Mathematical Modeling

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TYPES OF MODELS

Models are used not only in the natural sciences (such as physics, biology, life sciences, earth science, meteorology) and engineering-architecture disciplines, but also in the social sciences (such as economics, psychology, sociology and political science).

Here is a list:

- **Physical Models**
- **Analogic Models**
- **Provisional Theories**
  (e.g., molecular and atomic models)
- **Maps and Drawings**
  (e.g., PI&D, geographycal maps, etc.)
- **Mathematical and symbolic models**

📖 § 1.4 in Himmelblau D.M. e Bischoff K.B., "Process Analysis and Simulation", Wiley & Sons Inc., 1967

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Why modeling?
Some answers …

Models are usually more accessible to study than the actual system modeled.

- Changes in the structure of a model are easier to implement, and changes in the behavior of a model are easier to isolate, understand, and communicate to others.
- A model can be used to achieve insight when direct observation/experimentation with the actual system is too dangerous, disruptive, or demanding.
- A model can be used to answer questions about a system that has not yet been observed or built, or even one that cannot be observed or built with present technologies.

MATHEMATICAL MODELING

WIKIPEDIA

A **mathematical model** is a description of a system using mathematical concepts and language.

The process of developing a mathematical model is termed **mathematical modeling.**

Mathematical models are used not only in the NATURAL SCIENCES (such as physics, biology, earth science, meteorology) and ENGINEERING DISCIPLINES (e.g. computer science, artificial intelligence), but also in the SOCIAL SCIENCES (such as economics, psychology, sociology and political science);

physicists, engineers, statisticians, operations research analysts and economists use mathematical models most extensively.

A model may help to explain a system and to study the effects of different components, and to make predictions about behavior.

MATHEMATICAL MODELING

General statements

A mathematical model usually describes a system by a set of variables and a set of equations that establish relationships between the variables.
Relationships can be described by *operators*, such as algebraic operators, functions, differential operators, etc.
Anonymous

A mathematical model is a representation, in mathematical terms, of certain aspects of a non-mathematical system
Aris, 1999

A model may be prescriptive or illustrative, but, above all, it must be useful !
Wilson, 1991

Why Math Modeling ?

- Is it:
  - to design a controller?
  - to analyze the performance of the process?
  - to understand the process/system better?
  - to simplify the complexity of a system?

Mathematical model development strategy

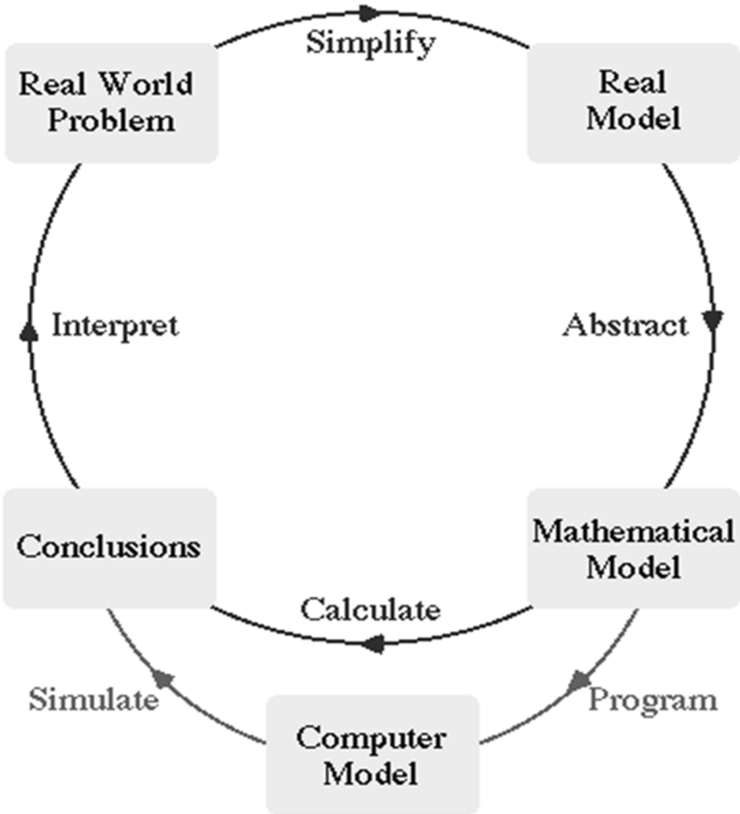
- The development of a model and its structure are intimately related to the goals of modeling.
- In other words, the complexity of a model should be commensurate with the ultimate application in which it will be used.
- In model development, always start by trying the simplest model and then only add complexity to the extent needed

Keep things as simple as possible, but not simpler
A. Einstein

Mathematical model development: *Complexity* vs. *Simplicity*

- ***Ratio of costs to benefits***

Mathematical model development strategy: cycling



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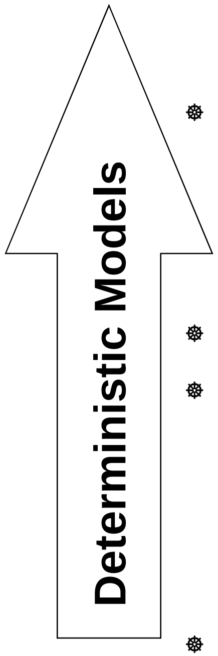
Mathematical Models 1st classification

(on the base of the approach adopted for model development)



- "*First principle Models*"
  - ☞ Basic models
  - ☞ Models involving transport phenomena
  - ☞ Models based on the "population balance approach"
- Empirical or "fitting" models
- Dynamic models
  - dynamic models with "input-output representation"
  - state-space dynamic models
  - black box dynamic models
- Time Series
- Statistical models

📖 rielaborated from § 1.4 in Himmelblau D.M. e Bischoff K.B., "Process Analysis and Simulation", Wiley & Sons Inc., 1967

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Mathematical Models
1st classification

(on the base of the approach adopted for model development)

- *First principles Models*

  or
  Fundamental Models
  (📖 Palazoglu & Romagnoli, 2005)
  or
  Mechanistic or White Box Models
  (📖 Roffel & Betlem, 2006)

  ☞ Modelli basati sui "fenomeni di trasporto"
- Modelli basati sul "bilancio di popolazione"
- Modelli empirici o di "*fitting*"
- Modelli dinamici
  - Modelli dinamici "con rappresentazione ingresso-uscita"
  - Modelli dinamici "con rappresentazione nello spazio di stato"
  - Modelli dinamici a scatola nera (*black box*)
- Serie temporali
- Modelli statistici

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FUNDAMENTAL LAW

GENERAL CONSERVATION PRINCIPLE

[IN] – [OUT] + [GEN] = [ACC]

NB: **GEN > 0** → formation

GEN < 0 → disappearance

SIMPLER CASES

For a chemical element:

IN - OUT = ACC

At steady-state:

IN - OUT + GEN = 0

At steady-state and without chemical/biochemical reactions:

IN - OUT = 0

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First principles models
(including population balance models)

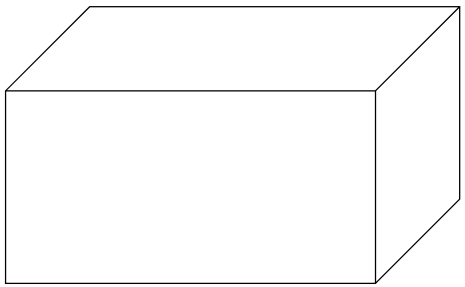
NB:

The description of such a **system** and the development of such a **model** require the concept of:

- **control volume**

or

- **system boundary**



First principles mathematical models.
Malthusian Growth Model

An Early and Very Famous Population Model

In 1798 the Englishman Thomas R. Malthus posited a mathematical model of population growth. He model, though simple, has become a basis for most future modeling of biological populations. His essay, "An Essay on the Principle of Population," contains an excellent discussion of the caveats of mathematical modeling and should be required reading for all serious students of the discipline. Malthus's observation was that, unchecked by environmental or social constraints, it appeared that human populations doubled every twenty-five years, regardless of the initial population size. Said another way, he posited that populations increased by a fixed proportion over a given period of time and that, absent constraints, this proportion was not affected by the size of the population.

By way of example, according to Malthus, if a population of 100 individuals increased to a population 135 individuals over the course of, say, five years, then a population of 1000 individuals would increase to 1350 individuals over the same period of time.

Malthus's model is an example of a model with one ***variable*** and one ***parameter****.* A variable is the quantity we are interested in observing. They usually change over time. Parameters are quantities which are known to the modeler before the model is constructed. Often they are constants, although it *is* possible for a parameter to change over time. In the Malthusian model the variable is the population and the parameter is the population growth rate.

First principles mathematical models.
Malthusian Growth Model

GENERAL CONSERVATION LAW applied to No. of individuals in a "closed system": ACC = GEN

GEN = birth - death

$$\dot{N} = cN(t)$$

INITIAL CONDITION: $CI: \ t = 0 \Rightarrow N = N_0$

STATE VARIABLES

$N \in \mathcal{N}$

where

$N(t) = $ No. individuals at time t

PARAMETERS

$c \in \Re$

$\downarrow$

3 cases:

$c < 0$

$c = 0$

$c > 0$

CLASSIFICATION

DYNAMIC AUTONOMOUS MATHEMATICAL MODEL

made by 1 *ODE* (Order =1) ,

LINEAR, CONSTANT COEFFICIENT MODEL

First principles mathematical models.
Logistic Model

GENERAL CONSERVATION LAW applied to No. of individuals in a "closed system": ACC = GEN

GEN = birth - death

$$\dot{N} = cN(t) - hN(t)^2$$

INITIAL CONDITION: $CI: \ t = 0 \Rightarrow N = N_0$

STATE VARIABLES

$N \in \mathcal{N}$

where

$N(t) = $ No. individuals at time t

PARAMETERS

$p^T = (c, h) \in \Re^+$

CLASSIFICATION

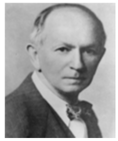
DYNAMIC AUTONOMOUS MATHEMATICAL MODEL

made by 1 *ODE* (Order =1) ,

NON LINEAR, CONSTANT COEFFICIENT MODEL

First principles mathematical models. The prey-predator model

BIBLIO REF.



Lotka A.J. (1925) *Elements of Physical Biology*. Baltimore: Williams & Wilkens.

Volterra V. (1926) "Variazioni e fluttuazioni del numero d'individui in specie animali conviventi", Mem.R.Accad.Naz.dei Lincei, Ser.VI, 2
1st president of National Research Council (CNR) of Italy

The idea is that, if left to themselves with an infinite food supply, the rabbits or zebras would live happily and experience exponential population growth.

On the other hand, if the foxes or lions were left with no prey to eat, they would die faster than they could reproduce, and would experience exponential population decline.

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First principles mathematical models. The prey-predator model

GENERAL CONSERVATION LAW applied to No. of individuals in a "closed system": ACC = GEN

GEN = birth - death

"maltusian" term

$$\begin{cases} \dot{x}_1 = +ax_1 - bx_1 x_2 \\ \dot{x}_2 = -cx_2 + dx_1 x_2 \end{cases}$$

interaction term

STATE VARIABLE VECTOR

$x^T = (x_1, x_2)$

$x_i \in R^+$

VECTOR OF PARAMETERS

$x_1 =$ No. of preys at time t

$x_2 =$ No. of predatorsat time t

$p^T = (a, b, c, d)$

$\forall i, p_i \geq 0$

INITIAL CONDITION

$x_1(0) = x_{10};\ x_2(0) = x_{20} \Rightarrow x^T(0) = (x_{10}, x_{20})$

CLASSIFICATION

DYNAMIC AUTONOMOUS MATHEMATICAL MODEL made by 2 *ODEs* (Order = 2) ,
NON LINEAR, CONSTANT COEFFICIENT MODEL

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First principles mathematical models. The prey-predator model with 2 parameters

$$\begin{cases} \dot{x}_1 = \left(1 - \dfrac{x_2}{\mu_2}\right) x_1 \\ \dot{x}_2 = -\left(1 - \dfrac{x_1}{\mu_1}\right) x_2 \end{cases}$$

carrying capacity

INITIAL CONDITION

$$x_1(0) = x_{10};\ x_2(0) = x_{20} \Rightarrow x^T(0) = (x_{10}, x_{20})$$

STEADY-STATE or EQUILIBRIUM POINTS

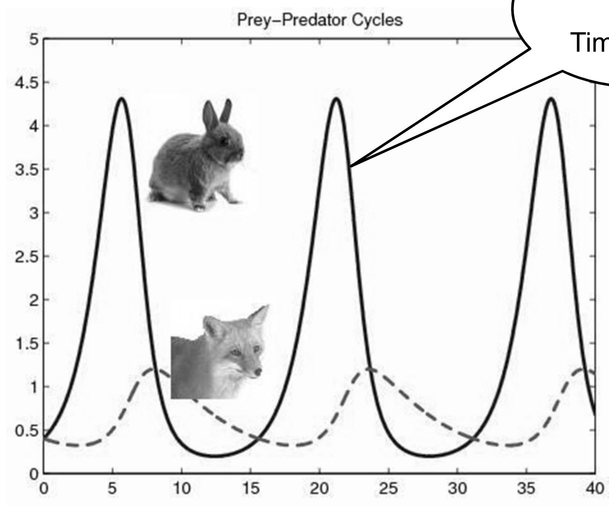
$$\begin{cases} x_{1,ss} = 0 \\ x_{2,ss} = 0 \end{cases} \qquad \begin{cases} x_{1,ss} = \mu_1 \\ x_{2,ss} = \mu_2 \end{cases}$$

☞ Cleve Moler, Experiments with MATLAB, 2009

http://www.mathworks.com/moler/exm/chapters.html

First principles mathematical models. The prey-predator model

- **Steady-state solutions**
- **Periodic solutions**



Time profile or Time series

http://www.scholarpedia.org/article/Predator-prey_model

First principles mathematical models.
The prey-predator model with 2 parameters

MatLab SOLUTION (1)

- **run *file* LOTKADEMO.M**

- **calling *function* LOTKA.M**

```
function yp = lotka(t,y)
%LOTKA  Lotka-Volterra predator-prey model.
%   Copyright 1984-2002 The MathWorks, Inc.
%   Revision: 5.9 by Michele MICCIO: May 8, 2008
% suggested parameters in the original file by MatLab:
% ALPHA=0.01
% BETA=0.02

yp = diag([1 - ALPHA*y(2), -1 + BETA*y(1)])*y;
```


First principles mathematical models.
The prey-predator model with 2 parameters

MatLab SOLUTION (2)

- **run *file* PREYPRED.M**

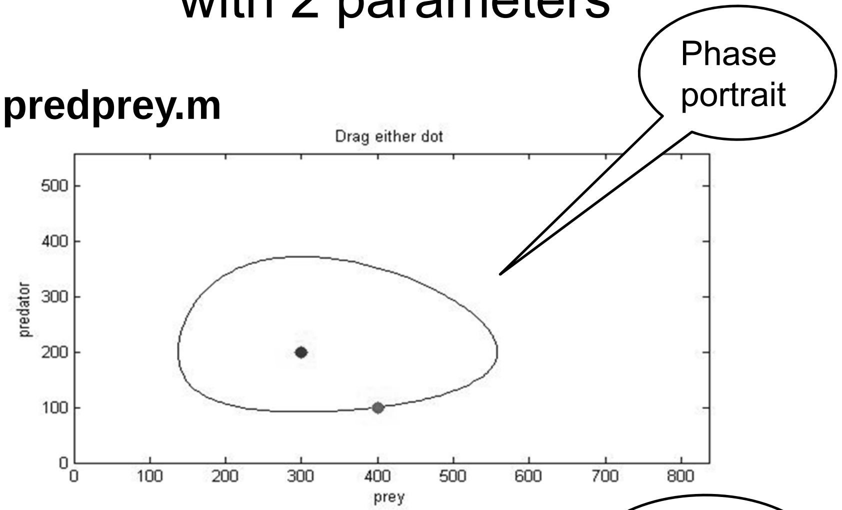
- **Use of graphycal interface**

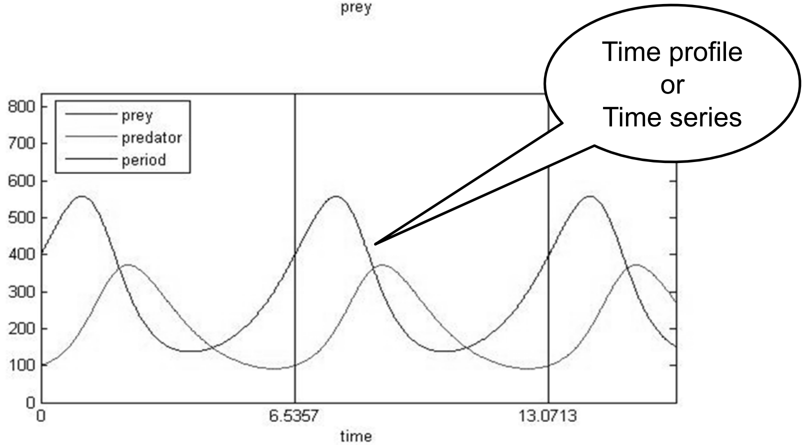
```
function predprey(action)
% PREDPREY  Predator-prey GUI.
% Drag the red dot to change equilibrium point.
% Drag the blue-green dot to change the initial conditions.

   % Default parameters.

   mu = [300 200]';      % Equilibrium.
   eta = [400 100]';     % Initial conditions.

   % Predator-prey ode

   function ydot = ppode(t,y);
      ydot = [(1-y(2)/mu(2))*y(1);
             -(1-y(1)/mu(1))*y(2)];
   end
```

First principles mathematical models.

The prey-predator model with 2 parameters

predprey.m





VARIABLES Definition

A variable represents a relevant property of the system, being modeled.

A variable can be, for example, physical or chemical quantities, measured system outputs often in the form of <u>signals</u>, timing data, counters, and event occurrence (yes/no).

The values of the variables can be practically anything; <u>real</u> or <u>integer</u> numbers, <u>boolean</u> values or even strings.

Mathematically, a variable can be an unknown appearing in equations and disequations or a function of one or more independent variables.

ⓘ The actual model is the set of functions that describe the relations between the different variables.

VARIABLES Examples

The most common variables in chemical and process engineering are:

1. composition/concentration
2. temperature
3. pressure
4. rate
5. repetition variable

Variables 1 to 3 are referred to as "intensive" as they do not depend on mass or size of the system being considered.
A rate can be related to matter (mass, mole, volume) or energy (heat) or momentum (force).
Rate is an "extensive" variable.
A repetition variable is used to account for realization of a given operation through a number of stages or units, being all equal in their working principle.
A variable can be "continuous" or "discrete".
Generally, each variable is defined in a given interval.

N_V = No. of variables in the model being considered.

COMPOSITION VARIABLES

Mass fraction

$$\omega_i \; [=] \; \frac{\text{mass of component i}}{\text{total mass}}$$

Molar fraction

$$x_i \; [=] \; \frac{\text{moles of component i}}{\text{total moles}}$$

Volume fraction

$$y_i \; [=] \; \frac{\text{volume of component i}}{\text{total volume}}$$

Implicit constraint

$$\sum_{i=1}^{c} \omega_i = 1; \quad \sum_{i=1}^{c} x_i = 1; \quad \sum_{i=1}^{c} y_i = 1$$

Molar concentration

$$c_i \; [=] \; \frac{\text{moles of component i}}{\text{total volume}}$$

Mass concentration

$$m_i \; [=] \; \frac{\text{mass of component i}}{\text{total volume}}$$

VARIABLES
Classification

Specified variables or Specifications

They are those variables that represent physical-chemical properties or that are fixed by designers, regulations, environmental considerations, etc. prior to the design phase.

Design variables

They are variables selected by designers.

Generally, their values are chosen in order to satisfy an optimum condition for a given "objective function".

Unknown or State variables

They are those variables that are calculated by the available system of equations once values for Design Variables have been fixed.

Mathematical Models
1st classification
(on the base of the approach adopted for model development)

- "*First principle Models*"
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📖 rielaborated from § 1.4 in Himmelblau D.M. e Bischoff K.B., "Process Analysis and Simulation", Wiley & Sons Inc., 1967

Transport Phenomena

General Law

$$(\text{flux}) = (\text{diffusion coeff.}) \cdot (\text{driving force})$$

Examples:

- Newton law of viscosity
- Fourier law of heat conduction
- 1st Fick law of diffusion

Transport and Kinetic Rate Equations

Momentum, Heat and Mass transfers

	Heat	**Mass**	**Momentum**
Flux	q	n_A	τ_{xy}
Diffusion transfer (microscopic scale)			
Law	Fourier's law	Fick's law	Newton's law
Driving force (gradient)	dT/dx	dC_A/dx	dv_y/dx
Key parameter (diffusion coefficient)	k_T (Thermal conductivity)	D_{AB} (Diffusivity)	μ (Viscosity)
Convection transfer (macroscopic scale)			
Driving force	ΔT	ΔC_A	ΔP

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🕮 rielaborated from § 1.4 in Himmelblau D.M. e Bischoff K.B., "Process Analysis and Simulation", Wiley & Sons Inc., 1967

Mathematical Models
2nd classification
(on the base of an approach typical of process engineering)

🕮 Ogunnaike B.A. and Ray W.H., "Process Dynamics, Modeling and Control", Oxford Univ. Press, 1994

🕮 Romagnoli & Palazoglu, "Introduction to Process Control"

- **Structured or Theoretical or White Box Models**
- **Unstructured or Empirical or Black Box Models**
- **Hybrid or Gray Box Models**

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Structured models

Characteristics:

Using mathematical equations describe the system

a) **Conservation equations** e.g. total mass, mass of individual chemical species, total energy, momentum and number of particles.

b) **Rate equations** e.g. transport rate and reaction rate equation.

c) **Equilibrium equation** e.g. reaction and phase equilibrium.

d) **Equations of state** e.g. ideal gas law

e) Other **constitutive relationships** e.g. Control valve flow equation, PID control law

☺ **Advantages:**

Being able of understanding the process in a fundamental way from this modeling

☹ **Disadvantages:**

It requires a good and reliable understanding of the physical and chemical phenomena that underlie the process

Accuracy of model depends on the assumptions and mathematical ability of the person constructing the model.

Unstructured models

Characteristic: constructing (***fitting***) a mathematical relationship among the variables that can explain the observed data.

a) Vary input variables and then measure the response of the output variables.

b) Enough experiments are required (a historical database of measurements or observations is needed)

c) Such models that rely solely on empirical information are considered as **black-box** models.

Example: A black-box model simulating the internal combustion engine operation and implemented into the control box of a modern car

☺ **Advantages:**

a) Good indicator to actual process (no assumption required).

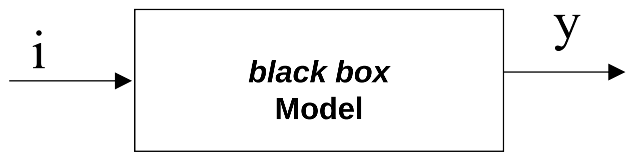
b) Just focus in on the range of conditions under the operating process.

☹ **Disadvantages:**

a) It requires an actual operating process and may become very time-consuming and costly

b) It doesn't allow extrapolation, generally

c) It never gives the engineer a fundamental understanding of the process.



Structured and unStructured Models: Comparison

- **Structured Models**

theory-rich and data-poor

- **Unstructured Models**

data-rich and theory-poor

"Hybrid" Models

- **Empirical Model II (*Gray-Box*)** is developed by incorporating empirical knowledge into the fundamental understanding of the process.

Such models blending fundamental and empirical knowledge are referred to as *gray-box* models.

Example

An example can be the use of mass and energy balances to develop a reactor model and the rate of the reaction will be based on expressions obtained from laboratory experiments.

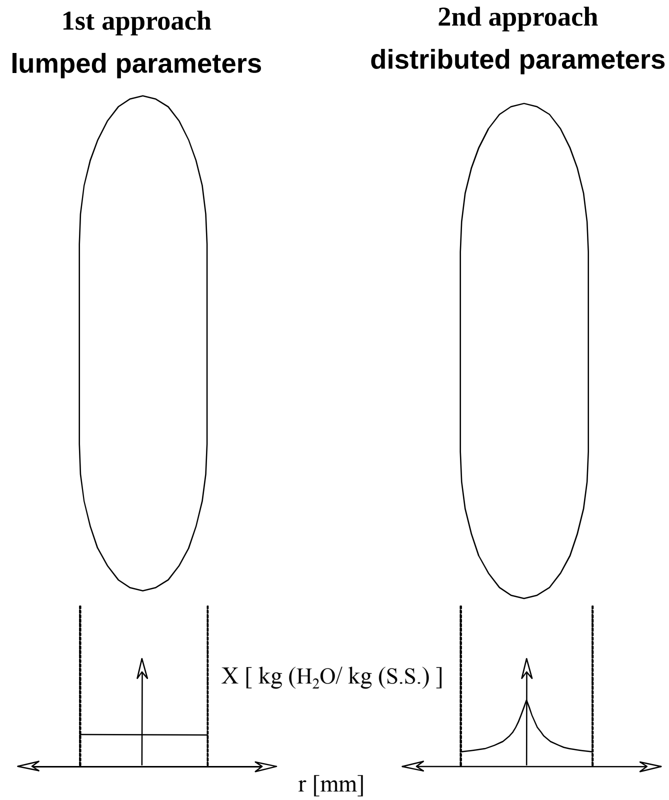
Mathematical Models
3rd classification

(on the base of
mathematical features of equations and variables,
also affecting type or easiness of solution)

Ch.3 of Himmelblau D.M. and Bischoff K.B., "Process Analysis and Simulation", Wiley, 1967

1. deterministic vs stocastic
2. lumped parameters vs distributed parameters
3. one dimension vs several dimensions
4. linear vs non linear
5. steady state vs time dependent
6. time-invariant vs time – varying
7. autonomous vs non – autonomous

First principles mathematical models. EXAMPLE of salami drying



X [=] mass of H_2O (liq.) / mass of dry solids

SIMPLIFIED MODEL: Assumptions

• Sausage is considered as a “Lumped body”:

• Uniform moisture concentration

• Uniform temperature

• Cylindrical shape

• All sausages have equal characteristics during drying.

• Weight loss is considered as the consequence of H_2O evaporation only.

• Heat generation by fermentation is negligible.

• Sausage size and shape remain unchanged during ripening.

• Heat transfer to sausage is under steady-state.

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SIMPLIFIED MODEL: Equations

Mass balance equation

for a single sausage:

$$\text{OUT} = \text{ACC}$$

$$\beta \cdot (a_{we} - RH) = -\frac{m_{ds}}{A} \cdot \frac{dX}{dt}$$

$$\text{IC}: \quad t = 0 \rightarrow X = X_0$$

m_{ds} is mass of dry solid in kg

A is the sausage outer surface in m²

X is the moisture content of the sausage in kg (H_2O)/kg (dry solid)

β is a mass transfer coefficient in kg/m^{2}s

a_w is the water activity corresponding to the equilibrium conditions with a humid solid

RH is the relative humidity of air

Mass transfer is considered as the result of a H_2O partial pressure difference between the outer surface of the sausage and air.

The desorption curve

The Oswin law is used:

$$X = K\left(\frac{a_{we}}{1 - a_{we}}\right)^n$$

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SIMPLIFIED MODEL: Equations

Heat balance equation

for a single sausage:

$$h \cdot (T_a - T) = \left(- \frac{m_{ds}}{A} \cdot \frac{dX}{dt} \right) \cdot \Delta H_{vap}(T)$$

h is the convective heat transfer coefficient in kW/m^2K

T_a is air temperature in K

T is sausage temperature in K at time t

ΔH_{vap} is H_2O latent heat of vaporization at temperature T in kJ/kg

NB:

It is an Algebraic eq.

SIMPLIFIED MODEL: Equations

Single sausage evaporation rate

The quantity of water which evaporates from the outer surface of a single sausage is given by:

$$\phi = - \frac{m_{ds}}{A} \frac{dX}{dt}$$

Weight loss

$$\Delta M(t) = A \cdot \int_0^t \phi \cdot dt$$

$$\Delta M_{fin} = A \cdot \int_0^{t_{fin}} \phi \cdot dt$$

SIMPLIFIED MODEL: Numerical resolution

- 4th order Runge-Kutta Method to solve the differential equation

- Trapezoidal rule to solve the following integral for weight loss

SIMPLIFIED MODEL: results

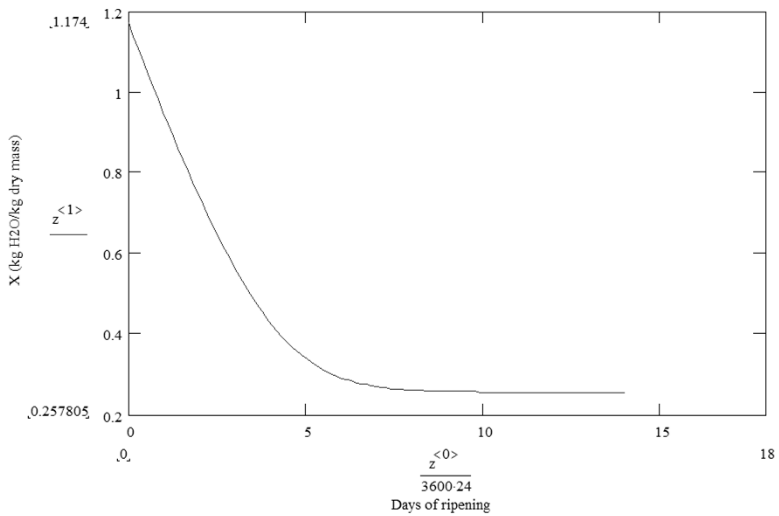
Moisture content versus drying time

"Turista Buonpiemonte"

RH=0.8

T_a=20° C

v_a=0.6 m/s



SIMPLIFIED MODEL: results

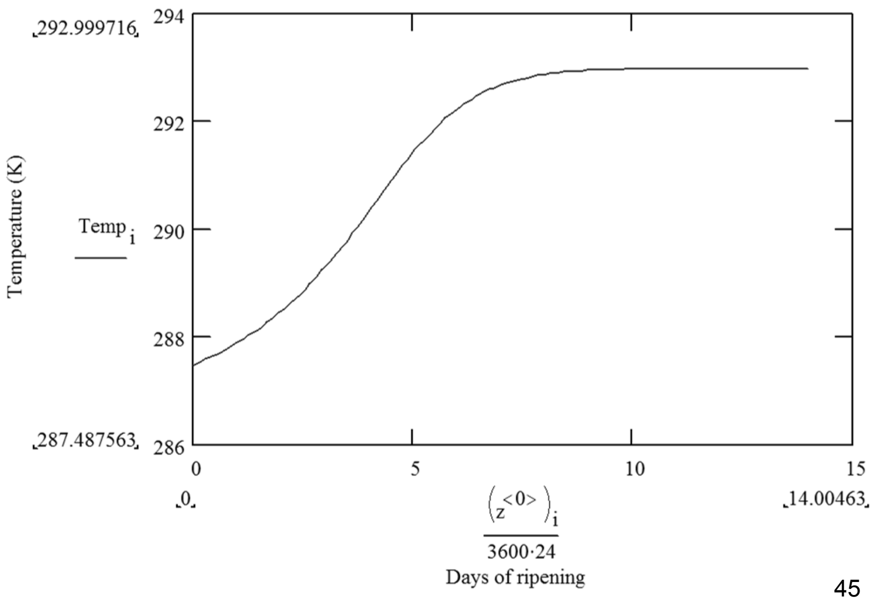
Salami temperature versus drying time

“Turista Buonpiemonte”

RH=0.8

T_a=20° C

v_a=0.6 m/s



SIMPLIFIED MODEL: results

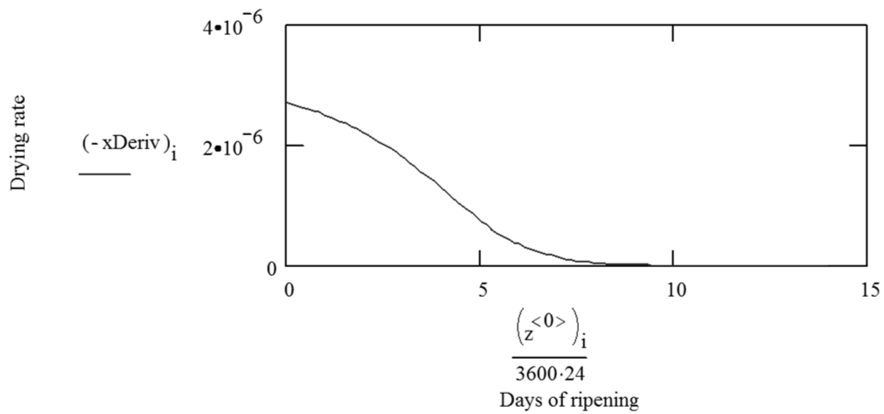
Drying rate versus drying time

“Turista Buonpiemonte”

RH=0.8

T_a=20° C

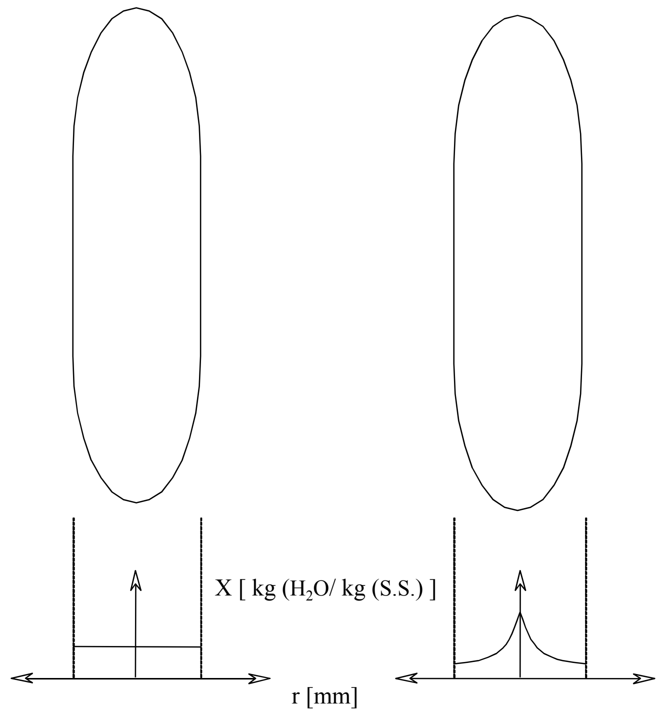
v_a=0.6 m/s



First principles mathematical models. EXAMPLE of salami drying

1st approach lumped parameters

2nd approach distributed parameters



X [=] mass of H_2O (liq.) / mass of dry solids

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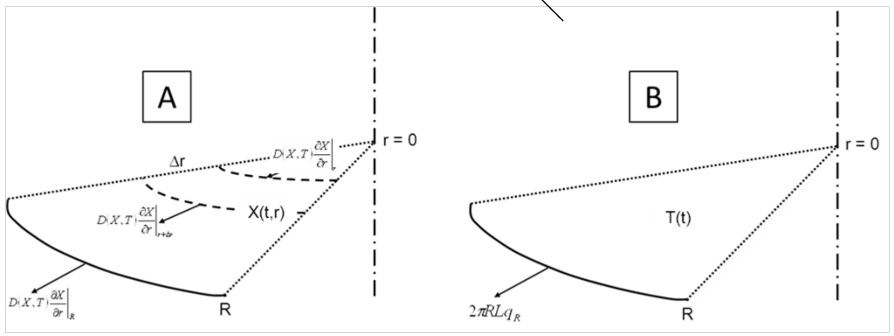
First principles mathematical models. EXAMPLE of salami drying

Distributed parameters approach

Water mass balance in a cylindrical shell

[IN] – [OUT] + [GEN] = [ACC]



where:

- D(X,T) is the mass diffusion coefficient depending on sausage moisture content and on sausage temperature (m^2/s)
- X is the moisture content on a dry basis (kg water/kg dry mass)

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First principles mathematical models. EXAMPLE of salami drying

Water mass balance,
with the corresponding initial and
boundary conditions

$$
\begin{cases}
\dfrac{\partial X}{\partial t} = \dfrac{D(X,T)}{r}\cdot\dfrac{\partial X}{\partial r} + \dfrac{\partial}{\partial r}\left(D(X,T)\cdot\dfrac{\partial X}{\partial r}\right) & (2.11)\\
-D(X,T)\cdot\left(\dfrac{\partial X}{\partial r}\right)_{r=R} = \dfrac{\beta}{\rho_{ds}}\cdot\left(a_{we} - RH\right) & (2.12)\\
\left(\dfrac{\partial X}{\partial r}\right)_{r=0} = 0 & (2.13)\\
X(0,r) = X_0 & (2.14)
\end{cases}
$$

where:

- $D(X,T)$ is the mass diffusion coefficient depending on sausage moisture content and on sausage temperature (m^2/s)
- ρ_{ds} is the dry mass density (kg/m^3)
- X is the moisture content on a dry basis (kg water/kg dry mass)

First principles mathematical models. EXAMPLE of salami drying

Energy balance,
with the corresponding initial condition

$$\pi R^2 L \rho(X) C_p(X) \frac{dT}{dt} = 2\pi R L q_r - 2\pi R L N_R M_w \Delta H(T)$$

lumped parameters Eq.

$$T(0) = T_0$$

where:

$$q = h(T_a - T)$$

$$q = \varepsilon\sigma(T_\infty^4 - T^4)$$

- N_R is the molar moisture flux at the sausage surface [$mol/(m^2\ s)$]
- $\Delta H(T)$ is the latent heat of water evaporation
- X is the moisture content on a dry basis (kg water/kg dry mass)

Mathematical Models
3rd classification

on the base of

- mathematical features of equations and variables,
- also affecting type or easiness of solution

Ch.3 of Himmelblau D.M. and Bischoff K.B., "Process Analysis and Simulation", Wiley, 1967

1. deterministic vs stocastic
2. lumped parameters vs distributed parameters
3. one dimension vs several dimensions

4.	linear	vs	non linear
5.	steady state	vs	time dependent
6.	time-invariant	vs	time – varying
7.	autonomous	vs	non–autonomous

Mathematical Models
3rd classification

Several levels are possible:

- Easy vs. difficult (*subjective*)
- Constant coefficients vs. variable coefficients
- Stiff system vs. non-stiff
- Linear vs. non-linear system (algebraic and differential).
- Homogeneous vs. Inhomogeneous
- Number of variables (e.g. binary and multicomponent systems)
- Order of differential equations (operators)
- Ordinary differential equations, partial differential equations, differential-algebraic equations, integrodifferential equations etc.
- Hyperbolic, parabolic and elliptic PDE
- Initial vs. boundary value problem

Adapted from: TEKNILLINEN KORKEAKOULU

Mathematical Models 3rd classification

Easy vs. difficult:

If this is estimated based on required time to solve the model with certain computational capacities, then this is actually a physical classification

Variable vs. constant coefficients:

$$\frac{\partial\left(D\frac{\partial c}{\partial h}\right)}{\partial h} \approx D\frac{\partial^2 c}{\partial h^2}$$

Mathematical Models 3rd classification

Stiff vs. non-stiff

- Formally, based on the ratio of eigenvalues
- In practice, if there are simultaneously very fast phenomena dictating step sizes, and very slow phenomena dictating simulation time, system is stiff.

Linear vs. non-linear

In principle, linear systems are easy. Natural systems are rarely linear, but often numerical solution is based on (local) linearizations

Linear Operator: Definition and first consequences

Formally, if *V* and *W* are vector spaces over the same ground field *K*, we say that $f : V \to W$ is a **linear transformation** if for any two vectors *x* and *y* in *V* and any scalar *a* in *K*, we have

$$f(x+y) = f(x) + f(y)$$

(**additivity**)

$$f(ax) = af(x)$$

(**homogeneity**).

This is equivalent to saying that *f* "preserves linear combinations", i.e., for any vectors x_1, ..., x_m and scalars a_1, ..., a_m, we have (**superposition**)

$$f(a_1x_1 + \cdots + a_mx_m) = a_1f(x_1) + \cdots + a_mf(x_m).$$

1st example (linear)

f : $w = a\,x$

2nd example (non linear)

f : $z = a^2\, b\, x\, y^{1/2}$

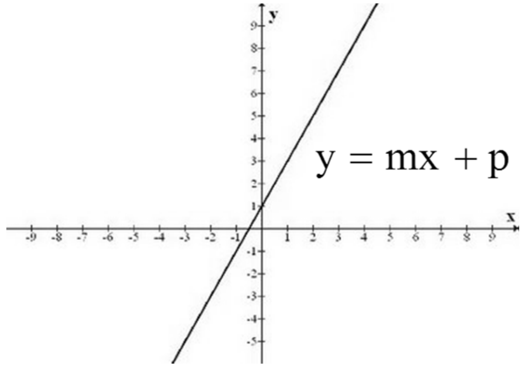
with *a, b* scalar constants

Linear Operator: Definition and first consequences

3rd example (non linear)

f : $y = mx + p$

with *m, p* scalar constants



NB:

It does not obey the **principle of superposition**

Mathematical Models
3rd classification

Homogeneous vs. inhomogeneous

If $f(\lambda x)= \lambda^n f(x)$ for every λ, then $f(x)$ is homogeneous to n:th degree.

Number of variables

- One-component system
- Two-component system
- Multi-component system

More components, more degrees of freedom.

Often one degree of freedom leads to scalar equations, more degrees to matrices.

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Mathematical Models
3rd classification

Order of differential equation

It is defined as the order of the highest derivative in the differenzial eq.

Ex.: n-th order ODE:

$$\frac{d^n y}{dx^n} + a_{n-1}\frac{d^{n-1} y}{dx^{n-1}} + \cdots + a_1 \frac{dy}{dx} + f(x,y) = 0$$

Can be linear or non-linear, depending on parameters a and function f.

If parameters a depend on x only (not on y), and function f is at most first order with respect to y, then the equation is linear

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Mathematical Models
3rd classification

Ordinary vs. partial differential equations

ordinary: variables are functions of only one independent variable

Ex.: Variable c is time invariant: $\partial \rightarrow d$

$$\frac{\partial c}{\partial t} = 0 = -v\frac{dc}{dh} + D\frac{d^2c}{dh^2} + r$$

partial: functions of several independent variables

Ex.:Variable c depends on time and on position

$$\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial h} + D\frac{\partial^2 c}{\partial h^2} + r$$

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Mathematical Models
3rd classification

Differential-algebraic equations (DAE)

In addition to the differential equations there are algebraic constraints.

Ex.:

$$f\left(\frac{dx}{dt}, x, y, t\right) = 0$$

for variables x there are both differential and algebraic equations

for variables y there are only algebraic equations

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Mathematical Models
3rd classification

Integro-differential equations

Involve both derivatives and integrals of the unknown variable.

Ex.:

Distributed systems: x is a density distribution with respect to s, and this distribution depends on t.

K is sometimes called a *Kernel* function

A reasonably general form:

$$\frac{dx(s,t)}{dt} = f(t,s,x(s,t)) + \int_a^b K(t,s,x(s,t))ds$$

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Mathematical Models
3rd classification

Initial vs. boundary value problems

Initial value problems usually easier: start from the initial values and ”march” forward in position or time.

Ex.:

*the **lumped parameters** salami drying model*

Boundary value problems are encountered usually in partial differential equations.

Ex.:

*the **distributed parameters** salami drying model*

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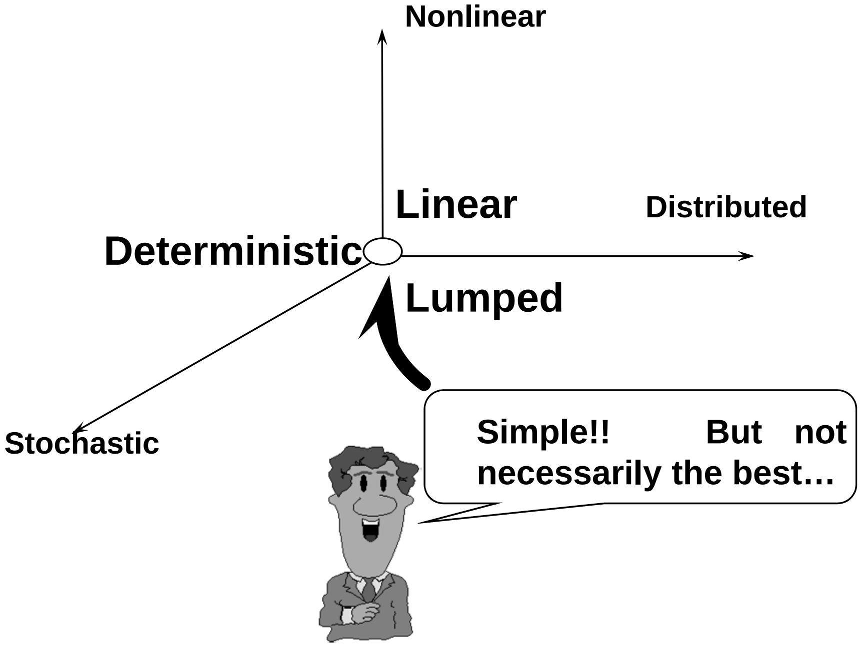
Linear-Lumped-Deterministic Model



"The theory of control is well developed for linear, deterministic, lumped-parameter models."

☞ Introduction to Process Control Romagnoli & Palazoglu

Mathematical Models 3rd classification

on the base of

- mathematical features of equations and variables,
- also affecting type or easiness of solution

Ch.3 of Himmelblau D.M. and Bischoff K.B., "Process Analysis and Simulation", Wiley, 1967

1. deterministic vs stocastic
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6. time-invariant vs time – varying
7. autonomous vs non – autonomous

Dynamical models (5–7)

Mathematical Models
1st classification

(on the base of the approach adopted for model development)

- Modelli a "principi primi" ("*First principle Models*")
  - ☞ Modelli basati sui "fenomeni di trasporto"
- Modelli basati sul "bilancio di popolazione"
- Empirical or "*fitting*" models
- Modelli dinamici
  - Modelli dinamici "con rappresentazione ingresso-uscita"
  - Modelli dinamici "con rappresentazione nello spazio di stato"
  - Modelli dinamici a scatola nera (*black box*)
- Serie temporali
- Modelli statistici

Mathematical Models
1st classification

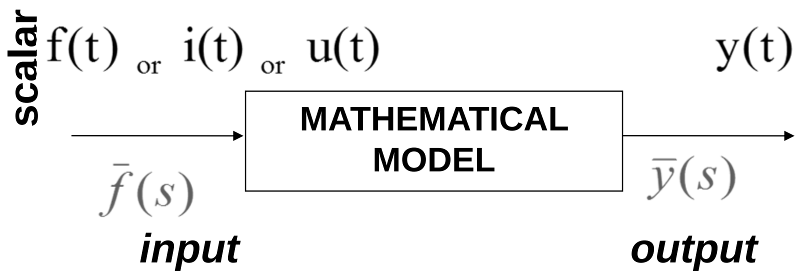
(on the base of the approach adopted for model development)

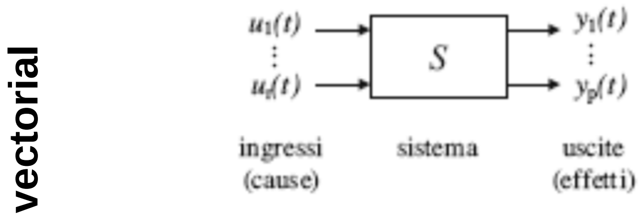
- Modelli a "principi primi" ("*First principle Models*")
  - ☞ Modelli basati sui "fenomeni di trasporto"
- Modelli basati sul "bilancio di popolazione"
- Modelli empirici o di "*fitting*"
- Dynamical models
  - input-output dynamic models
  - input-state-output dynamic models or state-space models
  - dynamic black box models
- Serie temporali
- Modelli statistici

Dynamic Models: definitions

- A dynamical system is a state space *S* , a set of times *T* and a rule *R* for evolution, $R{:}S \times T \rightarrow S$ that gives the consequent(s) to a state $s \in S$.
  - ❖ A dynamical system consists of an abstract phase space or state space, whose coordinates describe the state at any instant, and a dynamical rule that specifies the immediate future of all state variables, given only the present values of those same state variables.
  - ❖ For example the state of a pendulum is its angle and angular velocity, and the evolution rule is Newton's equation $F = ma$.
- A dynamical mathematical model can be considered to be a tool describing the temporal evolution of an actual dynamical system.
  - ❖ Dynamical systems are **deterministic** if there is a unique consequent to every state, or **stochastic** or **random** if there is a probability distribution of possible consequents (the idealized coin toss has two consequents with equal probability for each initial state).
  - ❖ A dynamical system can have discrete or continuous time.

Dynamic Models: input-output representation





🕮 Giua & Seatzu, "Analisi dei sistemi dinamici", 2006

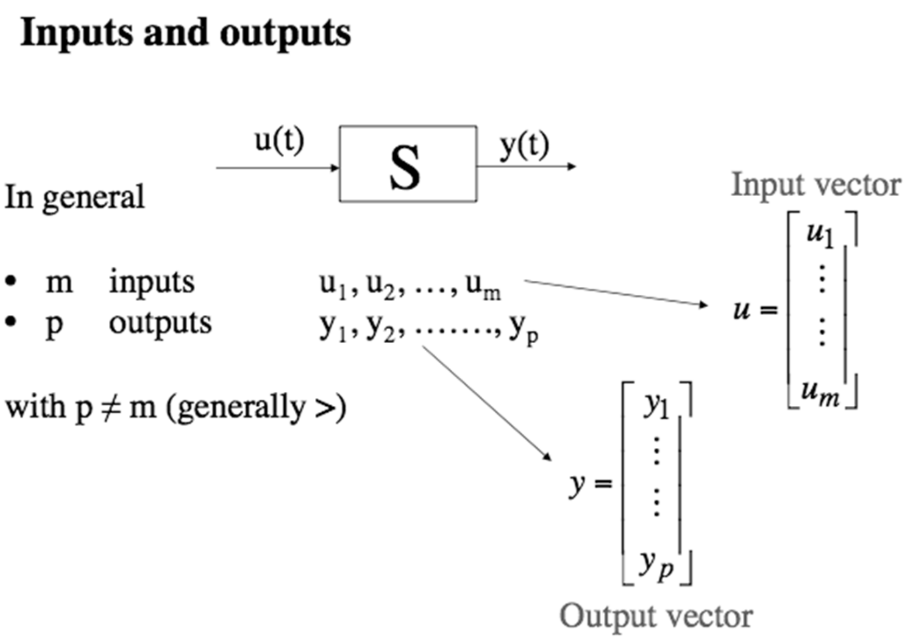
Fig. 2.1. Descrizione in ingresso-uscita

- An input-output equation reveals the direct relationship between the output variable desired, and the input variable.
- This relationship often includes the derivatives of one or both variables.
- Even with a higher order equation, the advantage is that the output variable is independent of (uncoupled from) any other variables except the inputs.

ⓘ typical of automatic process control

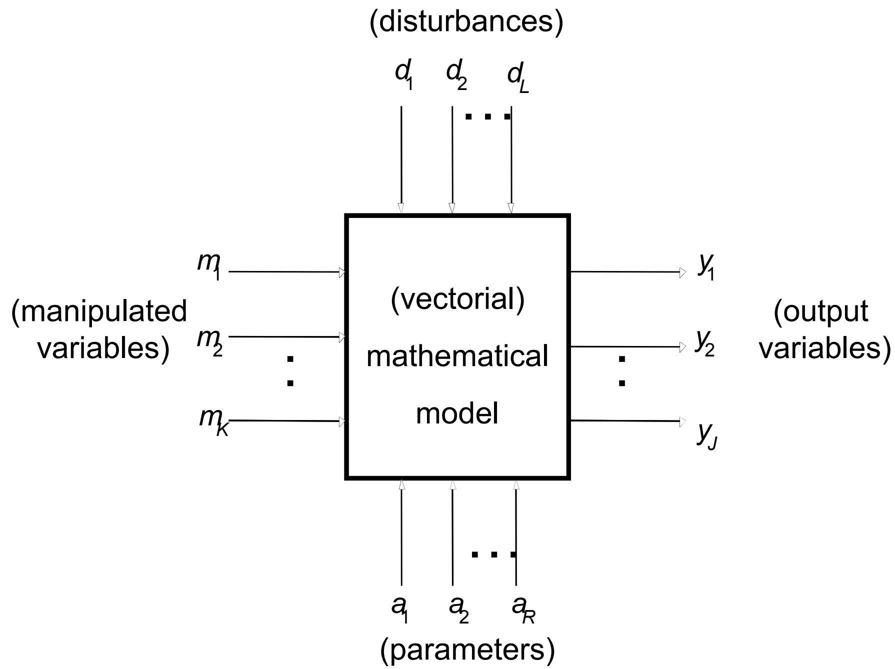
🕮 Roffel & Betlem, 2006

Input-Output representation Variables



Input-Output Models

General System Representation



typical of automatic process control

Romagnoli & Palazoglu, Introduction to Process Control, 2005

Definition of Linear dynamic system

From Wikipedia, the free encyclopedia: **http://it.wikipedia.org**

*A **linear dynamic system** is a model based on some kind of **linear operator H**. Linear systems typically exhibit features and properties that are much simpler than the general, **nonlinear** case. By definition, they satisfy the properties of **superposition** and **scaling**:*

Given two inputs:

$$i_1(t),\ i_2(t)$$

as well as their respective outputs:

$$y_1(t) = H\big(i_1(t)\big)$$

$$y_2(t) = H\big(i_2(t)\big)$$

then a linear system must satisfy:

$$\alpha y_1(t) + \beta y_2(t) = H\big(\alpha\, i_1(t) + \beta\, i_2(t)\big)$$

for any α *and* β.

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Definition of Time-invariant system

Retrieved from Simple Systems by Don Johnson: **http://cnx.org/content/m0006/latest/**

Systems that don't change their input-output relation with time are said to be **time-invariant**.

The mathematical way of stating this property is to use the **signal delay concept**:.

$$y(t) = S(i(t)) \quad \Rightarrow \quad y(t-\tau) = S(i(t-\tau))$$

If you delay (or advance) the input, the output is similarly delayed (advanced). Thus, a time-invariant system responds to an input you may supply tomorrow the same way it responds to the same input applied today; today's output is merely delayed to occur tomorrow.

Retrieved from Wikipedia, the free encyclopedia: **http://it.wikipedia.org**

A **time-invariant** system is one whose output does not depend explicitly on time.

Simple examples

To demostrate how to determine if a system is **time-invariant** then consider the two systems:

System A: $y_A(t) = t \cdot i(t)$

System B: $y_B(t) = 10 \cdot i(t)$

Since system A explicitly depends on *t* outside of *i*(*t*) then it is **time-variant**. System B, however, does not depend explicitly on *t* so it is **time-invariant**.

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Definition of Time-variant system

A time-variant system is one that is not time-invariant. The following things can be said about a time-variant system:

- It has explicit dependence on **time**.
- It is not **stationary**

ⓘ It does not have an **impulse response** (**transfer function**) in the normal sense. The system can be characterized by an impulse response except the impulse response must be known at each and every time instant.

Examples of time-variant systems

*The **human vocal tract** is a time variant system, with its transfer function at any given time dependent on the shape of the vocal organs. As with any fluid-filled tube, resonances (called formants) change as the vocal organs such as the tongue and velum move. Mathematical models of the vocal tract are therefore time-variant, with transfer functions often linearly interpolated between states over time.*

Table of Typical Math Operators

Retrieved from:

http://cnx.rice.edu/content/m0006/latest/

Input-Output Relation	Linear	Time-Invariant
$y(t) = d/dt\,[x(t)]$	yes	yes
$y(t) = d^2/dt^2\,[x(t)]$	yes	yes
$y(t) = (d/dt\,[x(t)])^2$	no	yes
$y(t) = d/dt\,[x(t)] + x(t)$	yes	yes
$y(t) = x_1+x_2$	yes	yes
$y(t) = x(t-\tau)$	yes	yes
$y(t) = \cos(2\pi ft)\,x(t)$	yes	no
$y(t) = x^2(t)$	no	yes
$y(t) = \|x(t)\|$	no	yes
$y(t) = mx(t) + b$	no	yes

Definition of Autonomous system (in theory of differential equations)

Retrieved from
"http://en.wikipedia.org/wiki/Autonomous_system_%28mathematics%29"

An **autonomous system** is an ODE equation of the form

$$\frac{d}{dt}x(t) = f(x(t))$$

Vector field

where *x* takes values in *n*-dimensional Euclidean space and *t* is usually time. It is distinguished from systems of differential equations of the form

$$\frac{d}{dt}x(t) = g(x(t), t)$$

in which the law governing the rate of motion of a particle depends not only on the particle's location, but also on **time**; such systems are **not autonomous**.

Simple examples

System A: $\frac{d}{dt}x(t) = tx(t)$

System B: $\frac{d}{dt}x(t) = 10x(t)$

Since system A explicitly depends on *t* outside of *x*(*t*) then the **dynamic system** is **not autonomous**. System B, however, does not depend explicitly on *t* so it is **autonomous.**

📖 *Retrieved from Luenberger, Introduction to Dynamic Systems*

A system of ODEs is called **autonomous** or **time invariant** if its vector field does not depend explicitly on time.

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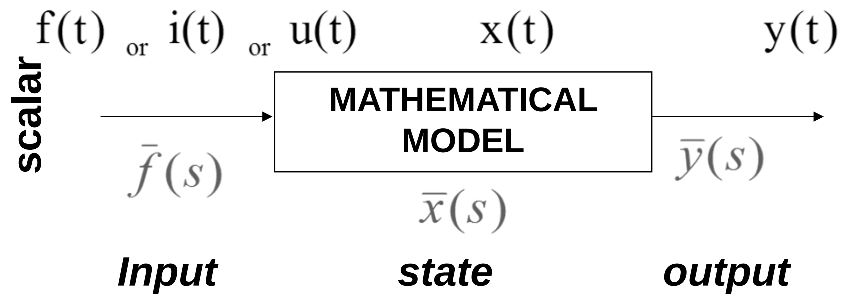
Dynamic Models: input-state-output representation



vectorial

Lo schema rappresentativo di un sistema descritto in termini di variabili di stato è del tipo riportato in Fig. 2.4.

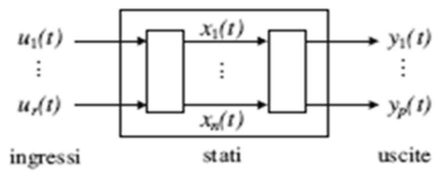


Fig. 2.4. Descrizione in variabili di stato

📖 Giua & Seatzu, "Analisi dei sistemi dinamici", 2006

Intuitively, the **state** of a system describes enough about the system to determine its future behavior.

ⓘ Behavioral models

☞ **"internal" model of the process**

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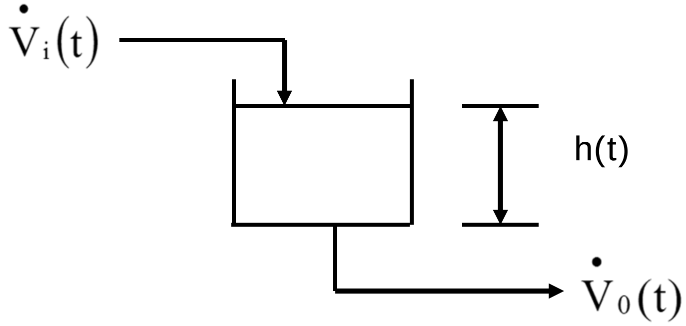
📖 Roffel & Betlem, 2006

Definition of State

The **state** of a **dynamic system** is defined through the smallest set of variables (called the *state variables*) such that the knowledge of these variables at $t=t_0$, together with the knowledge of the input for $t \geq t_0$, completely determines the behavior of the system for any time.

State variable ➔ $x(t)$

Example of input-state-output dynamic model: OPEN TANK FOR WATER STORAGE



VARIABLES
- IN : $\dot{V}_i(t)$
- STATE: $h(t)$
- OUT : $\dot{V}_0(t)$

Initial Condition: $\mathbf{h(0) = h_0}$

Input-state-output model

input u → evolution of y

"past values" ↗

Systems with "memory"

The same input produces different effects depending on the initial condition of the system.

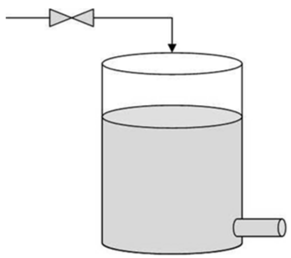
⇓

Dynamic systems

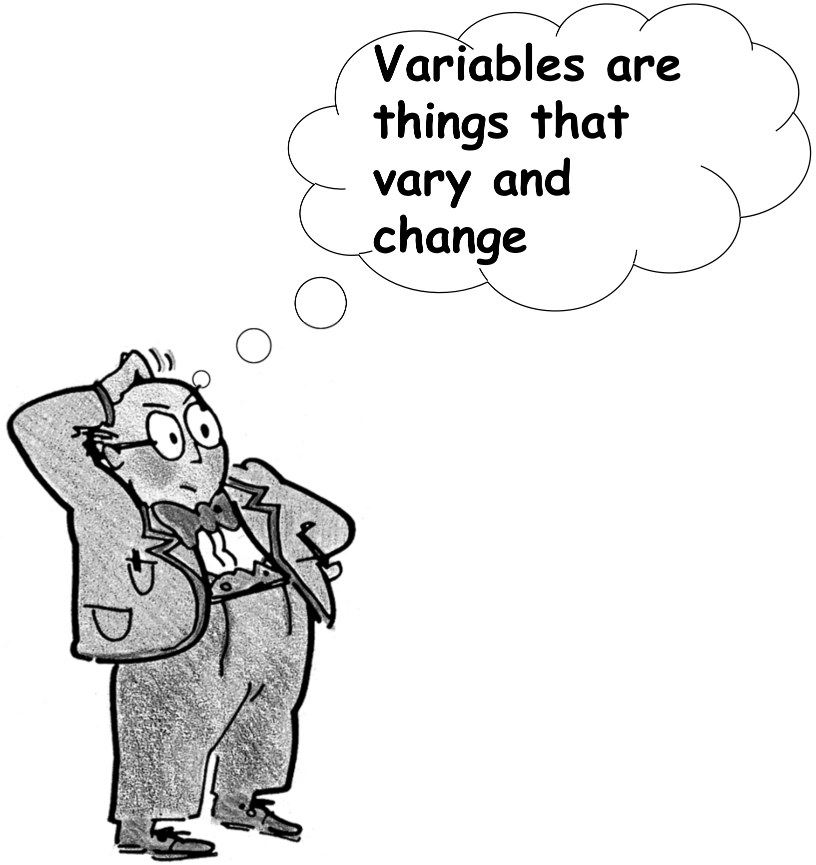
Ex: the reservoir model (A=area)

$dh(t)/dt = 1/A\ [q_1(t)-q_2(t)] = 1/A\ [q_1(t) - kh(t)]$ $\qquad h(t_0) = h°$

NOTE: the equation represents the evolution of the state *h*



VARIABLES



VARIABLES
Classification in dynamic models

INPUT:

time-varying quantities that change according to a known or prefixed law.

- The user (e.g., **manipulated variables**) or the outside environment (e.g., **disturbances**) decides how they change with time

OUTPUT:

quantities representing the observed or calculated results that the model yields to outside.

- They are originally unknown, but provide (typically as functions) results to outside once the input variables have been specified and the state variables have been calculated.

STATE:

quantities describing the present state of a system enough well to determine its future behavior.

- They provide a means to keep memory of the consequences of the past inputs to the system.
- They may be partly coincident with **output var.**
- The minimum number of state variables required to represent a given system, n, is usually equal to the order of the system's defining differential equation.

ⓘ **HINT**: The **state variables** are often given by the same variables appearing within the initial conditions of the system's ODEs

State Variables

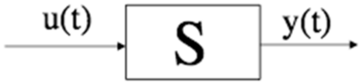
- It is necessary to know something else beside the evolution of input and output variables: initial conditions
- Such a *"memory",* required to define the initial condition, is called *the state of the system* at the time instant when the input is applied.
- Therefore, it is necessary to define the state variables to take into account the effects of initial conditions (as a matter of fact, also differential equations require an initial condition to be solved).

http://www.cds.caltech.edu/~murray/amwiki/index.php/FAQ:_What_is_a_state%3F_How_does_one_determine_what_is_a_state_and_what_is_not%3F

- The choices for variables to include in the state is highly dependent on the fidelity of the model and the type of system.
- One can see immediately that the choice of variables to be included in the state is not unique.

State Variables

State variables:



<u>Internal</u> variables whose knowledge at the time t_0 defines the minimum necessary information to determine univocally the output y(t) according to the input u(t), for every $t \geq t_0$

The state variables summarize the "past history" of the system.

$x_i(t) \quad i = 1,2,\ldots,n$ ⟹ $x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_n(t) \end{bmatrix}$

n is the system order

state vector

State-Space Models

State representation for continuous-time systems

$$\begin{cases} \dot{x}(t) = f(x(t),u(t),t) \\ y(t) = g(x(t),u(t),t) \end{cases}$$ ⟸ state equation ⟸ output transformation

$x(t_0) = x_0$ ⟸ initial state

$\mathbf{x}(t) \in \Re^n \quad \mathbf{u}(t) \in \Re^m \quad \mathbf{y}(t) \in \Re^p$

$\mathbf{f}(\cdot)$ is a vector function in $\Re^n$
$\mathbf{g}(\cdot)$ is a vector function in $\Re^p$
$\mathbf{f}(\cdot)$ and $\mathbf{g}(\cdot)$ can be time dependent functions

<u>A continuous-time dynamic system is described by differential equations</u>

State-Space Models

Example 1

$$
\begin{cases} \dot{x}(t) = -x^2(t) + u(t) \\ y(t) = 2x(t) - 2\sin(u(t)) \end{cases}
$$

$\leftarrow f(x(t),u(t))$

$\leftarrow g(x(t),u(t))$

$x(0) = 0$ $\leftarrow t_0 = 0$

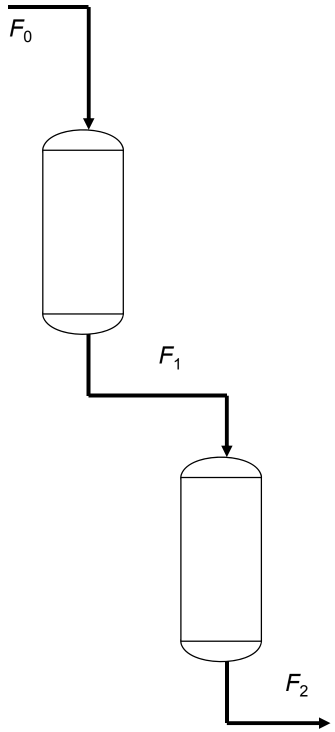
$x(t) \in \Re$
$u(t) \in \Re$
$y(t) \in \Re$

are scalars ($m=p=n=1$)

$f(\cdot)$ e $g(\cdot)$ are non linear functions of u and x, *but **not** of t*

ⓘ
it is a scalar model

Example 2: Pasteurized Milk Storage (Two Non-interacting Tanks)



- With a ***constant cross sectional***

area A, the volume of a tank can be expressed as:

V = Ah

where ***h*** represents the liquid level.

- Let us suppose that the ***control objective is to maintain a constant level in the second tank*** while the inlet flow rate to the first tank is varied.

- The ***liquid level $h_2(t)$*** is the variable that we want to be the **controlled variable**.

Example 2 – Two (Non-interacting) Tanks
State-space Model

mass balances

$$A_1 \frac{dh_1}{dt} = F_0 - F_1$$

$$A_2 \frac{dh_2}{dt} = F_1 - F_2$$

constitutive eqs.

$$F_1 = \frac{h_1}{R_1}, \quad F_2 = \frac{h_2}{R_2}$$

$\Rightarrow$

$$A_1 \frac{dh_1}{dt} = F_0 - \frac{h_1}{R_1}$$

$$A_2 \frac{dh_2}{dt} = \frac{h_1}{R_1} - \frac{h_2}{R_2}$$

IC:

$h_1(0)=h_{1s}$, $h_2(0)=h_{2s}$

Defining:

$x_1 = h_1$

$x_2 = h_2$

$m = F_0$

$a_1 = 1/A_1R_1$

$a_2 = 1/A_1$

$a_3 = 1/A_2R_1$

$a_4 = 1/A_2R_2$

$\Rightarrow$

State-space process model

$$\frac{dx_1}{dt} = -a_1 x_1 + a_2 m$$

$$\frac{dx_2}{dt} = a_3 x_1 - a_4 x_2$$

Example 2 – Two (Non-interacting) Tanks
State-space Model

vector field

$$\frac{dx_1}{dt} = -a_1 x_1(t) + a_2 m(t)$$

$$\frac{dx_2}{dt} = a_3 x_1(t) - a_4 x_2(t)$$

$y = x_2$ *(1st choice for output variable)*

OR

$y = \frac{x_2}{R_2}$ *(2nd choice for output variable)*

IC : $x_1(0) = x_{1s};\ x_2(0) = x_{2s}$

MODEL CLASSIFICATION:

DYNAMIC, LINEAR, CONSTANT-COEFFICIENT, NON-AUTONOMOUS, TIME-INVARIANT, 2 *ODE* SYSTEM.

ORDER = 2

State-space Models
Terminology

$$\frac{d}{dt}x(t) = f\big(t, x(t), u(t)\big)$$
$$IC : x\big(t_0\big) = x_0$$

- $n \in N$ is the order or size of the model
- x(t) is the vector of the state variables
- The n components of x(t) are phases
- The space spanned x(t) $\in \Re^n$ is the state-space or phase-space
- u(t) is the vector of the input variables with m components
- The function $f{:}\Omega \in \cdot \Re^{+} \Re^{n} \cdot \Re^{m} \rightarrow \Re^{n}$ is the vector field

Linear State-space Models.
Terminology

$$\frac{d}{dt}x(t) = Ax(t) + Bu(t)$$
$$y\big(t\big) = Cx(t) + Du(t)$$
$$IC : x\big(t_0\big) = x_0$$

- A is the is the state matrix (n•n)
- B is the is the input matrix (n•m)

Autonomous System
(definition in Theory of Systems)

An **autonomous system** is a system having the **state** not depending on **input**

OR

input constant with time

in its the mathematical model.

📖 adapted from "notecontrolli_PRATTICHIZZO.pdf"

NB:

For a dynamic model described by a system of ODEs, an **autonomous** system is also **time invariant**

Autonomous System
(in Non-Linear Dynamics)

A **dynamic system** is **autonomous** if its vector field depends on the state x(t), but does not explicitly depend on time.

$$\frac{d}{dt}x(t) = f(x(t)) \qquad \text{with } x(t) \in \Re^n$$

$$IC : x(t_0) = x_0 \qquad t \in \Re^+$$

Examples of 2nd order systems:

Autonomous system

$$\begin{cases} \dot{x}_1 = -x_1 + x_2 \\ \dot{x}_2 = -x_1 - x_2 \end{cases}$$

Non-autonomous system

$$\begin{cases} \dot{x}_1 = -x_1 + x_2 + \cos(2\pi t) \\ \dot{x}_2 = -x_1 - x_2 \end{cases}$$

Example 2 – Two (Non-interacting) Tanks
State-space Model

$$\dot{x}(t) = Ax(t) + Bm(t)$$

State-space (linear) process model

$$A = \begin{pmatrix} -a_1 & 0 \\ a_3 & -a_4 \end{pmatrix}$$

State matrix

$$B = \begin{pmatrix} a_2 \\ 0 \end{pmatrix}$$

Input matrix

$$CI : x(0) = x_0$$

$$x(t) = \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix}$$

State variables

$$y(t) = x_2(t)$$

Output variable

MODEL CLASSIFICATION:

DYNAMIC, LINEAR, NON-AUTONOMOUS, TIME-INVARIANT, 2 *ODE* SYSTEM.

ORDER = 2

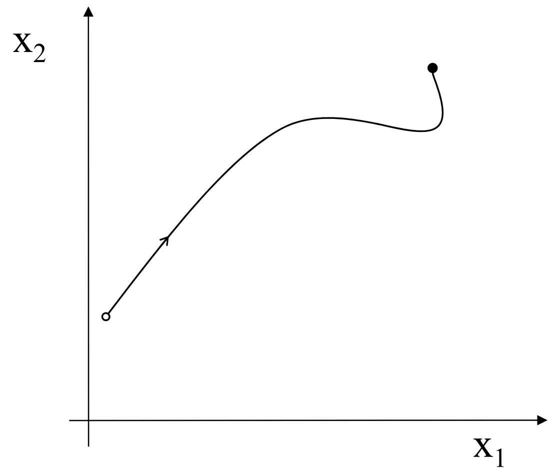
Orbits or Trajectories of a dynamic system

The **forward orbit** or **trajectory** of a state *x* is the time-ordered collection of states that x follow from an initial state x_0 using the system evolution rule.

•When both state space and time are continuous, the forward orbit is a curve *x*(*t*) parametric in *t* ≥ 0

•Different initial states result in different trajectories

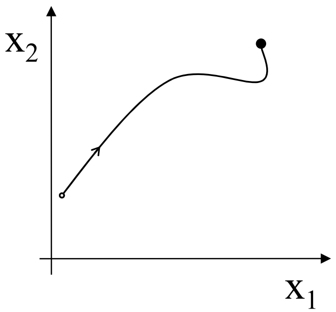
Example of an orbit (order n=2)



Phase portrait

The set of of all trajectories forms the **phase portrait** of a dynamical system.

- in practice, only representative trajectories are considered
- the **phase portrait** is usually built by numerical methods for nonlinear systems
- The analysis of phase portraits provides an extremely useful way for visualizing and understanding qualitative features of solutions.
- The **phase portrait** is particolarly useful for scalar (1st order) and planar systems (2nd order)



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Transients and regimes

- The **orbits** may have a bounded or unbounded asymptotic behavior (for $t \rightarrow \pm \infty$).
- If an orbit has a bounded asymptotic behavior for $t \rightarrow + \infty$, the part of the orbit describing such an asymptotic behavior is referred to as **regime** and the remaining part is referred to as **transient**.
- The simplest and most well known regime (bounded) is the **equilibrium point** (**steady-state point**), which is possible for every system order n

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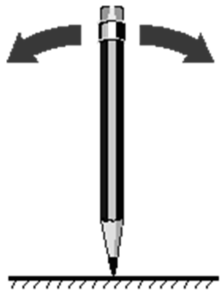
Stability of an equilibrium point

Adapted from *On-Line Lectures* ©Alexei Sharov, Department of Entomology, Virginia Tech, Blacksburg, VA
http://www.ento.vt.edu/~sharov/PopEcol/

*An **equilibrium** may be **stable** or **unstable** or **indifferent**.*

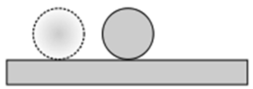
For example,

the equilibrium of a pencil standing on its tip is unstable;



the equilibrium of a picture on the wall is (usually) stable;

the equilibrium of a ball on a flat plane is (usually) indifferent.



ⓘ More formal definitions of stability do exist …

Example 2 – Two (Non-interacting) Tanks
Input-Output Model

$$\frac{dx_2}{dt} = a_3 x_1 - a_4 x_2$$

$$\frac{d^2x_2}{dt^2} = a_3\frac{dx_1}{dt} - a_4\frac{dx_2}{dt} = a_3(-a_1x_1 + a_2m) - a_4\frac{dx_2}{dt}$$

$$\frac{dx_1}{dt} = -a_1x_1 + a_2m$$

$$y = x_2$$

Finally, $$\frac{d^2y}{dt^2} = a_3\left(-a_1\left(\frac{1}{a_3}\frac{dy}{dt} + \frac{a_4}{a_3}y\right) + a_2m\right) - a_4\frac{dy}{dt}$$

m(t) →

$$\frac{d^2y}{dt^2} + (a_1 + a_4)\frac{dy}{dt} + a_1a_4y = a_2a_3m(t)$$

$$\text{IC}: \quad y(0)=h_{2s}; \quad \left.\frac{dy}{dt}\right|_{t=0} = 0$$

→ **y(t)**

A single equation describing the effect of the input on the output.

Mathematical Models
4th classification

(based on the type of description adopted for **time** as the independent variable)

☞ VALID for **DYNAMICAL SYSTEMS** only

1. continuous time models

2. discrete time models

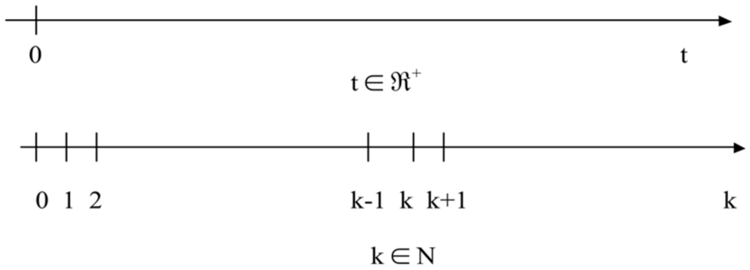
CONTINUOUS-TIME SYSTEMS

The time changes continuously. It is not possible to define a minimum time interval: it is always possible to consider a smaller time interval.

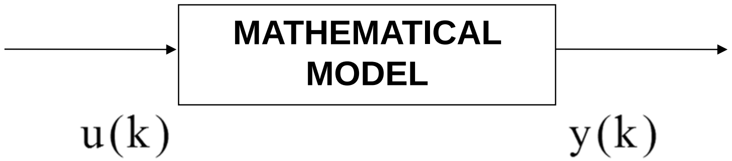
Accordingly, the theory of continuous-time systems has been defined and studied, where the variables of the system are continuous-time functions, that is, at every time instant *t*, it is possible to define and assign the variable value.

Continuous-time systems: $t \in \Re$

DISCRETE-TIME SYSTEMS

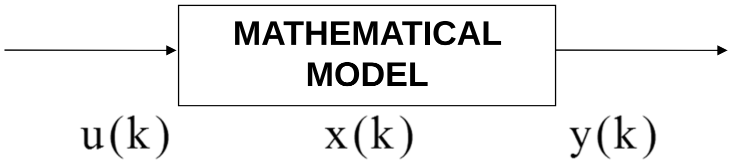


input – output representation



Ingresso **uscita**
Input ***output***

input – state – output representation



Ingresso **stato** **uscita**
Input ***state*** ***output***

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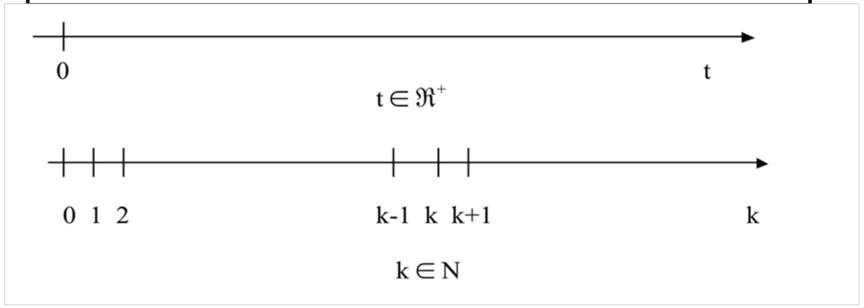
DISCRETE-TIME SYSTEMS



General representation of input–state–output discrete-time models

EXPLICIT TYPE

$$\begin{cases} x(k) = \varphi[k, k_0, x_0, u(k_0, k)] \\ y(k) = \eta[k, x(k), u(k)] \end{cases}$$

"IMPLICIT" TYPE

$$\begin{cases} x(k+1) = f[k, x(k), u(k)] \\ y(k) = \eta[k, x(k), u(k)] \end{cases}$$

$$CI : x(k_0) = x_0$$

SCALAR SYSTEMS: **x(k) is a scalar variable**
VECTOR SYSTEMS: **x(k) is a vector variable of size n**

ⓘ A deterministic system with discrete time is often defined a map.

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Example No. 1
Malthusian Growth Model (II)

If we let x(k) denote the population size during time period k and let c denote the population growth rate per unit time, the Malthusian model can be written mathematically in the following way:

$$x(k+1) = (1+c)\, x(k)$$

A model in this form, where the population at the next time period is determined by the population at the previous time period, is said to be a

***difference equation model** or a **map**.*

The initial condition is:

$$IC:\ x(0) = x_0$$

autonomous discrete-time system of order 1 (scalar model)

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Model Order

The **order n** is an integer number obtained as the product between the size of the space vector x and the time gap *in* the implicit model representation.

ⓘ The *time gap* is the max time distance in the implicit model representation

Example 1:

autonomous discrete-time system of order 1 (scalar model)

$$\begin{cases} x(k+1) = f(x(k)) \\ IC: \quad x(k_0) = x_0 \end{cases}$$

Example 2:

autonomous discrete-time system of order 2 (vectorial model)

$$\begin{cases} x(k+1) = g(x(k)) \\ IC: \quad x(k_0) = x_0 \end{cases}$$

$$\text{with} \quad x^T = (x_1 \quad x_2)$$

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Fixed Points
for autonomous systems
x(k+1) = f(x(k)

DEFINITION of a fixed point**:**

$$\mathbf{x(k+1) = x(k)}$$

ⓘ x(k) may be a scalar or vector variable

DETERMINATION of a fixed point**:**

The fixed points are determined as the solutions of the algebraic eq. (scalar) or system of eqns.(vector):

$$\mathbf{x^* = f\left(x^*\right)}$$

➢A fixed point can be stable or unstable.

➢A stable fixed point is an **attractor** for the trajectories originating in a reasonable neighborhood of it.

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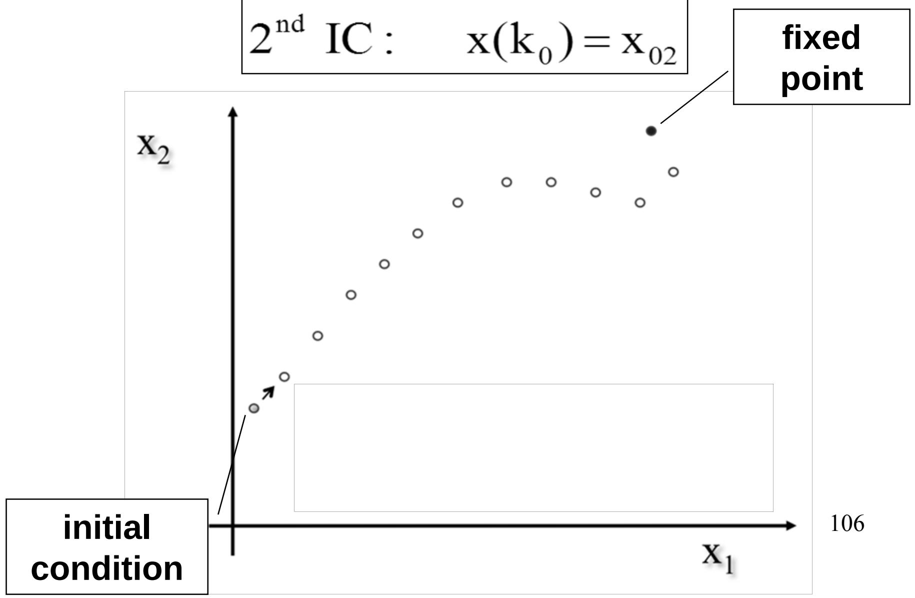
Orbits or Trajectories

Example:
autonomous non-linear, discrete-time model of order 2

$$x(k+1) = f(x(k))$$
$$\text{with } x^T = \begin{pmatrix} x_1 & x_2 \end{pmatrix}$$

$$1^{st}\ IC: \quad x(k_0) = x_{01}$$
$$2^{nd}\ IC: \quad x(k_0) = x_{02}$$



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Example No. 2
Logistic Model

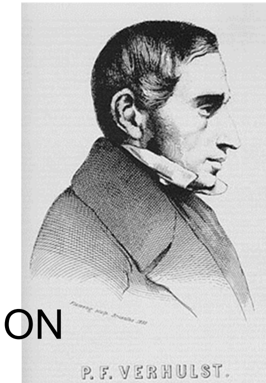
Differently from the Malthusian model …

- developed by Belgian mathematician Pierre Verhulst (1838)

HYPOTHESES

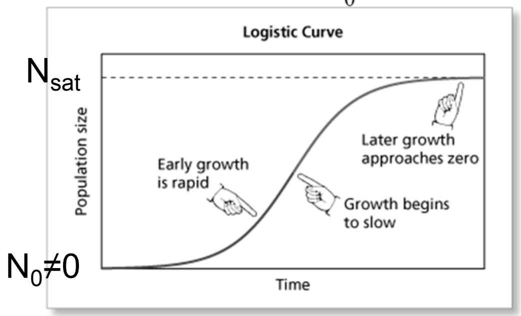
- resources are limited for growth: $N(t) \le N_{sat}$

$$\dot{N} = cN(t) - hN^2(t)$$
$$c > 0; h > 0$$
$$IC: \; N(t_0) = N_0$$



CLOSED-FORM SOLUTION

$$N(t) = \frac{N_{sat}}{1 + \frac{N_{sat} - N_0}{N_0} e^{-ct}}$$



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Example No. 2
Logistic Map

$$\dot{N} = cN(t) - hN(t)^2$$

$$\dot{N} = 0 \quad \text{if} \quad N(t) = N_{sat} \Rightarrow h = \frac{c}{N_{sat}}$$

$\downarrow$

discreti-zation

$$\frac{N(k+1) - N(k)}{(k+1) - k} = cN(k) - c\frac{N(k)^2}{N_{sat}} \qquad \text{where: } N(k) \in \mathcal{N}$$

$$N(k+1) = N(k) + cN(k) - c\frac{N(k)^2}{N_{sat}}$$

$$N(k+1) = (1+c)N(k) - c\frac{N(k)^2}{N_{sat}}$$

$\downarrow$

$$\frac{N(k+1)}{N_{sat}} = (1+c)\frac{N(k)}{N_{sat}} - \frac{c}{N_{sat}}\frac{N(k)^2}{N_{sat}}$$

$\downarrow$

adimen-siona-lization

$$x(k) = \frac{N(k)}{N_{sat}} \in [0,1]$$

$$x(k+1) = (1+c)x(k) - cx(k)^2$$

$$\text{let's assume: } c \gg 1$$

$$\text{let's set: } r = (1+c) = c$$

$$x(k+1) = rx(k)\left[1 - x(k)\right]$$
$$IC: \quad x(k_0) = x_0$$

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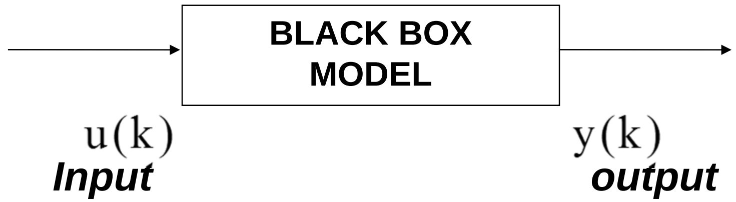
Mathematical Models 1st classification

(on the base of the approach adopted for model development)

- Modelli a “principi primi” (“*First principle Models*”)
  - ☞ Modelli basati sui “fenomeni di trasporto”
- Modelli basati sul “bilancio di popolazione”
- Modelli empirici o di “*fitting*”
- Dynamic models
  - input-output dynamic models
  - input-state-output dynamic models or state-space models
  - dynamic black box models
- Serie temporali
- Modelli statistici

Black-Box Model Structures



The model structures vary in complexity and order depending on the flexibility you need to account for the dynamics and on possible consideration of noise in your system.

The simplest black-box structures are:

1.Linear polynomial model, which is the simplest input-output model (e.g., ARX model)

$$y(t) + \alpha_1 y(t-1) + \ldots + \alpha_n y(t-n) = \beta_0 u(t) + \beta_1 u(t-1) + \ldots + \beta_n u(t-n)$$

2.Transfer function, with a given number of adjustable poles and zeros.

3.State-space model, with unknown system matrices, which you can estimate by specifying the number of model states

4.Non-linear parameterized functions

Black-Box Modeling

- Black-box modeling is usually a trial-and-error process, where you estimate the parameters of various structures and compare the results.
- Typically, you start with the simple linear model structure and progress to more complex structures.
- You might also choose a model structure because you are more familiar with this structure or because you have specific application needs.

ⓘ Black box models are not based on physical grounds and the equations do not reflect the internal structure of the process.

ⓘ Black box models usually have a linear structure, and because of this built-in linearity they have a limited validity range.

Dynamic black box. Linear polynomial models

Black box models may describe the system dynamics through a linear, time-invariant vector difference equation of finite dimension.

•The difference equation has some model parameters. The following difference equation represents a simple model structure:

$$y(k) + ay(k-1) = bu(k)$$

where *a* and *b* are adjustable parameters.

•Parameters are a crucial point in dynamic black box model development.

•In order to parameterize a black box model, only the input-output behavior is required; detailed knowledge about the internal behavior is not necessary.

•The parameters are estimated by minimizing a scalar function of the prediction error, i.e. the difference between the observed output and the model-predicted output.

Example No. 1
the ARMAX model

For a single-input/single-output system (SISO), the ARMAX (Auto-Regressive Moving-Average with eXogenous variable) model structure is:

Auto-Regression

$$\underbrace{}_{}y(t)+\overbrace{a_1 y(t-1)+\ldots+a_{na}\,y(t-n_a)}^{\text{Auto-Regression}} =$$
$$b_1 u(t-n_k)+\ldots+b_{nb}u(t-n_k-n_b+1)+$$
$$\underbrace{e(t)+c_1 e(t-1)+\ldots+c_{nc}e(t-n_c)}_{\text{Moving-Average}}$$

Moving-Average

where:
y(t) represents the output at time *t*,
u(t) represents the input (eXogenous variable) at time *t*,
n_a is the number of poles for the dynamic model,
n_b is the number of zeros plus 1,
n_c is the number of poles for the disturbance model,
n_k is the dead time (in terms of the number of samples) before the input affects output of the system,
e(t) is the white-noise disturbance (gaussian)

ⓘ here t≅k

MathWorks
Documentation center

System Identification

System identification is a methodology for building mathematical models of dynamic systems using measurements of the system's input and output signals/data.

The process of system identification requires that you:
1. Measure the input and output signals/data from your system in time or frequency domain.
2. Select a model structure.
3. Apply an estimation method to estimate value for the adjustable parameters in the candidate model structure.
4. Evaluate the estimated model to see if the model is adequate for your application needs.

•System identification uses the input and output signals you measure from a system to estimate the values of adjustable parameters in a given model structure.

•Obtaining a good model of your system depends on how well your measured data reflect the behavior of the system.

Mathematical Models
1st classification

(on the base of the approach adopted for model development)

- Modelli a "principi primi" ("*First principle Models*")
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- Modelli basati sul "bilancio di popolazione"
- Modelli empirici o di "*fitting*"
- Dynamic models
  - input-output dynamic models
  - input-state-output dynamic models or state-space models
  - dynamic black box models
- Serie temporali
- Modelli statistici

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Dynamical modeling
Final Statement

A way to distinguish the techniques used when modeling dynamic processes is to picture them on a scale with two extremes at the ends:

•at the one side
black box
system identification

•at the other side
theoretical modeling or
first principles modeling

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Mathematical Models
5th classification

(based on the type of solution,

with exclusion of empirical models)

1. ANALYTICAL SOLUTIONS
   → DIFFERENTIAL CALCULUS
   → ALGEBRA
2. NUMERICAL SOLUTIONS
   → NUMERICAL CALCULUS

Ex.: numerical methods for PDEs

1. FINITE DIFFERENCE METHODS (FDM)
2. FINITE ELEMENT METHODS (FEM)
3. COLLOCATION METHODS

Mathematical Models
1st classification

(on the base of the approach adopted for model development)

- Modelli a "principi primi" ("*First principle Models*")
  - ☞ Modelli basati sui "fenomeni di trasporto"
- Modelli basati sul "bilancio di popolazione"
- Modelli empirici o di "*fitting*"
- Modelli dinamici
  - Modelli dinamici "con rappresentazione ingresso-uscita"
  - Modelli dinamici "con rappresentazione nello spazio di stato"
  - Modelli dinamici a scatola nera (*black box*)
- **Time Series**
- Modelli statistici