1993).

Modeler's knowledge of hidden structure of the phenomenon O grows until the model satisfies the verification criteria at all levels, or an impasse is reached and modeling must stop until more background knowledge are gained or new observations are made of the modeled phenomenon.

Feedback loops: a summary

The process of model construction meanders through many feedback loops, as solutions to problems specific at a given step may require changes made to the constructions at the earlier steps.

Objects, properties, processes

The objects observed in O become the initial components of the model. New elements are added according to the knowledge-base). For instance, consider modeling a star by a steady-state model. A steady state model means that the values of different parameters that describe a single state have values that satisfy the basic laws.

Since the star surface radiates energy, background knowledge implies that radiation must be accompanied by energy transfer to the surface. The known mechanisms for energy transfer include internal radiation and convection. Modeling a system assumes that they occur, but it also tries to verify them by their observed symptoms in O. Since energy is generated and released in different places, we must introduce an energy transfer process (from higher to lower temperature). In that process, energy released is equal to energy generated (not conservation of energy but steady state requirement) When empirical data reveal the existence of absorption lines in the star's spectrum, the star atmosphere can be added to the list of objects. *The ultimate task is to select all objects, properties and processes which are relevant to the modeled phenomenon O.*

Model-diagram

But many details are reckoned not important, so that model-diagram is an idealization of O. The observed behavior of a physical system can be explained by a combination of many interactions.

Model-formalism

Basic laws and interactions lead to model-formalism. Each elementary interaction in a model-diagram corresponds to a specific mathematical expression that can be retrieved from the knowledge-base. Those expressions are put together into equation schemes such as conservation of mass, momentum or energy, and term-generating schemas such as additivity for scalar properties, vector additivity for force. When filled with terms specific to a given model, those equations become a model-formalism, that is, a system of equations that link different processes in model-diagram.

Solving the equations

Equation are refined to yield quantitative predictions. Model-formalism is simplified if the equations are not solvable, by recognizing negligible influence of certain components. Solved equations lead to quantitative predictions. In step f, the predicted and the measured values of parameters P are compared.

The process oscillates between solvability of equations and adequacy of description. An acceptable model is simple enough so that the equations of the model can be solved and complex enough to provide an adequate description of the investigated phenomenon.

Verification

Verification accompanies each cycle in model construction, providing feedback long before the final solution is reached. The most efficient evaluation occurs at the levels prior to the final verification, according to an AI principle: "evaluate partial solutions as early as possible".

If the equations are empirically disconfirmed, the difference between facts and predictions is analyzed. This can lead to changes in O, in model-diagram, as well as in model-formalism.

Prior to empirical confirmation, the consistency of the model is checked, because equations can be internally inconsistent or inconsistent with the previous knowledge. A solution is physically absurd when, for instance, the value of a measured parameter grows indefinitely. Each component used in the equation has a limited physical range of application. For instance, a particular mechanism of energy transfer applies within certain temperature limits.

Verification is not complete without demonstration that objects not included in the model do not bear observable influence. One of the ways is to construct a more complex model which includes additional objects and their interactions represented in model-formalism by additional expressions. Showing that those additions lead to the observationally indistinguishable results demonstrates their irrelevance. This is not possible when the original model has reached the limit of equations solvability. Still the system can be satisfied that it obtained a viable model if the model fits very well the observed data.

A model may reveal new phenomena and open new questions. Modeling may lead to new hypotheses about hidden structure suggested by a successful model. We also demonstrated, on Galileo's example, how models can be used to design new methods of measurement, that is, new operational definitions, leading to finer measurements and new instruments. In the advanced sciences, the majority of important new phenomena which lead to further scientific revolutions are noticed through differences between predictions of models and the observed phenomena. Those differences can be small, such as the part of precession of Mercury's perihelion, unexplained by the models based on classical mechanics. Similar discrepancies occur in our examples, but they may be explained by reference to the known phenomena.

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