Dynamic Process Models

Moritz Diehl

Overview

- Ordinary Differential Equations (ODE)
- Boundary Conditions, Objective
- Differential-Algebraic Equations (DAE)
- Multi Stage Processes
- Partial Differential Equations (PDE) and Method of Lines (MOL)

Dynamic Systems and Optimal Control

- "Optimal control" = **optimal choice of inputs for a dynamic system**

Dynamic Systems and Optimal Control

- "Optimal control" = **optimal choice of inputs for a dynamic system**
- What type of dynamic system?
  - Stochastic or deterministic?
  - Discrete or continuous time?
  - Discrete or continuous states?

Dynamic Systems and Optimal Control

- "Optimal control" $=$ **optimal choice of inputs for a dynamic system**
- What type of dynamic system?
  - Stochastic or deterministic?
  - Discrete or continuous time?
  - Discrete or continuous states?
- In this course, treat deterministic differential equation models (ODE/DAE/PDE)

(Some other dynamic system classes)

- Discrete time systems:

$$x_{k+1} = f(x_k, u_k), \quad k = 0, 1, \ldots$$

system states $x_k \in X$, control inputs $u_k \in U$. State and control sets X, U can be discrete or continuous.

- Games like chess: discrete time and state (chess figure positions), adverse player exists.
- Robust optimal control: like chess, but continuous time and state (adverse player exists in form of worst-case disturbances)
- Control of Markov chains: discrete time, system described by transition probabilities

$$P(x_{k+1}|x_k, u_k), \quad k = 0, 1, \ldots$$

- Stochastic Optimal Control of ODE: like Markov chain, but continuous time and state

Ordinary Differential Equations (ODE)

System dynamics can be manipulated by controls and parameters:

$$\boxed{\dot{x}(t) = f(t, x(t), u(t), p)}$$

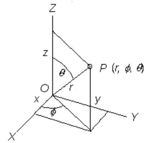
- simulation interval: $[t_0, t_{\mathrm{end}}]$
- time $t \in [t_0, t_{\mathrm{end}}]$
- state $x(t) \in \mathbb{R}^{n_x}$
- controls $u(t) \in \mathbb{R}^{n_u}$ $\longleftarrow$ manipulated
- design parameters $p \in \mathbb{R}^{n_p}$ $\longleftarrow$ manipulated

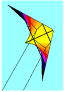
ODE Example: Dual Line Kite Model

- Kite position relative to pilot in spherical polar coordinates r, ϕ, θ. Line length r fixed.
- System states are $x = (\theta, \phi, \dot{\theta}, \dot{\phi})$.
- We can control roll angle $u = \psi$.
- Nonlinear dynamic equations:

$$
\begin{aligned}
\ddot{\theta} &= \frac{F_\theta(\theta, \phi, \dot{\theta}; \dot{\phi}, \psi)}{rm} + \sin(\theta)\cos(\theta)\dot{\phi}^2 \\
\ddot{\phi} &= \frac{F_\phi(\theta, \phi, \dot{\theta}; \dot{\phi}, \psi)}{rm\sin(\theta)} - 2\cot(\theta)\dot{\phi}\dot{\theta}
\end{aligned}
$$

- Summarize equations as $\dot{x} = f(x, u)$.





Initial Value Problems (IVP)

THEOREM [Picard 1890, Lindelöf 1894]:

Initial value problem in ODE

$$\dot{x}(t) = f(t, x(t), u(t), p), \quad t \in [t_0, t_{\mathrm{end}}],$$
$$\dot{x}(t_0) = x_0$$

- with given initial state x_0, design parameters p, and controls $u(t)$,
- and Lipschitz continuous $f(t, x, u(t), p)$

has **unique** solution

$$x(t), \quad t \in [t_0, t_{\mathrm{end}}]$$

NOTE: Existence but not uniqueness guaranteed if $f(t, x, u(t), p)$ only continuous [G. Peano, 1858-1932].
Non-uniqueness example: $\dot{x} = \sqrt{|x|}$

Boundary Conditions

Constraints on initial or intermediate values are important part of dynamic model.

STANDARD FORM:

$$\boxed{r(x(t_0), x(t_1), \ldots, x(t_{\mathrm{end}}), p) = 0, \quad r \in \mathbb{R}^{n_r}}$$

E.g. fixed or parameter dependent initial value x_0:

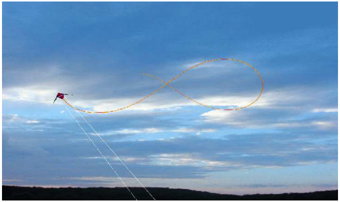
$$x(t_0) - x_0(p) = 0 \qquad (n_r = n_x)$$

or periodicity:

$$x(t_0) - x(t_{\mathrm{end}}) = 0 \qquad (n_r = n_x)$$

NOTE: Initial values $x(t_0)$ need not always be fixed!

Kite Example: Periodic Solution Desired



- Formulate periodicity as constraint.
- Leave $x(0)$ free.
- Minimize integrated power per cycle

$$\min_{x(\cdot),u(\cdot)} \int_0^T L(x(t), u(t))dt$$

subject to

$$x(0) - x(T) = 0$$
$$\dot{x}(t) - f(x(t), u(t)) = 0, \; t \in [0, T].$$

Objective Function Types

Typically, distinguish between

- *Lagrange term* (cost integral, e.g. integrated deviation):

$$\int_0^T L(t, x(t), u(t), p)dt$$

- *Mayer term* (at end of horizon, e.g. maximum amount of product):

$$E(T, x(T), p)$$

- Combination of both is called *Bolza objective*.

Differential-Algebraic Equations (DAE) - Semi-Explicit

Augment ODE by **algebraic equations** g and **algebraic states** z

$$\boxed{\begin{aligned} \dot{x}(t) &= f(t, x(t), z(t), u(t), p) \\ 0 &= g(t, x(t), z(t), u(t), p) \end{aligned}}$$

- differential states $x(t) \in \mathbb{R}^{n_x}$
- algebraic states $z(t) \in \mathbb{R}^{n_z}$
- algebraic equations $g(\cdot) \in \mathbb{R}^{n_z}$

Standard case: index one $\Leftrightarrow$ matrix $\frac{\partial g}{\partial z} \in \mathbb{R}^{n_z \times n_z}$ invertible.

Existence and uniqueness of initial value problems similar as for ODE.

Tutorial DAE Example

Regard $x \in \mathbb{R}$ and $z \in \mathbb{R}$, described by the DAE

$$\begin{aligned} \dot{x}(t) &= x(t) + z(t) \\ 0 &= \exp(z) - x \end{aligned}$$

- Here, one could easily eliminate $z(t)$ by $z = \log x$, to get the ODE

$$\dot{x}(t) = x(t) + \log(x(t))$$

Tutorial DAE Example

Regard $x \in \mathbb{R}$ and $z \in \mathbb{R}$, described by the DAE

$$\begin{aligned} \dot{x}(t) &= x(t) + z(t) \\ 0 &= \exp(z) - x + z \end{aligned}$$

- Now, z cannot be eliminated as easily as before, but still, the DAE is well defined because $\frac{\partial g}{\partial z}(x, z) = \exp(z) + 1$ is always positive and thus invertible.

(Fully Implicit DAE)

A fully implicit DAE is just a set of equations:

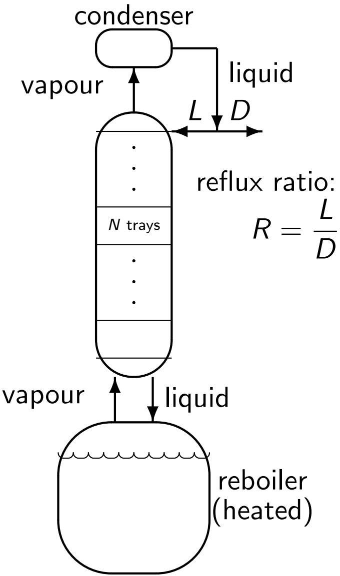
$$\boxed{0 \quad = \quad f(t, x(t), \dot{x}(t), z(t), u(t), p)}$$

- derivative of differential states $\dot{x}(t) \in \mathbb{R}^{n_x}$
- algebraic states $z(t) \in \mathbb{R}^{n_z}$

Standard case: fully implicit DAE of index one $\Leftrightarrow$ matrix $\frac{\partial f}{\partial(\dot{x}, z)} \in \mathbb{R}^{(n_x+n_z)\times(n_x+n_z)}$ invertible.

Again, existence and uniqueness similar as for ODE.

DAE Example: Batch Distillation



- concentrations $X_{k,\ell}$ as differential states x
- tray temperatures T_ℓ as algebraic states z
- T_ℓ implicitly determined by algebraic equations

$$1 - \sum_{k=1}^{3} K_k(T_\ell)\, X_{k,\ell} = 0, \quad \ell = 0, 1, \ldots, N$$

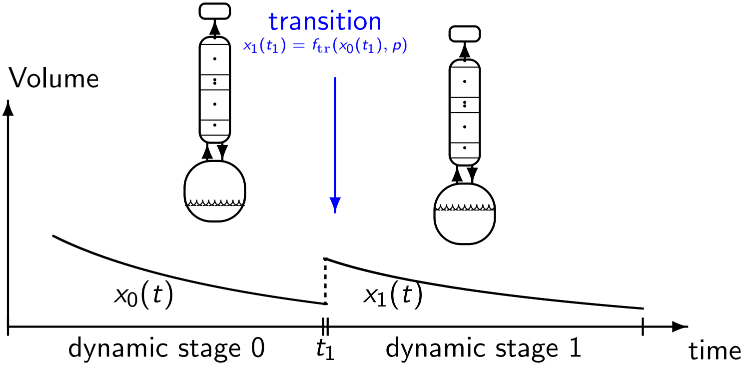
with

$$K_k(T_\ell) = \exp\left(-\frac{a_k}{b_k + c_k T_\ell}\right)$$

- reflux ratio R as control u

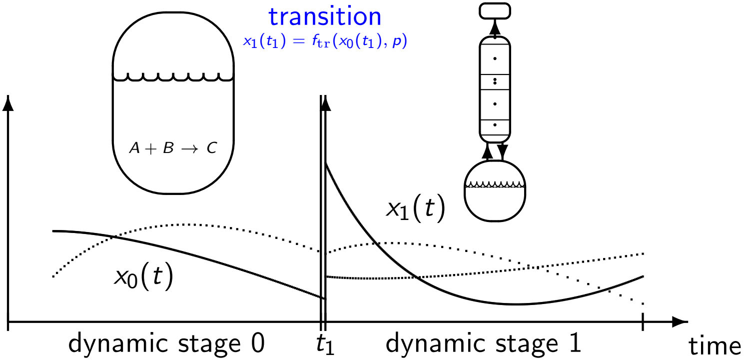
Multi Stage Processes

Two dynamic stages can be connected by a discontinuous "transition". **E.g. Intermediate Fill Up in Batch Distillation**



Multi Stage Processes II

Also **different** dynamic systems can be coupled. **E.g. batch reactor followed by distillation (different state dimensions)**



Partial Differential Equations

- Instationary partial differential equations (PDE) arise e.g in transport processes, wave propagation, ...
- Also called "distributed parameter systems"
- Often PDE of subsystems are coupled with each other (e.g. flow connections)
- Method of Lines (MOL): discretize PDE in space to yield ODE or DAE system.
- Often MOL can be interpreted in terms of compartment models.

Summary

Dynamic models for optimal control consist of

- differential equations (ODE/DAE/PDE)
- boundary conditions, e.g. initial/final values, periodicity
- objective in Lagrange and/or Mayer form
- transition stages in case of multi stage processes

PDE often transformed into DAE by Method of Lines (MOL)

DAE standard form:

$$\boxed{\begin{array}{rcl} \dot{x}(t) & = & f(t, x(t), z(t), u(t), p) \\ 0 & = & g(t, x(t), z(t), u(t), p) \end{array}}$$

References

- K.E. Brenan, S.L. Campbell, and L.R. Petzold: The Numerical Solution of Initial Value Problems in Differential-Algebraic Equations, SIAM Classics Series, 1996.
- U.M. Ascher and L.R. Petzold: Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations. SIAM, 1998.