

## Chapter 2

# MODELS AND HISTORY OF MODELING

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**Abstract** After a very fast tour through 30,000 years of modeling history, we describe the basic ingredients to models in general, and to mathematical models in particular.

**Keywords:** Modeling, History of Modeling, Model, Mathematical Model

### 2.1 The History of Modeling

The word “modeling” comes from the Latin word *modellus*. It describes a typical human way of coping with the reality. Anthropologists think that the ability to build abstract models is the most important feature which gave homo sapiens a competitive edge over less developed human races like homo neandertalensis.

Although abstract representations of *real-world objects* have been in use since the stone age, a fact backed up by cavemen paintings, the real breakthrough of modeling came with the cultures of the Ancient Near East and with the Ancient Greek.

The first recognizable models were *numbers*; counting and “writing” numbers (*e.g.*, as marks on bones) is documented since about 30.000 BC. *Astronomy* and *Architecture* were the next areas where models played a role, already about 4.000 BC.

It is well known that by 2.000 BC at least three cultures (Babylon, Egypt, India) had a decent knowledge of mathematics and used mathematical models

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to improve their every-day life. Most mathematics was used in an algorithmic way, designed for solving specific problems.

The development of philosophy in the Hellenic Age and its connection to mathematics lead to the deductive method, which gave rise to the first pieces of *mathematical theory*. Starting with *Thales of Miletus* at about 600 BC, *geometry* became a useful tool in analyzing reality, and analyzing geometry itself sparked the development of mathematics independently of its application. It is said that Thales brought his knowledge from Egypt, that he predicted the solar eclipse of 585 BC, and that he devised a method for measuring heights by measuring the lengths of shadows. Five theorems from elementary geometry are credited to him:

1. A circle is bisected by any diameter.
2. The base angles of an isosceles triangle are equal.
3. The angles between two intersecting straight lines are equal.
4. Two triangles are congruent if they have two angles and one side equal.
5. An angle in a semicircle is a right angle.

After Thales set the base, Pythagoras of Samos is said to have been the first pure mathematician, developing among other things the theory of numbers, and most important to initiate the use of *proofs* to gain new results from already known theorems.

Important philosophers like Aristotle, Eudoxos, and many more added lots of pieces, and in the 300 years following Thales, geometry and the rest of mathematics were developed further. The summit was reached by Euclid of Alexandria at about 300 BC when he wrote *The Elements*, a collection of books containing most of the mathematical knowledge available at that time. The Elements held among other the first concise axiomatic description of geometry and a treatise on number theory.

Euclid's books became the means of teaching mathematics for hundreds of years, and around 250 BC Eratosthenes of Cyrene, one of the first "applied mathematicians", used this knowledge to calculate the distances Earth-Sun and Earth-Moon and, best known, the *circumference of the Earth* by a mathematical/geometric model.

A further important step in the development of modern models was taken by Diophantus of Alexandria about 250 AD in his books *Arithmetica*, where he developed the beginnings of *algebra* based on symbolism and the notion of a *variable*.

For *astronomy*, Ptolemy, inspired by Pythagoras' idea to describe the celestial mechanics by circles, developed by 150 AD a mathematical model of the solar system with circles and epicycles to predict the movement of sun, moon, and the planets. The model was so accurate that it was used until the time of Johannes Kepler in 1619, when he finally found a superior, simpler model for planetary motions, that with refinements due to Newton and Einstein is still valid today.

Building models for real-world problems, especially mathematical models, is so important for human development that similar methods were developed independently in China, India, and the Islamic countries like Persia.

One of the most famous Arabian mathematicians is Abu Abd-Allah ibn Musa Al-Ḥwārizmī (late 8th century). His name, still preserved in the modern word *algorithm*, and his famous books *de numero Indorum* (about the Indian numbers — today called arabic numbers) and *Al-kitab al-muḥtaṣar fi ḥisāb al-ğabr wa'l-muqābala* (a concise book about the procedures of calculation by adding and balancing) contain many mathematical models and problem solving algorithms (actually the two were treated as the same) for real-life applications in the areas commerce, legacy, surveying, and irrigation. The term algebra, by the way, was taken from the title of his second book.

In the Occident it took until the 11th century to develop mathematics and mathematical models, in the beginning especially for surveying.

The probably first great western mathematician after the decline of Greek mathematics was *Fibonacci, Leonardo da Pisa* (ca. 1170–ca. 1240). As a son of a merchant, Fibonacci undertook many commercial trips to the the Orient, and in that time he got familiar with the Oriental knowledge about mathematics. He used the algebraic methods recorded in Al-Ḥwārizmī's books to improve his success as a merchant, because he realized the gigantic practical advantage of the Indian numbers over the Roman numbers which were still in use in western and central Europe at that time. His highly influential book *Liber Abaci*, first issued in 1202, began with a presentation of the ten "Indian figures" (0, 1, 2, ..., 9), as he called them. This date was especially important because it finally brought the number *zero* to Europe, an abstract model of *nothing*. The book itself was written to be an algebra manual for commercial use, and explained in detail the arithmetical rules using numerical examples which were derived, *e.g.*, from measure and currency conversion.

Artists like the painter Giotto (1267–1336) and the Renaissance architect and sculptor Filippo Brunelleschi (1377–1446) started a new development of geometric principles, *e.g.* perspective. In that time, *visual models* were used as well as mathematical ones (*e.g.*, for Anatomy).

In the later centuries more and more mathematical principles were detected, and the complexity of the models increased. It is important to note that despite the achievements of Diophant and Al-Ḥwārizmī the systematic use of variables was really invented by Vietá (1540–1603). In spite of that it took another 300 years until Cantor and Russell that the true role of variables in the formulation of mathematical theory was fully understood. *Physics* and the description of Nature's principles became the major driving force in modeling and the development of the mathematical theory. Later *economics* joined in, and now an ever increasing number of applications demand models and their analysis.

In the next section we will take a closer look at models, their function and their most prominent characteristics. Further information on mathematical history can, *e.g.*, be found in [81].

## 2.2 Models

As a basic principle we may say:

*A model is a simplified version of something that is real.*

The traits of the model can vary according to its use. They can vary in their *level of formality, explicitness, richness in detail, and relevance*. The characteristics depend on the basic function of the model and the *modeling goal*.

In building models, everything starts with the *real-world object* we are considering. In a *model* real-world objects are replaced by other, simpler objects, usually carrying the same names. The *knowledge* we possess about the real-world is *structured* by the model, and everything is *reduced* to those phenomena and aspects which are considered important. Of course, a model can only describe a part of the real-world phenomenon, and hence its usefulness is restricted to its *scope of application*.

Models can have many different functions.

**Explain Phenomena.** Most of the theories developed in physics belong to this category: Newton's mechanics, thermodynamics, Einstein's theory of relativity, quantum mechanics, the Standard Model of particle physics, and many more.

There is not only physics, however. The aggregate demand-price adjustment (AD-PA) model, the aggregate demand-inflation adjustment (AD-IA) model, or the Hicks-Hansen IS/LM Model are three examples of economic models describing macroeconomical equilibria.

Avalanche researchers build models based on statistical and phenomenological data to describe the state of snow on alpine slopes.

Biologists use predator-prey models or epidemiological models to investigate the relationship between various life-forms.

**Make Predictions.** After the models are built which explain the phenomena, these models can be used as a further step to make predictions about the future development of a real-world phenomenon.

The avalanche researchers, for example, take their state data and the topographical information of the slopes to make predictions on the probability that avalanches are triggered, on their likely strengths and their presumed places.

Aerodynamical models make *e.g.*, predictions about the maneuverability of a constructed airplane.

Climatic models are used to forecast the effects of the increased amount of greenhouse gases in the atmosphere.

**Decision Making.** A car driver uses a model of his surroundings and the typical traffic on the streets to decide which route to take. Of course, this model of the real world, reduced to streets and average traffic, is in no way a formal mathematical one. It is based on experience and rather vague, if it can be expressed in words at all.

A more formal model for decision making is the design problem for a chemical plant with hundreds of decision variables and thousands of additional variables and constraints, written as mathematical equations and inequalities. They represent space, capacity, cost limitations, and chemical principles like conservation of mass.

**Communication.** Another important aspect of models is that they can be used to communicate knowledge. If a person *A* wants to visit person *B*, he might ask for the way to drive. *B* will sketch the correct route on a sheet of paper with a few lines and some additional marks and text, like “here at the corner is a yellow house with small garden”. This sheet of paper is a visual model for the surroundings of *B*’s house; its purpose is to communicate a subset of *B*’s knowledge about his city to *A*.

**Others.** The detailed check-lists for airplane maintenance are (extremely detailed and explicit ones) models as well, as are the collections of formal norms (ANSI, DIN, EU Norm, . . .) used to regulate public life in modern countries.

## 2.3 Mathematical Models

The models of interest for us are mathematical models. Here, the real world object is represented by mathematical objects in a *formalized mathematical language*.

The advantage of mathematical models is that they can be analyzed in a precise way by means of *mathematical theory* and *algorithms*.

As we have seen in Section 2.1, mathematical models have been used long ago, and many problems have been formulated mathematically since hundreds of years. However, the sheer amount of computational work needed for solving the models restricted their use to qualitative analysis and to very small and simple instances.

The development of algorithms like the Runge-Kutta method or the Fast Fourier Transform made complex models accessible to computers. In the be-

ginning of the twentieth century human workers (most of the time low paid women) were used as “computers”, and the problem size was still very limited.

As ENIAC was started in 1945, models of previously unknown size became tractable. It was possible for the first time to use mathematical modeling for *solving* practical problems of significant size.

The improvements in computer technology in the years since and the enormous gain in storage capacity and speed have made mathematical modeling increasingly attractive for military and industry, and a special class of problems, *optimization problems*, became very important.

The success in solving real world problems increased the demand for better and more complex models, and the modeling process itself was investigated. There are now several books on modeling, *e.g.*, [228] and [123], and branches of mathematics completely devoted to solving practical problems and developing theory and algorithms for working on models, like operations research. See also [103] for a short treatise of this theme.

The structure of the models has changed throughout history, as the mathematical community gained increasing insight into the foundations of mathematics and formal logic. The introduction of variables, function spaces, and of all the mathematical structural theory has made mathematical models increasingly formal.

To date a mathematical model consists of *concepts* like

- variables:** These represent *unknown* or changing parts of the model, *e.g.*, whether to take a decision or not (decision variable), how much of a given product is being produced, the thickness of a beam in the design of a ceiling, an unknown function in a partial differential equation, an unknown operator in some equation in infinite dimensional spaces as they are used in the formulation of quantum field theory, etc.
- relations:** Different parts of the model are not independent of each other, but connected by relations usually written down as *equations* or *inequalities*. *E.g.*, the amount of a product manufactured has influence on the number of trucks needed to transport it, and the size of the trucks has an influence on the maximal dimensions of individual pieces of the product.
- data:** All numbers needed for specifying instances of the model. *E.g.* the maximal forces on a building, the prices of the products, and the costs of the resources.

## 2.4 The Modeling Process

As every textbook on modeling describes, the process of building a model from a real-world problem is a tedious task. It often involves many iterations in a cycle like in Fig. 2.4.1.

This is the traditional description of the modeling process, however as we will see in Chapter 3, the various stages of the *modeling cycle* appear interconnected, demanding even more interaction between the subtasks.

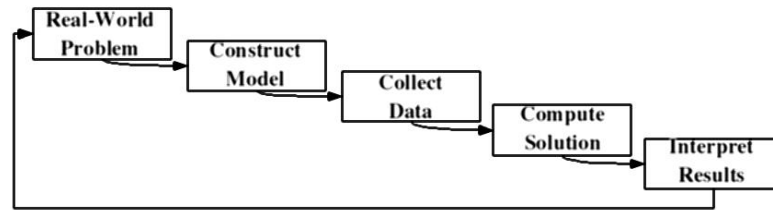


Figure 2.4.1. Modeling cycle

Several of these modeling steps require the help of the end user. For complex models, it is widely accepted that computers are needed in the *compute solution* process. For huge data sets or data which has to be retrieved from different sources, computer support for the *collect data* step is accepted, as well.

In this section we won't go into the details of the modeling process itself. This is done in the next chapter. We will rather focus on two aspects which have a strong influence on the structure of the model itself.

Until the first third of the twentieth century most of the mathematical models were used to describe phenomena and to make qualitative statements about the real world problems described. Since then the situation has changed dramatically. The tremendous increase in computing power has shifted the interest in mathematical models more and more from problem *description* towards problem *solving*.

This has an important consequence for mathematical modeling itself and for the structure of the models: If the most important conclusions which can be drawn from a model are qualitative statements, which are derived by analytic means using a lot of mathematical theory, it is important to formulate the model in a very concise way, especially tailored to the analytical methods available. In contrast to that, the urge for numerical solutions in the last decades, made it necessary to change the model structure, to adapt it to the solution algorithms available. Section 2.4.1 will focus on the impact solution methods have on the structure of the model. The adaption of the model and the connection with a computer based solution method made it further necessary to make the model machine accessible. This will be discussed in Section 2.4.2.

### 2.4.1 The Importance of Good Modeling Practice

Most important for the applicability of a model in real-life situations is, whether it can be used to solve problems of industry-relevant sizes. Whether this is possible greatly depends on the solution time of the algorithm. Although modern algorithms have made a bigger number of model classes solvable, it still makes a difference which model formulation is chosen, especially if solu-

tion time is considered, even if several mathematically equivalent formulations are compared. Choosing the “right” *structure* is a matter of experience and distinguishes good from bad modellers.

When we consider MIP or nonlinear problems, the solution time can often be reduced significantly by appropriate modeling. This is important since in contrast to ordinary LPs, effective solution of MIP or nonlinear problems depends critically upon good model formulation, the use of high level branching constructs, control of the Branch-and-Bound strategy, scaling and the availability of good initial values. The solution times can be greatly influenced by observing a few rules which distinguish “bad” from “good” modeling.

Good formulations in MIP models are those whose LP relaxation is as close as possible to the MILP relaxation, or, to be precise, those whose LP relaxation has a feasible region which is close to the *convex hull*, that is the smallest polyhedron including all feasible MILP points. In practice, this means, for example, that upper bounds should be as small as possible. If  $\alpha_1$  and  $\alpha_2$  denote integer variables, the inequality  $\alpha_1 + \alpha_2 \leq 3.7$  can be bound-tightened to  $\alpha_1 + \alpha_2 \leq 3$ . Another example: Expressions containing products of  $k$  binary variables can be transformed to MILP models according to

$$\left\{ \delta_p = \prod_{i=1}^k \delta_i \right\} \iff \left\{ \begin{array}{l} \delta_p \leq \delta_i, \quad i = 1, \dots, k \quad ; \\ \sum_{i=1}^k \delta_i - \delta_p \leq k - 1 \quad ; \quad \delta_i \in \{0, 1\} \end{array} \right\} . \quad (2.4.1)$$

However, the formulation (2.4.1) is superior to the alternative, and algebraically equivalent set of only two inequalities

$$\left\{ \delta_p = \prod_{i=1}^k \delta_i \right\} \iff \left\{ \begin{array}{l} k\delta_p \leq \sum_{i=1}^k \delta_i \quad ; \\ \frac{1}{k} \sum_{i=1}^k \delta_i - \left( k - \sum_{i=1}^k \delta_i \right) \leq \delta_p \end{array} \right\} \quad (2.4.2)$$

because the  $k + 2$  inequalities in (2.4.1) couple  $\delta_p$  and the individual variables  $\delta_i$  directly.

In many models, in addition, it might be possible, to derive *special cuts*, *i.e.*, *valid inequalities* cutting off parts of the LP relaxation’s feasible set but leaving the convex hull unchanged. If we detect inequalities of the form  $x + A\alpha \geq B$  with constants  $A$  and  $B$ , and variables  $x \in \mathbb{R}$  and  $\alpha \in \mathbb{N}$  in our model, we can enhance and tighten our model by the cuts

$$x \geq [B - (C - 1)A] (C - \alpha) \quad , \quad C := \left\lceil \frac{B}{A} \right\rceil = \text{ceil} \left( \frac{B}{A} \right) \quad , \quad (2.4.3)$$

where  $C$  denotes the rounded-up value of the ratio  $B/A$ . If a semi-continuous variable  $\sigma$ , *e.g.*,  $\sigma = 0$  or  $\sigma \geq 1$ , occurs in the inequality  $x + A\sigma \geq B$  it can be shown that  $\frac{x}{B} + \sigma \geq 1$  is a valid inequality tightening the formulation.

All these examples show that the quality of the model greatly depends on the care the modeler takes when designing its structure.



*Preprocessing* can also improve the model formulation. Preprocessing methods introduce model changes to speed up the algorithm. They apply to both continuous and MIP problems but they are much more important for MIP problems. Some common preprocessing methods are: *presolve* (logical tests on constraints and variables, bound tightening), *disaggregation of constraints*, *coefficient reduction*, and *clique and cover detection* (see [126] and references therein). However, it is important that preprocessing is used carefully, because for some classes of problems, especially if rigorous computing is needed (e.g., global optimization, see Section 4.2), the roundoff errors introduced by certain preprocessing techniques effectively change the model.

In models of industrial relevance, the number of variables and constraints which can be solved effectively usually makes the difference between success and failure of a model.

For very large problems, a second difficulty “lurks behind the corner”. Somebody has to put together all relevant variables, constraints, and the data, without making errors. If the model is designed once, then fixed, and only the data changes, this can be done by normal database tools. However, if the model itself changes from problem instance to problem instance the overall structure of the model has to be clearly arranged.

For example, optimization problems coming from resource optimization [207] tend to be very large and highly structured. However, from application to application neither the variables nor the constraints are fixed, not even parametrizable. In spite of that, all constraints can be generated from building blocks, and the data can be retrieved from databases.

There is a hierarchical system of models of increasing complexity and increasing non-linearity. Constraints for different resources are similar in structure but not identical, so they cannot be modeled by using loops or simple indexing.

Complicated resource optimization problems can have several 100,000 variables. A typical problem looks like in Figure ?? . There the  $s_i$  describe the resource streams needed for the amount  $p$  of end-product. Depending on the complexity of the materials these are linear or non-linear mixed integer problems. Most constraints can be constructed by general principles like resource conservation. The other constraints depend on the resources needed, their impact on the environment, and all this information could be retrieved from a database.

For this type of problem, a modeling system would be most convenient, in which large models can be constructed from smaller building blocks, and it is important that the modeler keeps the structure in the model description. Otherwise, the model will not be applicable for more than a few simple (and in practice irrelevant) examples.

Good modeling practice ([228], [126]) takes advantages from good use of structuring, presolve, scaling, and branching choice. Modeling appears more

$$\begin{aligned}
\min \quad & B(z_1, \dots, z_q) = \sum_{i \in I} b_i(s_i, z_1, \dots, z_q) \\
\text{s.t.} \quad & s_i = f_i(p) \quad \forall i \in I_0 \subseteq I \\
& s_i = S_i(p, z_1, \dots, z_q) \quad \forall i \in I_p \\
& s_i \leq 0 \quad \forall i \in I_{\text{in}} \subseteq I \setminus (I_0 \cup I_p) \\
& s_i \geq -M_i y_{n_i} \quad \forall i \in I_{\text{in}} \cap I_d \\
& s_i \geq 0 \quad \forall i \in I_{\text{out}} \subseteq I \setminus (I_0 \cup I_p) \\
& s_i \leq M_i y_{n_i} \quad \forall i \in I_{\text{out}} \cap I_d \\
& g_j(p, s_{j_1}, \dots, s_{j_n}) \leq 0 \quad \forall j \in J_u, j_1, \dots, j_n \in I \\
& h_k(p, s_{k_1}, \dots, s_{k_m}) = 0 \quad \forall k \in J_g, k_1, \dots, k_m \in I \\
& G_j(z_1, \dots, z_q) \leq 0 \quad \forall j \in J_u^z \\
& H_k(z_1, \dots, z_q) = 0 \quad \forall k \in J_g^z \\
& \sum_{i=1}^{m_r} y_{n_i} \leq e_r \quad \forall r \in R \\
& p, s_i, z_j \in \mathbb{R} \text{ (or } \mathbb{Z}) \quad \forall i \in I, j = 1, \dots, q \\
& y_n \in \{0, 1\} \quad \forall n \in E.
\end{aligned}$$

Figure 2.4.2. A typical model for resource optimization

as an art rather than a science. Experience clearly dominates. Remodeling and reformulations of problems (see, for instance, Section 10.4 in [126]) can significantly reduce the running time and factors like the *integrality gap*, *i.e.*, in a maximization problem the difference between the LP-relaxation and the best integer feasible point found. This task is still largely the responsibility of the modeler, although work has been done on automatically reformulating mixed zero-one problems [221]. For nonlinear problems this is much more difficult, though.

Especially, in nonlinear problems it is essential that the mathematical structure of the problem can be exploited fully. This is even more true if rigorous computing is involved. It is important that good initial values are made available by, for instance, exploiting homotopy techniques, or that good estimates for constraint propagation are provided by proper use of interval analytical techniques (see *e.g.* [128]).

## 2.4.2 Making Mathematical Models Accessible for Computers

As stated before, there is a second important consequence from computer assisted model solving. Somebody has to translate the model into a form accessible by the computer.

If we consider again the simple modeling cycle in Figure 2.4.1, we note that no step involving a computer is contained in this coarse grained view. In reality,

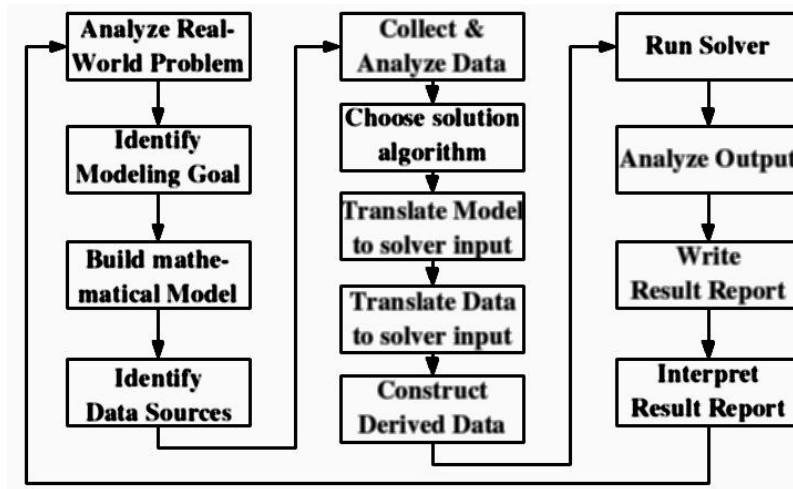


Figure 2.4.3. Detailed modeling cycle

the modeling process contains many more steps than described there. So let us consider the revised and more detailed model of the modeling process depicted in Fig. 2.4.3.

We observe that some of the additional steps in model building and solving involve translations from one format to another (*translate model to solver input format, translate data to solver input format, write status report*). These tasks are full of routine work and error prone. Furthermore, since during the various cycles sometimes the solution algorithm, and hence the solver, is changed, these “rewriting” steps have to be performed again and again.

A special case is the task *construct derived data*. Many solution algorithms need data which is a priori not part of the model, but which is also not provided by the solver. E.g. *gradients* of all functions involved are usually needed for an efficient local optimization algorithm. This not only involves routine but also mathematical work and additional translation steps.

As we have seen in Section 1.3 about the history of modeling languages, in the beginning all these translation steps were performed by hand and ended in the writing of *programs*, which would represent the mathematical model in an algorithmic way, almost like in Babylonian mathematics everything was described by means of algorithms. Data was stored in hand-written files. This method was very inflexible, error prone, and not re-usable. Maintenance of the models was close to impossible, and the models were not very scalable. This made the modeling process very expensive. In addition, a lot of expert knowledge in mathematics, modeling, and software engineering was necessary for building applicable models.

Many of the important models for military applications and for the industry were *optimization problems*, so methods were designed to reduce the modeling costs and to reduce the error rate in the translation steps, so many self-written modeling support systems were designed (and still are). However, using them still needed a lot of expert knowledge, and although scalability improved usually, flexibility did not.

Most of these problems now can be resolved by using a modeling language or modeling system, and the most important features of these will be analyzed in Chapter 4.

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