Modeling Time-Dependent Systems

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Types of Process Models

Time-dependent modeling concerns properties of a system changing through time.

Steady-state modeling addresses properties of a steady (equilibrium) state without explicit regard to time.

Forward modeling starts with the given state of a system at a time t_0 (often $t_0 = 0$) and predicts its properties at later times $t > t_0$. Some examples for demonstration:

- Val Pola rock avalanche
- Snow avalanche hitting a pond
- Evolution of the drainage system in and around the Alps

Backward modeling attempts to reconstruct properties at earlier times $t < t_0$ from the present state. This is in general difficult and non-unique, but one of the challenges in geology.

Variables

Time-dependent systems are described by a set of time-dependent variables, e. g.,

- $n(t)$ as the number of individuals in a population,
- $T(t)$ as the temperature of a gas, or
- $x(t)$, $y(t)$ und $z(t)$ for the motion of a particle in space.

In theory, $u(t)$ is often used for the time-dependent variable. If the system involves more than one variable, $u(t)$ is assumed to be a vector consisting of several components $u_1(t)$, $u_2(t)$, ..., $u_n(t)$.

Mathematical Description of Time-Dependent Systems

Discrete and Continuous Systems

The evolution of a system may take place in discrete steps or continuously. Large systems are often approximated by continuous descriptions.

Examples

- The movement of a particle is continuous.
- Radioactive decay is a discrete, stochastic process, but is often described by a continuous differential equation

$$\frac{d}{dt} u(t) \;=\; -\,\lambda\, u(t).$$

The Role of Derivatives

The time-derivative of a function $u(t)$ ($\frac{d}{dt}u(t)$, $\frac{\partial}{\partial t}u(t)$, $u'(t)$, $\dot{u}(t)$, $\ldots$) describes the rate of change in $u(t)$ per time.

Differential Equations

- Continuous time-dependent systems are described by (systems of) differential equations involving time-derivatives.
- A differential equation is an equation that involves the derivative(s) of an unknown function (and in many cases also the functions itself).
- A system characterized by more than one variable (i. e., if $u(t)$ is a vector) is described by a system of (coupled) differential equations.

Examples of Differential Equations

Radioactive decay:

$$\frac{d}{dt}u(t) \;=\; -\lambda\, u(t)$$

Unlimited growth (simplest model):

$$\frac{d}{dt}u(t) \;=\; \lambda\, u(t)$$

Logistic growth with limited resources:

$$\frac{d}{dt}u(t) \;=\; \lambda\, u(t) - \mu\, u(t)^2$$

Examples of Systems of Differential Equations

Radioactive decay chain:

$$\begin{aligned}
\frac{d}{dt} u_1(t) &= -\lambda_1\, u_1(t) \\
\frac{d}{dt} u_2(t) &= \lambda_1\, u_1(t) - \lambda_2\, u_2(t) \\
&\cdots \\
\frac{d}{dt} u_{n-1}(t) &= \lambda_{n-2}\, u_{n-2}(t) - \lambda_{n-1}\, u_{n-1}(t) \\
\frac{d}{dt} u_n(t) &= \lambda_{n-1}\, u_{n-1}(t)
\end{aligned}$$

Examples of Systems of Differential Equations

Chemical reaction (simplest version):

$$\begin{aligned}
\frac{d}{dt}A(t) &= -k_1\, A(t)\, B(t) + k_2\, C(t) \\
\frac{d}{dt}B(t) &= -k_1\, A(t)\, B(t) + k_2\, C(t) \\
\frac{d}{dt}C(t) &= k_1\, A(t)\, B(t) - k_2\, C(t)
\end{aligned}$$

Examples of Systems of Differential Equations

Predator-prey model in biology:

$$\begin{aligned}\frac{d}{dt}P(t) &= \lambda\left(1-\frac{P(t)}{c}\right)P(t) - s\,P(t)\,Q(t)\\ \frac{d}{dt}Q(t) &= \mu\left(\frac{s\,P(t)}{n}-1\right)Q(t)\end{aligned}$$

Differential Equations of First and Second Order

- A system of differential equations of first order involves only first-order derivatives. It can be written in the form

$$\frac{d}{dt}u(t) \; = \; F(u(t), t)$$

and directly defines the actual rate of change in the variables.

- A second-order system of differential equations involves first and second-order derivatives and can be written in the form

$$\frac{d^2}{dt^2}u(t) \; = \; F\left(u(t), \frac{d}{dt}u(t), t\right).$$

Mechanical systems are often described by second-order differential equations (why?).

Differential Equations of First and Second Order

- Second-order systems can be transformed to first order by introducing (an) additional variable(s) $v(t) = \frac{d}{dt}u(t)$:

$$\begin{aligned}\frac{d}{dt}u(t) &= v(t) \\ \frac{d}{dt}v(t) &= F(u(t), v(t), t)\end{aligned}$$

- Systems of higher order than two hardly occur.

Initial Conditions

Each variable in a first-order system requires a given initial value at a time t_0.

Linear and Nonlinear Differential Equations

A differential equation (or a set of differential equations) is called linear if it satisfies the following conditions:

- If $u(t)$ and $\tilde{u}(t)$ are solutions, then their sum $u(t) + \tilde{u}(t)$ is also a solution.
- If $u(t)$ is a solution, then any multiple $\lambda u(t)$ is also a solution.

Most of the theory of differential equations refers to linear differential equations.

Analytical Solution of Differential Equations

Although this topic fills books and classes for engineers, only a small number of differential equations can be solved analytically, mainly:

Several linear problems ➔ exp, sin, cos, ...

Separable equations:

$$\frac{d}{dt}u(t) = F(u(t), t) \quad \text{with} \quad F(u(t), t) = f(u(t))\, g(t)$$

$$\Downarrow$$

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

$$\Downarrow$$

$$\int g(t)\, dt = \int \frac{\frac{d}{dt}u(t)}{f(u(t))}\, dt = \int \frac{1}{f(u)}\, du$$

Numerical Simulation

- Very few (systems of) differential equations can be solved analytically.
- Numerical simulation of a continuous evolution requires a discrete approximation.

The Finite-Difference Method

- An approximate solution is computed for only at given times t_1, t_2, t_3, ..., starting from the given initial state t_0.
- Computing the solution at the time t_{n+1} using the known solution at the time t_n is called a (forward) time step.
- In many cases, equidistant time steps of the same length δt are used, so that $t_1 = t_0 + \delta t$, $t_2 = t_1 + \delta t$, $t_3 = t_2 + \delta t$, ...

Difference Quotients

The time derivative must be approximated by a suitable difference quotient. The common difference quotients are:

Right-hand difference quotient:

$$\frac{d}{dt}u(t) \approx \frac{u(t+\delta t) - u(t)}{\delta t}$$

Left-hand difference quotient:

$$\frac{d}{dt}u(t) \approx \frac{u(t) - u(t-\delta t)}{\delta t}$$

Difference Quotients

Central (symmetric) difference quotient:

$$\frac{d}{dt}u(t) \approx \frac{u(t+\delta t) - u(t-\delta t)}{2\delta t}$$

or

$$\frac{d}{dt}u(t+\tfrac{\delta t}{2}) \approx \frac{u(t+\delta t) - u(t)}{\delta t}$$

The accuracy of all these approximations decreases with increasing timestep length δt.

The Explicit Euler Scheme

Inserting the finite-difference approximation with a right-hand difference quotient into the differential equation leads to

$$\frac{u(t+\delta t)-u(t)}{\delta t} \;\approx\; F(u(t),t),$$

$$\Downarrow$$

$$u(t+\delta t) \;\approx\; u(t)+\delta t\, F(u(t),t).$$

Interpretation:
$u(t)$ is known. From this, the rate of change $\frac{d}{dt}u(t)$ at the time t is computed, and this rate is assumed to persist up to the time $t+\delta t$.

The Fully Implicit Euler Scheme

Using a left-hand difference quotient leads to

$$\frac{u(t+\delta t)-u(t)}{\delta t} \;\approx\; F(u(t+\delta t), t+\delta t),$$

$$\Downarrow$$

$$u(t+\delta t) - \delta t\, F(u(t+\delta t), t+\delta t) \;\approx\; u(t).$$

Interpretation:
The rate of change at the end of the interval $t+\delta t$ is valid throughout the interval $[t, t+\delta t]$.

Problem:
$u(t+\delta t)$ and thus $F(u(t+\delta t), t+\delta t)$ is not known.

Examples of Explicit and Implicit Discretization

Radioactive decay:

Explicit:

$$u(t + \delta t) \approx u(t) + \delta t\,(-\lambda\, u(t))$$

Fully implicit:

$$u(t + \delta t) \approx u(t) + \delta t\,(-\lambda\, u(t + \delta t))$$

$$\Downarrow$$

$$u(t + \delta t) \approx \frac{u(t)}{1 + \delta t\,\lambda}$$

Examples of Explicit and Implicit Discretization

Logistic growth:

Explicit:

$$u(t+\delta t) \;\approx\; u(t) + \delta t\,\lambda \left(1 - \frac{u(t)}{c}\right) u(t)$$

Fully implicit:

$$u(t+\delta t) \;\approx\; u(t) + \delta t\,\lambda \left(1 - \frac{u(t+\delta t)}{c}\right) u(t+\delta t)$$

$$\Downarrow$$

$$u(t+\delta t) \;\approx\; -\frac{c\,(1-\delta t\lambda)}{2\delta t\lambda} \pm \sqrt{\left(\frac{c\,(1-\delta t\lambda)}{2\delta t\lambda}\right)^2 + \frac{c}{\delta t\lambda}\, u(t)}$$

Mixed Schemes

Explicit and implicit discretizations can also be combined, e. g., for logistic growth

$$u(t+\delta t) \;\approx\; u(t) + \delta t\,\lambda\left(1 - \frac{u(t)}{c}\right) u(t+\delta t)$$

$$\Downarrow$$

$$u(t+\delta t) \;\approx\; \frac{u(t)}{1 - \delta t\,\lambda\left(1 - \frac{u(t)}{c}\right)}$$

or

$$u(t+\delta t) \;\approx\; u(t) + \delta t\,\lambda\left(1 - \frac{u(t+\delta t)}{c}\right) u(t)$$

$$\Downarrow$$

$$u(t+\delta t) \;\approx\; \frac{(1+\delta t\,\lambda)\,u(t)}{1 + \frac{\delta t\,\lambda}{c}\,u(t)}$$

The Crank-Nicholson Scheme

Specific mixture of explicit and fully implicit Euler scheme:

$$\frac{u(t+\delta t) - u(t)}{\delta t} \;\approx\; \frac{F(u(t), t) + F(u(t+\delta t), t+\delta t)}{2},$$

so that

$$u(t+\delta t) - \frac{\delta t}{2} F(u(t+\delta t), t+\delta t) \;\approx\; u(t) + \frac{\delta t}{2} F(u(t), t).$$

Advantages of the Different Schemes

Explicit: simple

Fully implicit: often stable for large δt

Crank-Nicholson: high accuracy for $\delta t \to 0$; convergence of second order, i. e., error $\propto \delta t^2$ instead of δt

Explicit Schemes of Higher Order

An error $\propto \delta t^n$ with $n > 1$ can also be achieved by appropriate explicit schemes, e. g., by the 4th order Runge-Kutta scheme

$$u(t+\delta t) \approx u(t) + \delta t \frac{k_1 + 2k_2 + 2k_3 + k_4}{6}$$

with

$$\begin{aligned}
k_1 &= F(u(t), t) \quad \text{(like explicit Euler scheme)} \\
k_2 &= F(u(t) + \tfrac{\delta t}{2} k_1, t + \tfrac{\delta t}{2}) \\
k_3 &= F(u(t) + \tfrac{\delta t}{2} k_2, t + \tfrac{\delta t}{2}) \\
k_4 &= F(u(t) + \delta t k_3, t + \delta t)
\end{aligned}$$

Analytical Considerations

Motivation

Even if the equations cannot be solved analytically, several properties of the solution can often be obtained without numerical simulations.

Fixed Points

A fixed point is a solution which remains constant through time. The fixed points of a (system of) differential equation(s) are computed by solving

$$\frac{d}{dt}u(t) \;=\; F(u(t)) \;=\; 0.$$

Analytical Considerations

Stability of Fixed Points

A fixed point u_f is stable if the system approaches the fixed point if it is close to it. Stable fixed points are also called attractors.

For a single differential equation of first order: u_f is stable if

$$\begin{array}{rclcrcl} F(u) & > & 0 & \multirow{2}{*}{for} & u & < & u_f \\ F(u) & < & 0 & & u & > & u_f \end{array}$$

Alternative criterion:

$$\frac{d}{du}F(u)|_{u=u_f} \; < \; 0$$

Fixed Points and the Stability of the Fully Implicit Euler Scheme

A time step of the fully implicity Euler scheme cannot cross a stable fixed point.

Analytical Considerations

Nondimensional Variables

Idea: If the differential equation has a characteristic time t_c and / or a characteristic value u_c of the solution $u(t)$ (e. g., a fixed point), introduce nondimensional variables

$$\hat{t} = \frac{t}{t_c}$$

$$\hat{u}(\hat{t}) = \frac{u(t)}{u_c}$$

$$\Downarrow$$

$$\frac{d}{d\hat{t}}\hat{u}(\hat{t}) = \frac{t_c}{u_c}\frac{d}{dt}u(t)$$

Advantage: Each of the transforms reduces the number of model parameters by one.