Introduction to Simulation

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Introduction to Mathematical Modelling

Goals

- Taste of the types of models
- Why do we need a to use the computer?

Notation

Consider an autonomous system of the form

$$F = f(p(t, x, y, z))$$

When the parameter p and hence F depend on both the spatial coordinates and time, the models are called **time-dependent**, **nonautonomous** or **dynamic**.

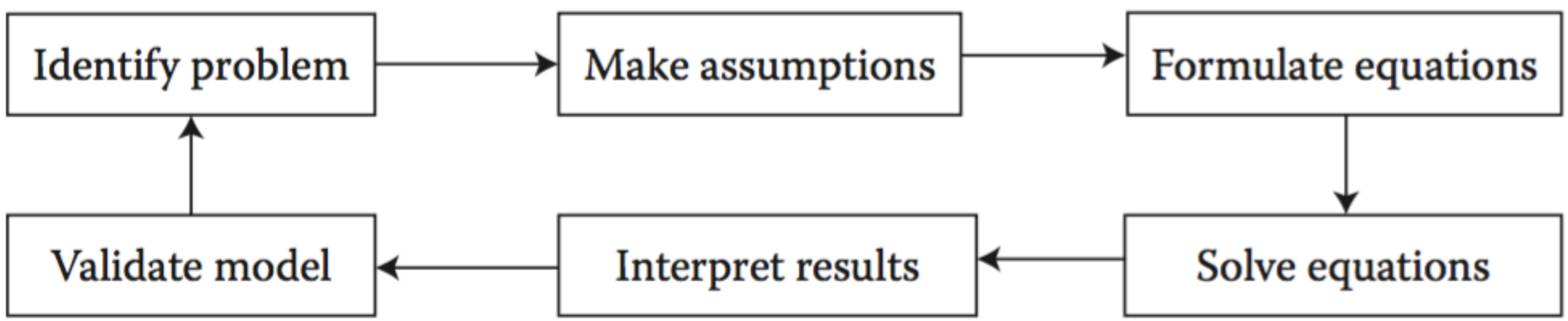
When the parameter p and hence F are independent of time t, the models are called **stationary**, **autonomous**, or **static**.

The basic equations may be **stochastic** or **deterministic** as the **chance** factors are or are not taken into account.

When the generalized argument forms a distribution of the possible values, characterized by **statistical indexes** such as mean, dispersion, and standard deviation, a model is called **stochastic**.

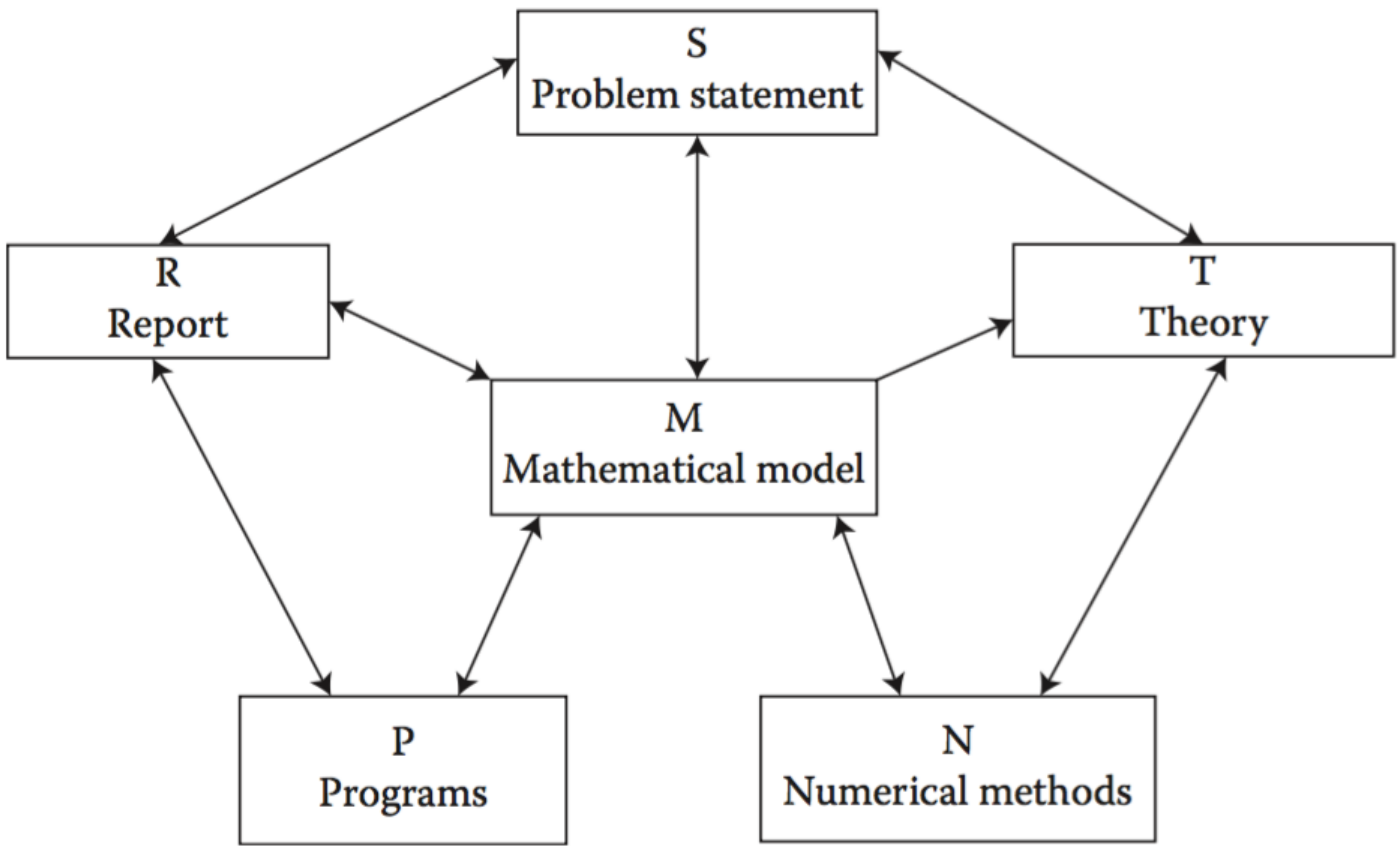
When an exact calculation is possible, such a model would be called **deterministic**.

Modeling/Cyclic Processes



Schematic diagram of a modeling cycle. (From Barnes, B., Fulford, G. R. 2002. *Mathematical Modeling with Case Studies*. Taylor & Francis, Boca Raton, FL.

A Modeling Diagram



Modeling diagram as suggested by Arnold Neumaier. (From Neumaier, A. 2004. Mathematical model building, Chapter 3. In: *Modeling Language in Mathematical Optimization*, J. Kallrath, ed. Kluwer, Boston.

Classification of Mathematical Models

- A mathematical model can be classified either as per the **mathematical technique used**, such as
  - differential equations and/or stochastic differential equations,
  - statistical techniques,
  - numerical data analysis,
  - graphs,
  - …..
- Or as per the subject matter, such as
  - physics,
  - medicine,
  - anthropology,
  - engineering,
  - …

Examples

Compartmental

Example 1

If 10% of a radioactive material disintegrates in 100 years, how long does it take for 90% of the material to disintegrate?

Optimization

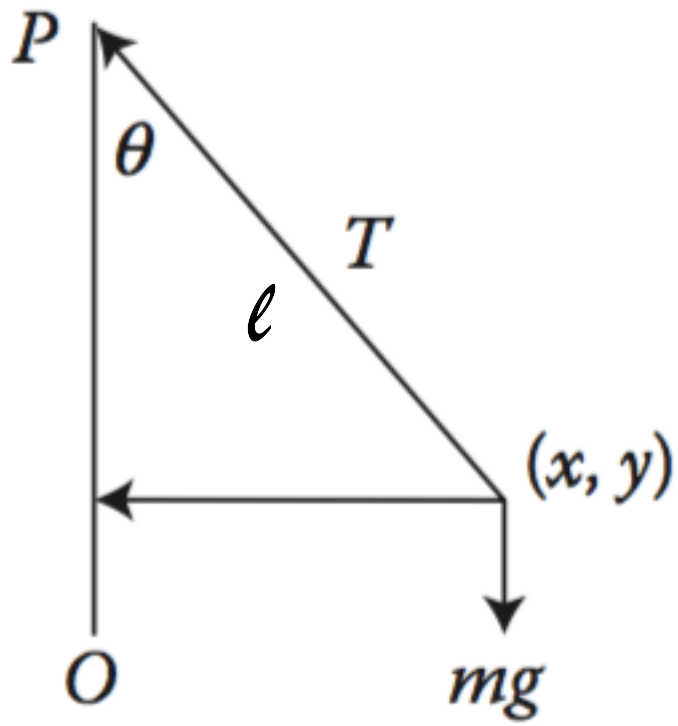
Example 2

A sealed can, cylindrical in shape, is to hold 10 L of oil. Find the dimensions that will minimize the cost of the material for manufacturing the can.

Theoretical

Example 3

Oscillations of a **simple pendulum**. The assumptions are that (i) the string has negligible mass, and (ii) the air resistance is negligible. The only forces acting on the system are (i) tension T in the string, and (ii) gravitational force mg, which acts vertically downward



Mathematical Preliminaries

Mathematical Preliminaries

Consider an autonomous system of the form

$$\frac{dx}{dt} = x' = f(x), \quad \text{where } f \in C[R^n, R^n] \tag{1.2}$$

in the variables $x_1, x_2, \ldots, x_n$. We assume that $f(x)$ is sufficiently smooth and the solution of system (1.2) exists and is unique. Let $f(0) = 0$ and $f(x) \neq 0$ for x in the neighborhood of the origin. Then, system (1.2) admits the zero solution, $x \equiv 0$, which is an isolated critical point of the system.

Function Properties

Let $V(x)$ be a real-valued scalar continuous function in the variables $x_1, x_2, \ldots, x_n$. Let Γ be an open set containing the origin in R^n. Then, $V(x)$ is said to be

i. *Positive definite* on Γ if and only if $V(0) = 0$ and $V(x) > 0$ at all points $x \neq 0$ on Γ.

ii. *Positive semidefinite* on Γ if and only if $V(0) = 0$, $V(x) = 0$ at a few points $x \neq 0$ in Γ, and $V(x) > 0$ at all of the remaining points $x \neq 0$ in Γ.

iii. *Negative definite* on Γ if and only if $-V(x)$ is positive definite on Γ.

iv. *Negative semidefinite* on Γ if and only if $-V(x)$ is positive semidefinite on Γ.

Let $V(t, x)$ be a real-valued time-varying scalar continuous function in the variables $t, x_1, x_2, \ldots, x_n$. Then, $V(t, x)$ is said to be

i. *Positive definite* if there exists a positive-definite function $V(x)$ such that $V(t, 0) \equiv 0$ and $V(t, x) \geq V(x)$ at all points $x \neq 0$.

ii. *Positive semidefinite* if $V(t, 0) \equiv 0$, $V(t, x) = 0$ at a few points $x \neq 0$, and $V(t, x) > 0$ at all the remaining points $x \neq 0$.

iii. *Negative definite* if and only if $-V(t, x)$ is positive definite.

iv. *Negative semidefinite* if and only if $-V(t, x)$ is positive semidefinite.

Quadratic Form

we consider the quadratic form

$$Q = V(x) = x^T A x = \sum_{i,\, j\, =\, 1}^{n} a_{ij} x_i x_j ,$$

where A is an $n \times n$ matrix $A = (a_{ij})$.

The quadratic form $V(x)$ is positive definite if A is positive definite. A necessary and sufficient condition is that the leading minors of A are positive.

If $x = x(t)$ is any solution of the autonomous system (1.2), then

$$\begin{aligned} \frac{d}{dt} V(x(t)) &= \frac{\partial V}{\partial x_1} \frac{dx_1}{dt} + \frac{\partial V}{\partial x_2} \frac{dx_2}{dt} + \cdots + \frac{\partial V}{\partial x_n} \frac{dx_n}{dt} \\ &= \frac{\partial V}{\partial x_1} f_1(x(t)) + \frac{\partial V}{\partial x_2} f_2(x(t)) + \cdots + \frac{\partial V}{\partial x_n} f_n(x(t)) \\ &= V^*(x(t)). \end{aligned}$$

Stability Discussion

Consider an autonomous system of the form

$$x' = f(x)$$

1. Theorem

If there exists a positive definite scalar function $V(x)$ such that $V^*(x) \leq 0$ on S_r, then the zero solution of the system is **stable**.

2. Theorem

If there exists a positive-definite scalar function $V(x)$ such that $V^*(x)$ is negative definite on S_r, then the zero solution of the system is **asymptotically stable**.

3. Theorem [Chetayev]

If there exists a scalar function $V(x)$ such that $V(0) = 0$, $V^*(x)$ is positive definite on S_r, and if in every neighborhood N of the origin, $N \subset S_r$, there is a point x_0 where $V(x_0) > 0$, then the zero solution of the system is **unstable**.

Examples

Stability Discussion Based on the Linearization Procedure

Consider the linearized system as

$$x' = Ax$$

An equilibrium point x_0 is called a:

- **Stable node or sink:** If all of the eigenvalues of matrix *A* have **negative real parts**.
- **Unstable node or source:** If all the eigenvalues of *A* have **positive real parts**.
- **Hyperbolic equilibrium point:** If all the eigenvalues of matrix *A* have **nonzero real parts.**
- **A saddle point:** If it is a hyperbolic equilibrium point and *A* has **at least one eigenvalue with a positive real part and at least one eigenvalue with a negative real part.**

Stability Discussion

Consider an autonomous system of the form

$$x' = f(x)$$

We linearize system about x_0 as

$$x' = Ax + R(x) \qquad (*)$$

The smallness of the higher-order partial derivatives is defined by the inequality

$$||R(x)|| \leq N||x||^{1+2\alpha}$$

in the neighborhood of x_0, N and α are positive constants and the usual Euclidean norm is used

4. Theorem

Let R satisfy inequality. Then, if A is a stable matrix, the zero solution $x(t) = 0$ of Equation (*) is asymptotically stable.

5. Theorem

Let R satisfy inequality. Then, if A has at least one eigenvalue whose real part is positive, then the zero solution $x(t) = 0$ of Equation (*) is unstable.

Examples

Stability Discussion

$$x_i' = f_i(x_1, x_2, \ldots, x_n), \quad i = 1, 2, \ldots, n \qquad (**)$$

$$f_i(0, 0, \ldots, 0) = 0$$

Stability of a *limit cycle*: Let the periodic solution C of nonlinear system (**) be a closed curve. We define the following:

Stable limit cycle: If the periodic solution C is the positive limit set of the solutions contained in the interior and also of the solutions contained in the exterior of C, then the limit cycle is said to be stable.

Unstable limit cycle: If the periodic solution C is the negative limit set of the solutions contained in the interior and also the solutions contained in the exterior of C, then the limit cycle is said to be unstable.

Semistable limit cycle: If the periodic solution C is the negative limit set of the solutions contained in the interior but is the positive limit set of the solutions contained in the exterior of C, then the limit cycle is said to be semistable.

Stability Discussion

Consider the two-dimensional autonomous system:

$$x_1' = f_1(x_1, x_2), \quad x_2' = f_2(x_1, x_2).$$

Let C be a periodic solution of period T of this system whose closed orbit is defined by x1 = α(t), x2 = β(t). The linear system corresponding to this solution is

$$\begin{bmatrix} x_1' \\ x_2' \end{bmatrix} = \begin{bmatrix} \partial f_1/\partial x_1 & \partial f_1/\partial x_2 \\ \partial f_2/\partial x_1 & \partial f_2/\partial x_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix},$$

where the partial derivatives are evaluated at (x_1= α(t), x_2= β(t)). Apart from the unity, the other characteristic exponent is given by

$$I = \frac{1}{T} \int_0^T [a_{11}(t) + a_{22}(t)]\, dt.$$

The limit cycle C is stable if I is negative and unstable if I is positive. If I = 0, C may or may not be semistable and we need to study the effect of the nonlinear terms.

- The stability or instability of limit cycles depends on the asymptotic behaviour of neighbouring paths.
- Often, linearized systems may not provide any indication of the existence of periodic solutions or limit cycles.

Poincaré–Bendixson Theorem

Consider the two-dimensional autonomous system:

$$x_1' = f_1(x_1, x_2), \quad x_2' = f_2(x_1, x_2).$$

If C^+ is a bounded positive semiorbit of the system and $L(C^+)$ does not contain the critical points of the system, then $L(C^+)$ is a periodic orbit. Moreover, if C^+ and $L(C^+)$ have no common regular point, then $L(C^+)$ is a limit cycle.

References

1. R. K. Upadhyay & S.R. K. Iyengar, "*Introduction to Mathematical Modeling and Chaotic Dynamics*", CRC Press, 2014.