

CHEM-E7225
2024

Dynamical
models

Continuous-time
Discrete-time

Numerical
simulations



Aalto University

Dynamical models and numerical simulations

CHEM-E7225 (was E7195), 2024

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Chemical and Metallurgical Engineering
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Dynamical models

Dynamical models and numerical simulations

Dynamical models

We focus on deterministic differential equation models of dynamical systems, in time

- All numerical simulation methods executed on a computer discretise time

We highlight some relevant properties of continuous-time systems

- How to convert them to discrete-time systems

Continuous-time systems are often described by ordinary differential equations (ODE)

- ↪ Other common forms of ODEs (delayed ODE)
- ↪ Differential-algebraic equations (DAE)
- ↪ Partial differential equations (PDE)

Continuous-time models (cont.)

We describe controlled dynamical systems in continuous-time with a first-order ODE

$$\dot{x}(t) = f(t, x(t), u(t)|\theta_x)$$

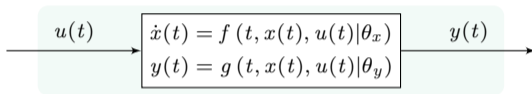
$$\rightsquigarrow x(t) \in \mathcal{R}^{N_x}$$

$$\rightsquigarrow u(t) \in \mathcal{R}^{N_u}$$

$$\rightsquigarrow \theta_x \in \mathcal{R}^{N_{\theta_x}}$$

$$\rightsquigarrow t \in \mathcal{R}$$

Nonlinear time-varying systems



$$\rightsquigarrow y(t) \in \mathcal{R}^{N_y}$$

$$\rightsquigarrow \theta_y \in \mathcal{R}^{N_{\theta_y}}$$

Function f is a general map from time t , state $x(t)$, controls $u(t)$ and parameters θ_x

- $f : [0, T] \times \mathcal{R}^{N_x} \times \mathcal{R}^{N_u} \mapsto \mathcal{R}^{N_x}$, to the rate of change of the state
- Because t is an explicit argument, function f is time-varying

$$\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \vdots \\ \dot{x}_{N_x}(t) \end{bmatrix} = \begin{bmatrix} f_1(x_1(t), x_2(t), \dots, x_{N_x}(t), u_1(t), u_2(t), \dots, u_{N_u}(t), t|\theta_x) \\ f_2(x_1(t), x_2(t), \dots, x_{N_x}(t), u_1(t), u_2(t), \dots, u_{N_u}(t), t|\theta_x) \\ \vdots \\ f_{N_x}(x_1(t), x_2(t), \dots, x_{N_x}(t), u_1(t), u_2(t), \dots, u_{N_u}(t), t|\theta_x) \end{bmatrix}$$

Continuous-time models (cont.)

$$\underbrace{\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \vdots \\ \dot{x}_{N_x}(t) \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} f_1(x_1(t), x_2(t), \dots, x_{N_x}(t), u_1(t), u_2(t), \dots, u_{N_u}(t), t | \theta_x) \\ f_2(x_1(t), x_2(t), \dots, x_{N_x}(t), u_1(t), u_2(t), \dots, u_{N_u}(t), t | \theta_x) \\ \vdots \\ f_{N_x}(x_1(t), x_2(t), \dots, x_{N_x}(t), u_1(t), u_2(t), \dots, u_{N_u}(t), t | \theta_x) \end{bmatrix}}_{f(x(t), u(t), t | \theta_x)}$$

We are interested in the conditions under which the differential equation has a solution

- Given a fixed initial value $x(0)$ for the state, and controls $u(t)$ with $t \in [0, T]$

The dependence of f on the the controls $u(t)$ is equivalent to another time-dependence

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t), t | \theta_x) \\ &:= \bar{f}(x(t), t | \bar{\theta}_x) \end{aligned}$$

A time-varying uncontrolled (autonomous, or time-homogeneous) differential equation

Continuous-time models (cont.)

$$\dot{x}(t) = f(x(t), t | \bar{\theta}_x)$$

An **initial value problem (IVP)** consists of a differential equation (ODE) and a restriction

- At $t = 0$, we constrain $x(t)$ to be some fixed value $x(0) = x_0$

A solution to the initial value problem on the open interval $[0, t)$ that contains the origin $t = 0$ is the differentiable function $x(\cdot)$ with $x(0) = x_0$ and $\dot{x}(t) = \bar{f}(x(t), t | \bar{\theta}_x)$

The solution to the IVP is equivalent to the solution to an integral equation,

$$x(t) = x_0 + \int_0^t f(x(\tau), \tau | \bar{\theta}_x) d\tau$$

Continuous-time models (cont.)

For notational simplicity, we leave away the dependence of function f on controls $u(t)$

- We can keep them fixed in time, together with the other parameters θ_x
- (The initial condition, $x(t=0) = x_0$, is also fixed)

Then, we have the uncontrolled dynamical system

$$\begin{aligned}\dot{x}(t) &= f(t, x(t)|\theta_x), \quad t \in [0, T] \\ x(0) &= x_0\end{aligned}$$

The solution,

$$x(t) = x_0 + \int_0^t f(x(\tau), \tau|\theta_x) d\tau$$

Existence and uniqueness of the solution to the IVP are implied by the properties of f

- Existence is guaranteed by the continuity of f with respect to $x(t)$ and t
- For continuous-time systems, existence is not a granted property

Continuous-time models (cont.)

Theorem

Existence and uniqueness

Let $f : [t_{\text{ini}}, t_{\text{fin}}] \times \mathcal{R}^{N_x} \rightarrow \mathcal{R}^{N_x}$ be some continuous function in $x(t)$ and t

Consider the initial value problem with initial value

$$\begin{aligned}\dot{x}(t) &= f(t, x(t)|\theta_x), \quad t \in [t_{\text{ini}}, t_{\text{fin}}] \\ x(t_{\text{ini}}) &= x_0\end{aligned}$$

The IVP has a solution $x : [t_{\text{ini}}, t_{\text{fin}}] \rightarrow \mathcal{R}^{N_x}$ and that solution is the unique solution to the IVP problem if and only if function f is Lipschitz continuous with respect to $x(t)$

That is, there exists a constant value $L \in (0, \infty)$ such that for any pair $(x(t), x'(t))$,

$$\|f(x(t), t|\theta_x) - f(x'(t), t|\theta_x)\| \leq L\|x(t) - x'(t)\|, \quad \forall t \in [t_{\text{ini}}, t_{\text{fin}}]$$

Or, equivalently, for any pair $(x(t), x'(t))$

$$\frac{\|f(x(t), t|\theta_x) - f(x'(t), t|\theta_x)\|}{\|x(t) - x'(t)\|} \leq L, \quad \forall t \in [t_{\text{ini}}, t_{\text{fin}}]$$

Continuous-time models (cont.)

$$\frac{\|f(x(t), t|\theta_x) - f(x'(t), t|\theta_x)\|}{\|x(t) - x'(t)\|} \leq L, \quad \forall t \in [t_{\text{ini}}, t_{\text{fin}}], x(t) \in \mathcal{R}^{N_x}, x'(t) \in \mathcal{R}^x$$

Lipschitz continuity of f with respect to $x(t)$ is a property that is difficult to determine

- It is difficult to determine a global (over the time-interval) Lipschitz constant L

A simpler property to be verified is the differentiability of f with respect to $x(t)$

Because every function f which is differentiable with respect to $x(t)$ is locally Lipschitz continuous, we define the condition for local existence and uniqueness of the solution

Continuous-time models (cont.)

Theorem

Local existence and uniqueness

Let $f : [t_{\text{ini}}, t_{\text{fin}}] \times \mathcal{R}^{N_x} \rightarrow \mathcal{R}^{N_x}$ be some continuous function in $x(t)$ and t

Consider the initial value problem with initial value

$$\begin{aligned}\dot{x}(t) &= f(t, x(t) | \theta_x), \quad t \in [t_{\text{ini}}, t_{\text{fin}}] \\ x(t_{\text{ini}}) &= x_0\end{aligned}$$

If f is continuously differentiable with respect to $x(t)$ for all $t \in [t_{\text{ini}}, t'_{\text{fin}}]$, there exists a non-empty interval $[t_{\text{ini}}, t'_{\text{fin}}]$ with $t'_{\text{fin}} \in (t_{\text{ini}}, t_{\text{fin}}]$ where the IVP has a unique solution

Continuous-time models (cont.)

Example

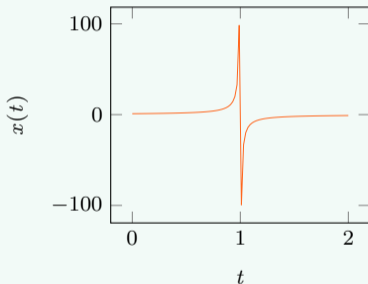
Consider the initial value problem

$$\begin{aligned}\dot{x}(t) &= x^2(t), \quad t \in [0, 2] \\ x(0) &= 1\end{aligned}$$

The explicit closed-form solution

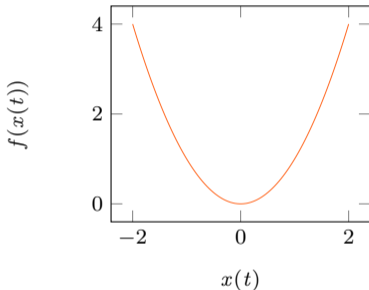
$$x(t) = \frac{1}{1-t}$$

$x(t)$ is only defined for $t \in [0, 1)$



Over the shorter interval $[0, T']$ with $T' < 1$, the solution exists and it is also unique

Continuous-time models (cont.)



Function $f(x(t)) = x^2(t)$ is not a globally Lipschitz continuous function

$$\frac{\|f(x^{\clubsuit}(t)) - f(x^{\spadesuit}(t))\|}{\|x^{\clubsuit}(t) - x^{\spadesuit}(t)\|} \not\leq L$$

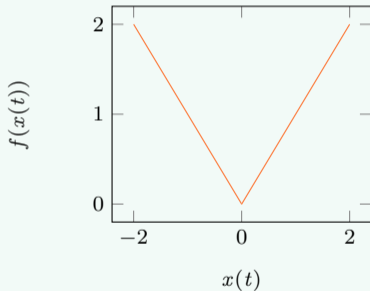
There is no single L that satisfies the inequality for all pairs $(x^{\clubsuit}(t), x^{\spadesuit}(t))$

Function $x^2(t)$ is continuously differentiable with respect to $x(t)$, thus locally Lipschitz



Continuous-time models (cont.)

Example



Is function $f(x(t)) = |x(t)|$ a globally Lipschitz continuous function?

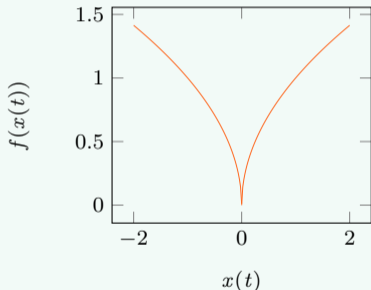
$$\frac{\|f(x_{\clubsuit}(t)) - f(x_{\spadesuit}(t))\|}{\|x_{\clubsuit}(t) - x_{\spadesuit}(t)\|} \leq L \quad (?)$$

If not, is it at least locally Lipschitz?



Continuous-time models (cont.)

Example



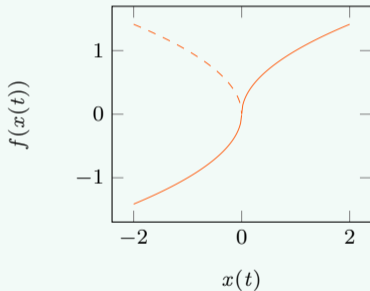
Is function $f(x(t)) = |x(t)|^{1/2}$
globally Lipschitz continuous?

$$\frac{\|f(x_{\clubsuit}(t)) - f(x_{\spadesuit}(t))\|}{\|x_{\clubsuit}(t) - x_{\spadesuit}(t)\|} \leq L \quad (?)$$

If not, is it at least locally Lipschitz?



Example



Is function $f(x(t)) = \text{sign}(x)|x|^{1/2}$ globally Lipschitz continuous?

$$\frac{\|f(x_{\clubsuit}(t)) - f(x_{\spadesuit}(t))\|}{\|x_{\clubsuit}(t) - x_{\spadesuit}(t)\|} \leq L \quad (?)$$

If not, is it at least locally Lipschitz?



Continuous-time models (cont.)

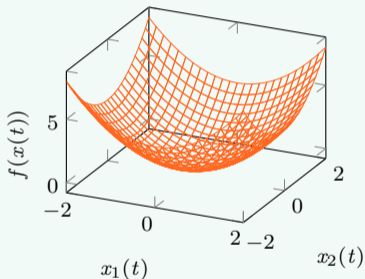
Dynamical
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Example



Is $f(x(t)) = \|x(t)\|_2^2$ a globally Lipschitz continuous function?

$$\frac{\|f(x^\clubsuit(t)) - f(x^\spadesuit(t))\|}{\|x^\clubsuit(t) - x^\spadesuit(t)\|} \leq L \quad (?)$$

If not, is it at least locally Lipschitz?



Continuous-time models (cont.)

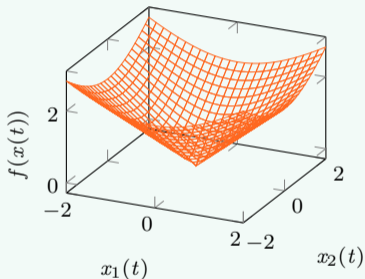
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Example



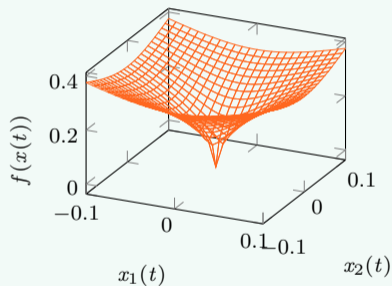
Is $f(x(t)) = \|x(t)\|_2$ a globally Lipschitz continuous function?

$$\frac{\|f(x^\clubsuit(t)) - f(x^\spadesuit(t))\|}{\|x^\clubsuit(t) - x^\spadesuit(t)\|} \leq L \quad (?)$$

If not, is it at least locally Lipschitz?



Example



Is $f(x(t)) = \|x(t)\|_2^{1/2}$ a globally Lipschitz continuous function?

$$\frac{\|f(x^\clubsuit(t)) - f(x^\spadesuit(t))\|}{\|x^\clubsuit(t) - x^\spadesuit(t)\|} \leq L \quad (?)$$

If not, is it at least locally Lipschitz?



Continuous-time models (cont.)

Conditions for global and local existence, and uniqueness of the solution of an IVP are extended to systems with finitely many discontinuities of function f with respect to t

- The solution must be defined separately on each of the continuous subintervals
- At the discontinuity time-points, the derivative is not (strongly) defined

Continuity of the state trajectory is used to enforce the transition between subintervals

- (The end-state of one interval need be the initial state for the next one)

Continuous-time models (cont.)

Steady-state (stationary, equilibrium, or fixed) points

- Values of x (fixed θ_x and u) such that $f(x(t)|\theta_x) = 0$

$$\begin{aligned}\frac{dx(t)}{dt} &= f(x(t)|\theta_x) \\ &= 0\end{aligned}$$

Stability

Consider the time evolution of a (set of) variable(s) of a system starting at steady-state

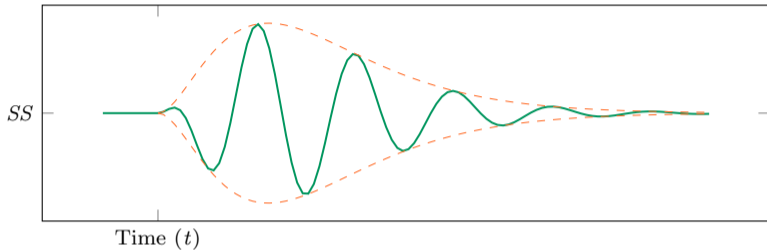
- At some point in time, the system is perturbed, some change occurs
- ↪ The system will respond to the perturbation, move away from SS

A *system is stable* if its variable(s) return autonomously to their steady-state value(s)

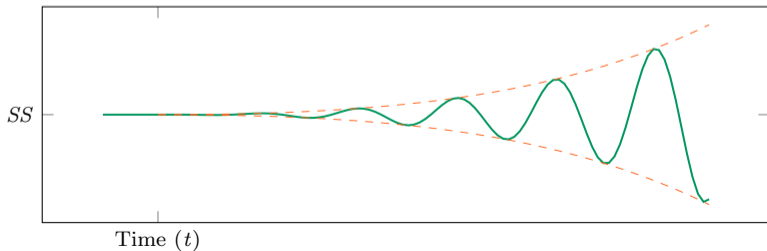
- ↪ A *stable system* is also said to be a self-regulating process
- A stable system would not need a controller, in general
- (If the steady-state condition is the desired state)
- (And, if we have an infinite amount of time)

Continuous-time models (cont.)

Stable



Unstable



Continuous-time models | LTIs

Dynamical
models

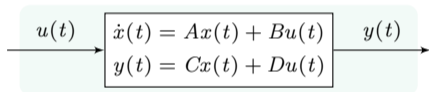
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A very important class of dynamical system are linear time-invariant systems, or LTIs

Linear time-invariant systems, LTI



$$\rightsquigarrow t \in \mathcal{R}$$

$$\rightsquigarrow x(t) \in \mathcal{R}^{N_x}$$

$$\rightsquigarrow u(t) \in \mathcal{R}^{N_u}$$

$$\rightsquigarrow A \in \mathcal{R}^{N_x \times N_x}$$

$$\rightsquigarrow B \in \mathcal{R}^{N_x \times N_u}$$

$$\rightsquigarrow \{A, B\} = \theta_x \in \mathcal{R}^{(N_x \times N_x) + (N_x \times N_u)}$$

$$\rightsquigarrow y(t) \in \mathcal{R}^{N_y}$$

$$\rightsquigarrow C \in \mathcal{R}^{N_y \times N_x}$$

$$\rightsquigarrow D \in \mathcal{R}^{N_y \times N_u}$$

$$\rightsquigarrow \{C, D\} = \theta_y \in \mathcal{R}^{(N_y \times N_x) + (N_y \times N_u)}$$

Linear time-invariant systems $f = Ax + Bu$ are Lipschitz continuous with respect to x

- The global Lipschitz constant $L = \|A\|$

Continuous-time models | LTIs (cont.)

The solution to the analysis, for $t \geq t_{\text{ini}}$, an initial state $x(t_{\text{ini}})$ and an input $u(t \geq t_{\text{ini}})$

$$x(t) = e^{A(t-t_{\text{ini}})}x(t_{\text{ini}}) + \int_{t_{\text{ini}}}^t e^{A(t-\tau)}Bu(\tau)d\tau$$
$$y(t) = \underbrace{Ce^{A(t-t_{\text{ini}})}x(t_{\text{ini}}) + C \int_{t_{\text{ini}}}^t e^{A(t-\tau)}Bu(\tau)d\tau}_{Cx(t)} + Du(t)$$

The solution is known as the **Lagrange formula**

↪ Based on the **state transition matrix**, e^{At}

Continuous-time models | LTIs (cont.)

Definition

Controllability of linear time-invariant systems

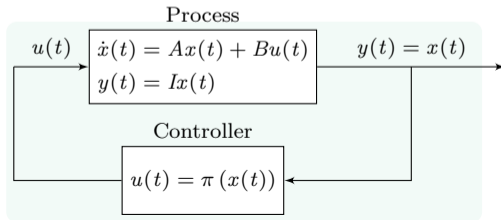
Consider a linear and time-invariant system (A, B) , with $x(t) \in \mathcal{R}^{N_x}$ and $u(t) \in \mathcal{R}^{N_u}$

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

The system is said to be **controllable**, if and only if it is possible to transfer the state of the system from any initial value $x_0 = x(0)$ to any other final value $x_f = x(t_f)$

- ..., only by manipulating the input $u(t)$
- ..., in some finite time $t_f \geq 0$

The final state x_f is called the **zero-state** or the **target-state**



Continuous-time models | LTIs (cont.)

Definition

Controllability gramian

Consider the linear and time-invariant system (A, B) , with $x(t) \in \mathcal{R}^{N_x}$ and $u(t) \in \mathcal{R}^{N_u}$

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

The system's **controllability gramian** is a $(N_x \times N_x)$ matrix, real and symmetric

$$W_c(t) = \int_0^t e^{A\tau} BB^T e^{A^T \tau} d\tau$$

Theorem

Controllability test (I)

Consider the linear and time-invariant system (A, B) , with $x(t) \in \mathcal{R}^{N_x}$ and $u(t) \in \mathcal{R}^{N_u}$

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

Let $W_c(t) = \int_0^t e^{A\tau} BB^T e^{A^T \tau} d\tau$ be the controllability gramian of the system

- The system is controllable iff $W_c(t)$ is non-singular, for all $t > 0$

State feedback (cont.)

Theorem

Controllability matrix and controllability test (II)

Consider a linear and time-invariant system (A, B) , with $x(t) \in \mathcal{R}^{N_x}$ and $u(t) \in \mathcal{R}^{N_u}$

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

We define the $(N_x \times (N_u \times N_x))$ **controllability matrix**

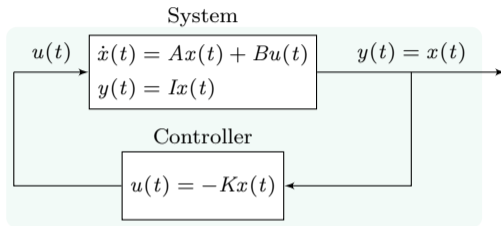
$$\mathcal{C} = [B \quad | \quad AB \quad | \quad A^2B \quad | \quad \dots \quad | \quad A^{N_x-1}B]$$

Necessary and sufficient condition for controllability

$$\text{rank}(\mathcal{C}) = N_x$$

State feedback (cont.)

We have system $\dot{x}(t) = Ax(t) + Bu(t)$, we can perfectly measure its state $x(t) = y(t)$



We design controllers that define an optimal control action $u(t)$, given the state $x(t)$

$$\rightsquigarrow u(t) = -Kx(t)$$

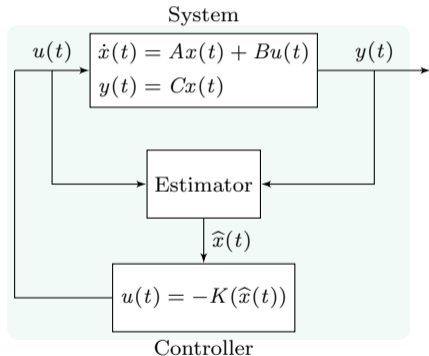
Linear-quadratic regulators (LQR) are model-based controllers

$$K = (B'Q_fB + R)^{-1} B'Q_fA$$

State estimation (cont.)

When we cannot measure the state, $x(t) \neq y(t)$, we design a device capable to estimate it from measurable quantities (data) and knowledge about the dynamics (a model)

The device that approximates the system's state is a **state observer**, or **estimator**



Were the state estimate $\hat{x}(t)$ accurate, we could use it with the optimal controller $(-K)$

Continuous-time models | LTIs (cont.)

Definition

Observability of linear-time-invariant systems

Consider a linear and time-invariant system (A, C) with $x(t) \in \mathcal{R}^{N_x}$ and $u(t) \in \mathcal{R}^{N_y}$

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

$$y(t) = Cx(t)$$

The system is said to be **observable** if and only if it is possible to determine its state $x(t)$ from the force-free response of its measurements over a finite time ($t_f < \infty$)

- ..., from any arbitrary initial state $x(t_0)$

Definition

Observability gramian

Consider the linear and time-invariant system (A, C) , with $x(t) \in \mathcal{R}^{N_x}$ and $y(t) \in \mathcal{R}^{N_y}$

$$\begin{cases} \dot{x}(t) = Ax(t) \\ y(t) = Cx(t) \end{cases}$$

The system's **observability gramian** is a $(N_x \times N_x)$ matrix, real and symmetric

$$W_o(t) = \int_0^t e^{A^T \tau} C^T C e^{A \tau} d\tau$$

Continuous-time models | LTIs (cont.)

Theorem

Observability test (I)

Consider the linear and time-invariant system (A, C) , with $x(t) \in \mathcal{R}^{N_x}$ and $y(t) \in \mathcal{R}^{N_y}$

$$\begin{cases} \dot{x}(t) = Ax(t) \\ y(t) = Cx(t) \end{cases}$$

Let $W_o(t) = \int_0^t e^{A^T \tau} C^T C e^{A \tau} d\tau$ be the observability gramian of the system

- The system is observable iff $W_o(t)$ is non-singular, for all $t > 0$

Continuous-time models | LTIs (cont.)

Proof (Sufficient condition)

From the second Lagrange equation, we have the force-free evolution of the output

$$y(\tau) = Ce^{A\tau}x(0)$$

We left-multiply the equation by $e^{A^T\tau}$, then we integrate between 0 and some t_f

$$\begin{aligned}\int_0^{t_f} e^{A^T\tau}y(\tau)d\tau &= \int_0^{t_f} e^{A^T\tau}Ce^{A\tau}x(0)d\tau \\ &= W_o(t_f)x(0)\end{aligned}$$

Thus, we have

$$x(0) = W_o^{-1}(t_f) \int_0^{t_f} e^{A^T\tau}Cy(\tau)d\tau$$

The initial state is given as a function of the inverse of the observability gramian $W_o(t_f)$ and the integral $\int_0^{t_f} e^{A^T\tau}Ce^{A\tau}y(\tau)d\tau$ which can be computed from measurements $y(\tau)$

- The observability gramian need be non-singular for the inverse to exist



Continuous-time models | LTIs (cont.)

Theorem

Observability matrix and observability test (II)

Consider a linear and time-invariant system (A, C) , with $x(t) \in \mathcal{R}^{N_x}$ and $y(t) \in \mathcal{R}^{N_y}$

$$\begin{cases} \dot{x}(t) = Ax(t) \\ y(t) = Cx(t) \end{cases}$$

We define the $(N_x \times (N_y \times N_x))$ **observability matrix**

$$\mathcal{O} = \begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^{N_x-1} \end{bmatrix}$$

Necessary and sufficient condition for observability,

$$\text{rank}(\mathcal{O}) = N_x$$

Definition

Luenberger observer

Consider a linear and time-invariant system, $x(t) \in \mathcal{R}^{N_x}$, $u(t) \in \mathcal{R}^{N_u}$, and $y(t) \in \mathcal{R}^{N_y}$

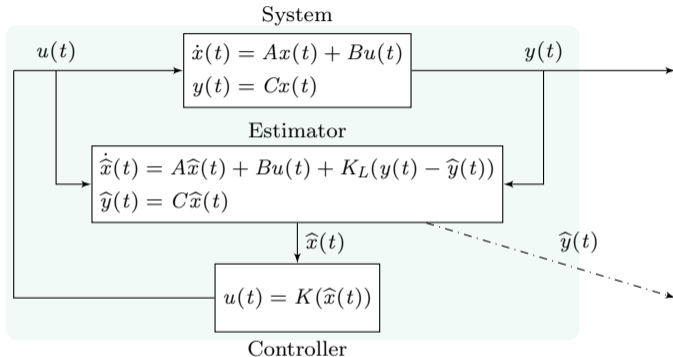
$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ y(t) = Cx(t) \end{cases},$$

The linear and time-invariant dynamical system

$$\begin{cases} \dot{\hat{x}}(t) = A\hat{x}(t) + Bu(t) + K_L(y(t) - \hat{y}(t)) \\ \hat{y}(t) = C\hat{x}(t) \end{cases},$$

with $\hat{x} \in \mathcal{R}^{N_x}$, $\hat{y}(t) \in \mathcal{R}^{N_y}$ is a Luenberger observer of the system iff $K_L \in \mathcal{R}^{N_x \times N_y}$ is any matrix such that the eigenvalues of matrix $A - K_L C$ all have a negative real part

Continuous-time models | LTIs (cont.)



Luenberger observers are asymptotic state observers that are also model-based

- Kalman filters are stochastic counterpart, linear-quadratic estimators

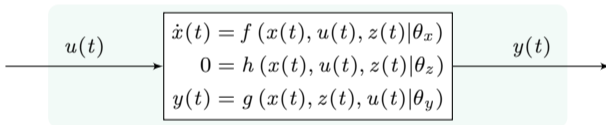


Continuous-time models | DAEs

A class of system models combine differential states $x(t)$ and algebraic states $z(t)$

- The derivative of function $z(t)$ is not expressed explicitly in the model
- $z(t)$ is determined implicitly by an algebraic (set of) equation(s), h

(Time-invariant) Differential algebraic systems, DAE



$$\rightsquigarrow x(t) \in \mathcal{R}^{N_x}$$

$$\rightsquigarrow u(t) \in \mathcal{R}^{N_u}$$

$$\rightsquigarrow z(t) \in \mathcal{R}^{N_z}$$

$$\rightsquigarrow \theta_x \in \mathcal{R}^{N_{\theta_x}}$$

$$\rightsquigarrow \theta_z \in \mathcal{R}^{N_{\theta_z}}$$

$$\rightsquigarrow t \in \mathcal{R}$$

$$\rightsquigarrow y(t) \in \mathcal{R}^{N_y}$$

$$\rightsquigarrow \theta_y \in \mathcal{R}^{N_{\theta_y}}$$

The algebraic equations cannot be solved independently of the differential equations

Continuous-time models | DAE (cont.)

$$\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \vdots \\ \dot{x}_{N_x}(t) \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} f_1(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_x) \\ f_2(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_x) \\ \vdots \\ f_{N_x}(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_x) \\ h_1(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_z) \\ h_2(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_z) \\ \vdots \\ h_{N_z}(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_z) \end{bmatrix}$$

Uniqueness of a numerical solution requires non-singularity of the Jacobian of h wrt z

$$\det \left(\frac{\partial h(x(t), u(t), z(t))}{\partial z} \right) \neq 0$$

These specific differential algebraic equations are known as index-one DAE

Continuous-time models | DAE (cont.)

Function $h : \mathcal{R}^{N_x} \times \mathcal{R}^{N_u} \times \mathcal{R}^{N_z} \rightarrow \mathcal{R}^{N_z}$,

$$h(x(t), u(t), z(t) | \theta_x) =$$

$$\begin{bmatrix} h_1(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_z) \\ h_2(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_z) \\ \vdots \\ h_{N_z}(x_1(t), \dots, x_{N_x}(t), u_1(t), \dots, u_{N_u}(t), z_1(t), \dots, z_{N_z}(t) | \theta_z) \end{bmatrix}$$

The Jacobian of h with respect to the algebraic state variables z

$$\frac{\partial h(x(t), u(t), z(t))}{\partial z} = \underbrace{\begin{bmatrix} [\partial h_1(x, u, z) / \partial z_1 \quad \cdots \quad \partial h_1(x, u, z) / \partial z_{n_z} \quad \cdots \quad \partial h_1(x, u, z) / \partial z_{N_z}] \\ [\partial h_2(x, u, z) / \partial z_1 \quad \cdots \quad \partial h_2(x, u, z) / \partial z_{n_z} \quad \cdots \quad \partial h_2(x, u, z) / \partial z_{N_z}] \\ \vdots \\ [\partial h_{n_z}(x, u, z) / \partial z_1 \quad \cdots \quad \partial h_{n_z}(x, u, z) / \partial z_{n_z} \quad \cdots \quad \partial h_{n_z}(x, u, z) / \partial z_{N_z}] \\ \vdots \\ [\partial h_{N_z}(x, u, z) / \partial z_1 \quad \cdots \quad \partial h_{N_z}(x, u, z) / \partial z_{n_z} \quad \cdots \quad \partial h_{N_z}(x, u, z) / \partial z_{N_z}] \end{bmatrix}}_{N_z \times N_z} (t)$$

Continuous-time models | DAE (cont.)

Any index-one differential-algebraic equation can be differentiated with respect to time

- This allows for a practical numerical solution using ODE integrators

Because we have that $h(x(t), z(t)) = 0$, we also have

$$\frac{dh(x(t), z(t))}{dt} = 0$$

For the total derivative of the algebraic equations, we have

$$\begin{aligned} \frac{dh(x(t), z(t))}{dt} &= \frac{\partial h(x(t), z(t))}{\partial z} \underbrace{\frac{dz(t)}{dt}}_{\dot{z}(t)} + \frac{\partial h(x(t), z(t))}{\partial x} \underbrace{\frac{dx(t)}{dt}}_{f(x(t), z(t))} \\ &= 0 \end{aligned}$$

Using the non-singularity of the Jacobian with respect to z , we have

$$\dot{z}(t) = - \underbrace{\left(\frac{\partial h(x(t), z(t))}{\partial z} \right)^{-1}}_{\text{Jacobian inverse}} \frac{\partial h(x(t), z(t))}{\partial x} f(x(t), z(t))$$



Continuous-time models (cont.)

$$\dot{x}(t) = f(x(t)|\bar{\theta}_x)$$

An **initial value problem (IVP)** consists of a differential equation (ODE) and a restriction

- At $t = 0$, we constrain $x(t)$ to be some fixed value $x(0) = x_0$

A differential model describes the microscopic (in time) behaviour of process $(x(t))_{t \geq 0}$

Let us consider the motion of the state over an certain time interval such that $t \in [0, \Delta t]$

$$x(\Delta t) = x_0 + \int_0^{\Delta t} f(x(t)) dt$$

Consider a tiny time interval Δt , then $f(x(t))$ is approximately constant over $[0, \Delta t]$

$$\begin{aligned} x(\Delta t) &= x_0 + \int_0^{\Delta t} f(x(t)) dt \\ &\approx x_0 + f(x(0)) \int_0^{\Delta t} dt \\ &= x_0 + f(x_0) [t]_0^{\Delta t} \\ &= x_0 + f(x_0) \Delta t \end{aligned}$$

Continuous-time models (cont.)

More generally, the discretisation of infinitesimal dynamics over intervals $[t, t + \Delta t]$

$$\begin{aligned}x(t + \Delta t) &= x(t) + \int_t^{t+\Delta t} f(x(\tau)) d\tau \\ &\approx x(t) + f(x(t)) \Delta t\end{aligned}$$

Equivalently, we have

$$\underbrace{x(t + \Delta t) - x(t)}_{\Delta x(t)} \approx f(x(t)) \Delta t$$

Continuous-time models (cont.)

$$x(t + \Delta t) \approx x(t) + f(x(t)) \Delta t$$

To approximate the evolution of process $(x(t))_{t=0}^T$, we divide the interval in K pieces

- For simplicity, we would typically let the size of each piece be $\Delta t = \frac{T - 0}{K}$
- We apply the discretisation scheme on each piece, from x_0 at $t = 0$

$$x(0\Delta t) = x_0$$

$$x(1\Delta t) = x(0) + f(x(0)) \Delta t$$

$$x(2\Delta t) = x(1\Delta t) + f(x(1\Delta t)) \Delta t$$

$$\dots = \dots$$

$$x(k\Delta t) = x((k-1)\Delta t) + f(x((k-1)\Delta t)) \Delta t$$

$$\dots = \dots$$

$$x(\underbrace{(K-1)\Delta t}_{T-\Delta t}) = x(\underbrace{(K-2)\Delta t}_{T-2\Delta t}) + f\left(x(\underbrace{(K-2)\Delta t}_{T-2\Delta t})\right) \Delta t$$

$$x(\underbrace{K\Delta t}_T) = x(\underbrace{(K-1)\Delta t}_{T-\Delta t}) + f\left(x(\underbrace{(K-1)\Delta t}_{T-\Delta t})\right) \Delta t$$

Continuous-time models (cont.)

$$x(t) = x_0 + \int_0^t f(x(\tau), u(\tau)) d\tau$$

Consider a tiny time interval Δt , then $f(x(t), u(t))$ is approximately constant in $[0, \Delta t]$

$$\begin{aligned} x(\Delta t) &= x_0 + \int_0^{\Delta t} f(x(t), u(t)) dt \\ &\approx x_0 + f(x(0), u(0)) \int_0^{\Delta t} dt \\ &= x_0 + f(x_0, u_0) \Delta t \end{aligned}$$

The discretisation of infinitesimal dynamics over intervals $[t, t + \Delta t]$

$$\begin{aligned} x(t + \Delta t) &= x(t) + \int_t^{t+\Delta t} f(x(\tau), u(\tau)) d\tau \\ &\approx x(t) + f(x(t), u(t)) \Delta t \end{aligned}$$

After we divide the interval in K pieces, the approximation of the evolution of $(x(t))_{t=0}^T$

$$x(k\Delta t) = x((k-1)\Delta t) + f(x((k-1)\Delta t), u((k-1)\Delta t)) \Delta t \quad (k = 1, \dots, K)$$



Continuous-time models (cont.)

The inputs are generated by a computer and implemented as piecewise constant signals

Zero-order hold controls

That is, the input $u(t)$ is kept constant between two equally spaced times, t_k and t_{k+1}

- We define the times when the control is applied as **sampling times**
- We let the sampling times be $\{t_k = k\Delta t\}_{k=0}^K$
- Δt denotes the (common) duration

The sampling interval Δt need not be the same one we used for approximating $(x(t))$

$$\{x(t_k = k\Delta t)\}_{k=0}^K$$

Zero-order holding is the operation of keeping a signal constant for $t \in [t_k, t_{k+1})$

Continuous-time models (cont.)

Dynamical
models

Continuous-time

Discrete-time

Numerical
simulations

Suppose that $\dot{x}(t) = f(x(t), u(t)|\theta_x)$ is differentiable and that the inputs are piecewise constant with fixed values $u(t) = u_k$ with $u_k \in \mathcal{R}^{N_u}$ over each interval, for $t \in [t_k, t_{k+1})$

We can treat the transition from state $x(t_k)$ to $x(t_{k+1})$ as a discrete-time system

- The time in which the system evolves takes values only on a time grid

$$0 \cdots t_1 \cdots t_2 \cdots \cdots t_{k-1} \cdots \underbrace{t_k \cdots t_{k+1}}_{\Delta t} \cdots \cdots t_{K-1} \cdots t_K$$

In each interval $(t_k, t_{k+1}]$, the solution to the individual IVP exists and it is unique

- With initial value $x(t_k) = x_{\text{init}}$

Continuous-time models (cont.)

We consider the initial value problem, $x(0) = x_{\text{ini}}$ and constant control $u(t) = u_{\text{const}}$

$$\begin{aligned}\dot{x}(t) &= f(x(t), u_{\text{const}} | \theta_x), \quad t \in [0, \Delta t] \\ x(0) &= x_{\text{ini}}\end{aligned}$$

The unique solution $x : [0, \Delta t] \mapsto \mathcal{R}^{N_x}$ to the IVP with x_{init} and u_{const} is a function

The solution is the state trajectory over the short interval $[0, \Delta t]$

$$x(t \mid x_{\text{ini}}, u_{\text{const}}; \theta_x), \quad t \in [0, \Delta t]$$

The map from pair $(x_{\text{init}}, u_{\text{const}})$ to process $(x(t))_0^{\Delta t}$ is denoted as the **solution map**

- The arguments are: 1) the initial state x_{ini} and 2) the constant control u_{const}

The final value $x(t = \Delta t | x_{\text{init}}, u_{\text{const}}, \theta_x)$ of this short trajectory is important

- $x(\Delta t)$ defines the initial state of the next initial value problem

$$\begin{aligned}\dot{x}(t) &= f(x(t), u_{\text{const}} | \theta_x), \quad t \in [\Delta t, 2\Delta t] \\ x(\Delta t) &= x_{\text{ini}}\end{aligned}$$

Continuous-time models (cont.)

We define the **transition function** which returns that final value $x(\Delta t|x_{\text{ini}}, u_{\text{const}}; \theta_x)$

$$f_{\Delta t} : \mathcal{R}^{N_x} \times \mathcal{R}^{N_u} \rightarrow \mathcal{R}^{N_x}$$

The transition function returns the state $x(\Delta t|x_{\text{ini}}, u_{\text{const}}; \theta_x)$, given x_{ini} and u_{const}

$$x(\Delta t|x_{\text{ini}}, u_{\text{const}}; \theta_x) = f_{\Delta t}(x_{\text{ini}}, u_{\text{const}}|\theta_x)$$

$f_{\Delta t}$ is used to define a discrete-time system whose evolution describes the state at $\{t_k\}$

$$x(t_{k+1}) = f_{\Delta t}(x(t_k), u_k|\theta_x) \quad (k = 0, 1, \dots, K)$$

When we discuss general dynamical system, we will often refer to discrete-time systems

- The transition function $f_{\Delta t}$ may be only available implicitly
- (Often, we will define it as a computer routine/function)

Continuous-time models (cont.)

Dynamical
models

Continuous-time

Discrete-time

Numerical
simulations

For linear and time-invariant dynamical systems $\dot{x}(t) = Ax(t) + Bu(t)$ with $x(0) = x_{\text{init}}$ and constant input u_{const} , the solution map $x(t|x_{\text{ini}}, u_{\text{ini}}, \theta_x)$ is explicitly known

$$\begin{aligned}x(t|x_{\text{ini}}, u_{\text{ini}}, \theta_x) &= e^{At} x_{\text{ini}} + \int_0^t e^{A(t-\tau)} Bu_{\text{const}} d\tau \\ &= e^{At} x_{\text{ini}} + \left(\int_0^t e^{A(t-\tau)} d\tau \right) Bu_{\text{const}}\end{aligned}$$

The corresponding discrete-time system with sampling time Δt is linear time-invariant

$$x(t_{k+1}) = \underbrace{A_{\Delta t} x(t_k) + B_{\Delta t} u_k}_{f_{\Delta t}(x(t_k), u_k | \theta_x)}, \quad (k = 0, 1, \dots, K-1)$$

$$\rightsquigarrow A_{\Delta t} = e^{A\Delta t} \text{ and } B_{\Delta t} = \left(\int_0^{\Delta t} e^{A(\Delta t-\tau)} d\tau \right) B$$

Since Δt is fixed, also $A_{\Delta t}$ and $B_{\Delta t}$ are fixed (their elements are not function of time)

- LTI continuous-time system (A, B) maps to LTI discrete-time system $(A_{\Delta t}, B_{\Delta t})$



Discrete-time models

Dynamical
models

Continuous-time

Discrete-time

Numerical
simulations

We describe a controlled dynamical system in discrete-time with a difference equation

$$x_{k+1} = f_k(x_k, u_k | \theta_x), \quad k \in \mathcal{N}_{0 \rightsquigarrow K-1}$$

- ↪ $K + 1$ state vectors, $x_0, x_1, \dots, x_k, \dots, x_K \in \mathcal{R}^{N_x}$
- ↪ K input vectors, $u_0, u_1, \dots, u_k, \dots, u_{K-1} \in \mathcal{R}^{N_u}$
- ↪ Some time-horizon of length K
- ↪ Parameter vector $\theta_x \in \mathcal{R}^{N_{\theta_x}}$
- ↪ (Time-varying dynamics)

Given the initial state x_0 and all the controls u_0, u_1, \dots, u_{K-1} , we could recursively call the functions $f_k(x_k, u_k | \theta_x)$ and sequentially obtain all the other states x_1, x_2, \dots, x_K

- This recursion is known as **forward simulation** of the system dynamics

Discrete-time models (cont.)

Definition

Forward simulation

The forward simulation of the system dynamics is formally defined as a function

- The argument are x_0 and the collection u_0, u_1, \dots, u_{K-1}
- The image is the collection x_0, x_1, \dots, x_K

That is, we have

$$\begin{aligned} f_{\text{sim}} : \mathcal{R}^{N_x + (K \times N_u)} &\rightarrow \mathcal{R}^{(K+1)N_x} \\ &: (x_0, u_0, u_1, \dots, u_{K-1}) \mapsto (x_0, x_1, \dots, x_K) \end{aligned}$$

Function f_{sim} is defined by the recursive solution of the problem

$$x_{k+1} = f_k(x_k, u_k | \theta_x) \quad (\text{for all } k \in \mathcal{N}_{0 \rightsquigarrow K-1})$$

Discrete-time models | LTI

Dynamical
models

Continuous-time

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Numerical
simulations

Linear time-invariant systems, LTI

$$x_{k+1} = Ax_k + Bu_k, \quad k \in \mathcal{N}_{0 \rightsquigarrow K-1}$$

- $x_0, x_1, \dots, x_{-K}, \dots, x_K \in \mathcal{R}^{N_x}$
- $u_0, u_1, \dots, u_k, \dots, u_{K-1} \in \mathcal{R}^{N_u}$
- $A \in \mathcal{R}^{N_x \times N_x}$
- $B \in \mathcal{R}^{N_x \times N_u}$
- $\{A, B\} = \theta_x \in \mathcal{R}^{(N_x \times N_x) + (N_x \times N_u)}$

The forward simulation map of linear time-invariant systems with horizon of length K

$$\begin{aligned}
 f_{\text{sim}}(x_0, u_0, \dots, u_{K-1}) &= \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_K \end{bmatrix} \\
 &= \begin{bmatrix} x_0 \\ Ax_0 + Bu_0 \\ A^2x_0 + ABu_0 + Bu_1 \\ \vdots \\ A^Kx_0 + \sum_{k=0}^{K-1} A^{K-1-k} Bu_k \end{bmatrix}
 \end{aligned}$$

Dynamical
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simulations

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_K \end{bmatrix} = \begin{bmatrix} x_0 \\ Ax_0 + Bu_0 \\ A^2x_0 + ABu_0 + Bu_1 \\ \vdots \\ \underbrace{A^K x_0 + \sum_{k=0}^{K-1} A^{K-1-k} Bu_k}_{f_{\text{sim}}(x_0, u_0, \dots, u_{K-1})} \end{bmatrix}$$

Consider the terminal value x_K after K steps from x_0 and subjected to $u_0 \rightsquigarrow u_{K-1}$,

$$x_K = A^K x_0 + \underbrace{\begin{bmatrix} A^{K-1}B & A^{K-2}B & \dots & B \end{bmatrix}}_{C_K} \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{K-1} \end{bmatrix}$$

Matrix C_K is the discrete-time controllability matrix of the linear time-invariant system

- The discrete-time version, because based on the pair (A, B)

Affine time-varying systems are an important generalisation of the plain LTI model

Affine time-varying systems

$$x_{k+1} = A_k x_k + B_k u_k + c_k, \quad k \in \mathcal{N}_{0 \rightsquigarrow K-1}$$

- $x_0, x_1, \dots, x_k, \dots, x_K \in \mathcal{R}^{N_x}$
- $u_0, u_1, \dots, u_k, \dots, u_{K-1} \in \mathcal{R}^{N_u}$
- $A_0, A_1, \dots, A_k, \dots, A_K \in \mathcal{R}^{N_x \times N_x}$
- $B_0, B_1, \dots, B_k, \dots, B_K \in \mathcal{R}^{N_x \times N_u}$
- $\{A_k, B_k\} = \theta_x \in \mathcal{R}^{(N_x \times N_x) + (N_x \times N_u)}$

Affine time-varying systems arise from trajectory linearisations of nonlinear models

$$x_{k+1} = f_k(x_k, u_k | \theta_x)$$

- Linearisation of nonlinear (and time-varying) dynamics around point (\bar{x}_k, \bar{u}_k)
- We assume the that point (\bar{x}_k, \bar{u}_k) is a term in a trajectory $\{(x_k, u_k)\}$
- (For example, $\{\bar{x}_0, \bar{x}_1, \dots, \bar{x}_K\}$ and $\{\bar{u}_0, \bar{u}_1, \dots, \bar{u}_{K-1}\}$)

$$\dot{x}(t) = f_f(x(t), u(t)|\theta_x)$$

In continuous-time, we would approximate (nonlinear and time-varying) dynamics f^t with a first-order Taylor's expansion around the point $(\bar{x}(t), \bar{u}(t))$ along the trajectory

After defining the deviation variables $x'(t) = x(t) - \bar{x}(t)$ and $u'(t) = u(t) - \bar{u}(t)$,

$$\underbrace{\begin{bmatrix} x'_1(t) \\ \vdots \\ x'_{N_x}(t) \end{bmatrix}}_{x'(t)} = \underbrace{\begin{bmatrix} \frac{\partial f_1^t}{\partial x_1} & \cdots & \frac{\partial f_1^t}{\partial x_{N_x}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_{N_x}^t}{\partial x_1} & \cdots & \frac{\partial f_{N_x}^t}{\partial x_{N_x}} \end{bmatrix}}_{A^t}(\bar{x}(t), \bar{u}(t)) \underbrace{\begin{bmatrix} x'_1(t) \\ \vdots \\ x'_{N_x}(t) \end{bmatrix}}_{x'(t)} + \underbrace{\begin{bmatrix} \frac{\partial f_1^t}{\partial u_1} & \cdots & \frac{\partial f_1^t}{\partial u_{N_u}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_{N_x}^t}{\partial u_1} & \cdots & \frac{\partial f_{N_x}^t}{\partial u_{N_u}} \end{bmatrix}}_{B^t}(\bar{x}(t), \bar{u}(t)) \underbrace{\begin{bmatrix} u'_1(t) \\ \vdots \\ u'_{N_u}(t) \end{bmatrix}}_{u'(t)} + \underbrace{\begin{bmatrix} f_1^t \\ f_2^t \\ \vdots \\ f_{N_x}^t \end{bmatrix}}_{c^t}(\bar{x}(t), \bar{u}(t))$$

- A^t is the Jacobian of f^t with respect to x , at $(\bar{x}(t), \bar{u}(t))$
- B^t is the Jacobian of f^t with respect to u , at $(\bar{x}(t), \bar{u}(t))$
- c^t is f^t evaluated at $(\bar{x}(t), \bar{u}(t))$

The affine continuous-time approximation expressed in terms of deviation variables,

$$\underbrace{\begin{bmatrix} x'_1(t) \\ \vdots \\ x'_{N_x}(t) \end{bmatrix}}_{\dot{x}'(t)} = \underbrace{\begin{bmatrix} a_{1,1}^t & \cdots & a_{1,N_x}^t \\ \vdots & \ddots & \vdots \\ a_{N_x,1}^t & \cdots & a_{N_x,N_x}^t \end{bmatrix}}_{(N_x \times N_x)} \underbrace{\begin{bmatrix} x'_1(t) \\ \vdots \\ x'_{N_x}(t) \end{bmatrix}}_{(N_x \times 1)} + \underbrace{\begin{bmatrix} b_{1,1}^t & \cdots & b_{1,N_u}^t \\ \vdots & \ddots & \vdots \\ b_{N_x,1}^t & \cdots & b_{N_x,N_u}^t \end{bmatrix}}_{(N_x \times N_u)} \underbrace{\begin{bmatrix} u'_1(t) \\ \vdots \\ u'_{N_u}(t) \end{bmatrix}}_{(N_u \times 1)} \\
 + \underbrace{\begin{bmatrix} c_1^t \\ c_2^t \\ \vdots \\ c_{N_x}^t \end{bmatrix}}_{N_x \times 1}$$

Discrete-time models | Affine (cont.)

$$x_{k+1} = f_k(x_k, u_k | \theta)$$

Similarly, we can approximate nonlinear and time-varying dynamics in discrete-time

We have the affine time-varying system,

$$\underbrace{x_{k+1} - \bar{x}_{k+1}}_{x'_{k+1}} = f_k(x_k, u_k) - \bar{x}_{k+1}$$

$$\approx \underbrace{\frac{\partial f}{\partial x} \Big|_{(\bar{x}_k, \bar{u}_k)}}_{A_k \in \mathcal{R}^{N_x \times N_x}} \underbrace{(x_k - \bar{x}_k)}_{x'_k} + \underbrace{\frac{\partial f}{\partial u} \Big|_{(\bar{x}_k, \bar{u}_k)}}_{B_k \in \mathcal{R}^{N_x \times N_u}} \underbrace{(u_k - \bar{u}_k)}_{u'_k} + \underbrace{f_k(\bar{x}_k, \bar{u}_k) - \bar{x}_{k+1}}_{c_k \in \mathcal{R}^{N_x \times 1}}$$

The forward simulation map of affine time-varying systems, for a horizon of length K

$$x_K = (A_{K-1} \cdots A_0) x_0 + \sum_{k=0}^{K-1} \left(\prod_{j=k+1}^{K-1} A_j \right) (B_k u_k + c_k)$$

Dynamical
models

Continuous-time

Discrete-time

Numerical
simulations

Numerical simulations

Dynamical models and numerical simulations

Numerical simulations

Dynamical
models

Continuous-time

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Numerical
simulations

The design/deployment of optimal controllers depends on the availability of efficient/accurate numerical simulation tools that build discretisations of continuous dynamics

We know that the IVP $\dot{x}(t) = f(x(t), u(t)|\theta_x)$ with $x(0) = x_0$ has a unique solution when f is Lipschitz continuous with respect to $x(t)$ and continuous with respect to t

↪ A solution exists on the interval $[0, T]$, even if time $T > 0$ is arbitrary small

Numerical simulation methods compute approximate solutions to some well-posed IVP

- (Well-posedness is in the sense of the existence/uniqueness theorem)
-

For practical reasons, numerical simulation methods can be categorised in two groups

- Single-step methods and multi-step methods

Typically, each group is then divided into two main subgroups

- Explicit methods and implicit methods

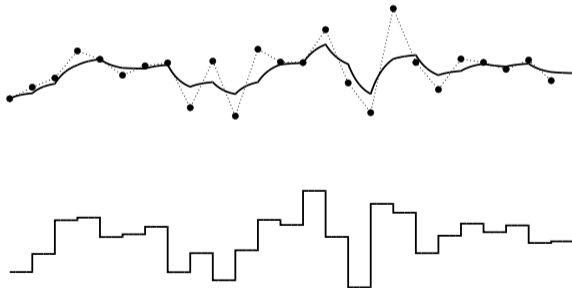
Numerical simulations (cont.)

The idea of a numerical simulation method is to compute an approximation to a solution map $x(t|x_{\text{ini}}, u_{\text{const}}; \theta_x)$ for $t \in [0, T]$, the computation is known as an **integrator**

↪ Remember, the function from pair $(x_{\text{ini}}, u_{\text{const}})$ to process $\{x(t)\}_0^T$

An intuitive way to compute an approximation for $x(t|x_{\text{init}}, u_{\text{const}}; \theta_x)$ when $t \in [0, T]$

- Perform a linear extrapolation, based on the time derivative of $x(t)$
- From the initial point x_{init} , under constant controls u_{const}
- (The time-derivative is the $\dot{x}(t) = f(x(t), u(t)|\theta_x)$)



The approach is an explicit Euler integration step, a good approximation if T is tiny

$$\begin{aligned}x(t|x_{\text{init}}, u_{\text{const}}; \theta_x) &\approx \underbrace{x(0|x_{\text{init}}, u_{\text{const}}; \theta_x)}_{x_{\text{ini}}} + \underbrace{f(x_{\text{init}}, u_{\text{const}}|\theta_x)(t-0)}_{tf(x_{\text{init}}, u_{\text{const}}|\theta_x)} \quad t \in [0, T] \\ &= \widehat{x}(t|x_{\text{ini}}, u_{\text{const}}; \theta_x)\end{aligned}$$

The error of the explicit Euler integration step is of order T^2 , it grows as T^2 grows

- Or informally, the approximation error is small if T is very small
- The error is directly related to the truncation in the expansion

Numerical simulations | Explicit Euler (cont.)

The practical implementation of the explicit **explicit Euler integration method**

We consider a now longer interval with $t \in [0, T]$ and we divide it in K subintervals

$$0 \cdots 1 \cdots 2 \cdots \cdots (k-1) \cdots \underbrace{k \cdots (k+1)}_{\Delta t} \cdots \cdots (K-1) \cdots K$$

- Typically, we set each subinterval to have the same time-length

$$\Delta t = \frac{T}{K}$$

- We denote the K time points $\{t_k\}$ as nodes in the time grid

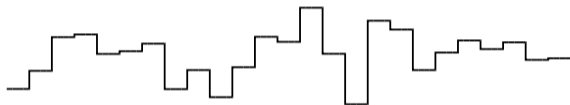
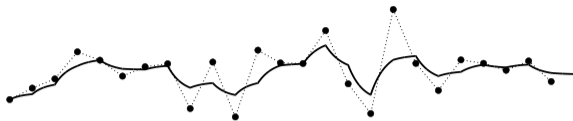
Starting from $\hat{x}_0 = x_{\text{init}}$, we then perform K sequential linear extrapolation steps

$$\hat{x}_{k+1} = \hat{x}_k + f(\hat{x}_k, u_{\text{const}} | \theta_x) \Delta t, \quad k = 0, 1, \dots, K-1$$

For notational simplicity, we set the indexing for k to start from zero

- This allows us to start the sequence with $\hat{x}_0 = x_{\text{ini}}$

Numerical simulations | Explicit Euler (cont.)



Sequentially, the individual integration steps

↪ $k = 0$

$$\hat{x}_1 = \hat{x}_0 + f(\hat{x}_0, u_{\text{const}} | \theta_x) \Delta t$$

↪ $k = 1$

$$\hat{x}_2 = \hat{x}_1 + f(\hat{x}_1, u_{\text{const}} | \theta_x) \Delta t$$

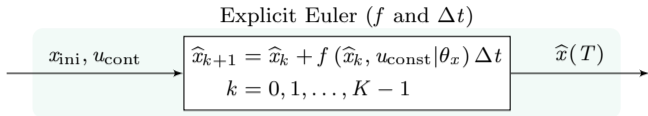
↪ ...

...

↪ $k = K - 1$

$$\hat{x}_K = \hat{x}_{K-1} + f(\hat{x}_{K-1}, u_{\text{const}} | \theta_x) \Delta t$$

Numerical simulations | Explicit Euler (cont.)



To compute the approximation \hat{x}_{k+1} at node $k + 1$, an explicit Euler integration only requires information related to node k , specifically the numerical approximation \hat{x}_k

- (The method is presented assuming that the dynamics are time-invariant)

The local (at k) approximation error gets smaller with the ‘length’ of the subintervals

- Using smaller (more) subintervals would lead to more accurate approximations

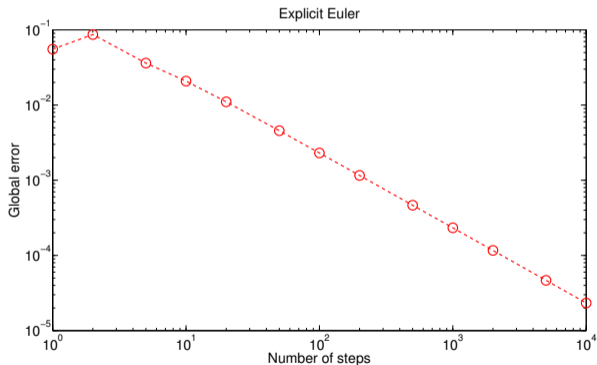
The Euler method is stable as the propagation of local errors is bounded by a constant

$$\underbrace{\|\hat{x}(T|x_{\text{init}}, u_{\text{const}}, \theta_x) - x(T|x_{\text{init}}, u_{\text{const}}, \theta_x)\|}_{\text{Accumulated approximation error}}$$

Numerical simulations | Explicit Euler (cont.)

The consistency error of each subinterval is of order $(\Delta t)^2$ and there are $\frac{T}{\Delta t}$ subintervals

- The global, accumulated, error at the final time has order $(\Delta t)^2 \frac{T}{\Delta t} = T \Delta t$



The error function is linear in the number of function evaluations, slope equal to one

Numerical simulations | Explicit Euler (cont.)

This would suggest running integration procedures with many small-sized subintervals

↪ The scheme requires the evaluation of function $f(x_{\text{ini}}, u_{\text{const}} | \theta_x)$ at each step

↪ Good approximations with many steps require many function evaluations

(Other methods can achieve the desired accuracy levels with lower computational cost)



Numerical simulations | Explicit Runge-Kutta

The **order-4 Runge-Kutta integration method, RK4** generates a sequence of values \hat{x}_k , by evaluating (and storing) function f four times for each node k , from $\hat{x}_0 = x_{\text{init}}$

From approximation \hat{x}_k and with constant input u_{const} , at each node k we have

$$\begin{aligned}\kappa_1 &= f(\hat{x}_k, u_{\text{const}}|\theta_x) \\ \kappa_2 &= f\left(\hat{x}_k + \frac{\Delta t}{2}\kappa_1, u_{\text{const}}|\theta_x\right) \\ \kappa_3 &= f\left(\hat{x}_k + \frac{\Delta t}{2}\kappa_2, u_{\text{const}}|\theta_x\right) \\ \kappa_4 &= f(\hat{x}_k + \Delta t\kappa_3, u_{\text{const}}|\theta_x)\end{aligned}$$

Each function evaluation is explicit and performed around the approximation point \hat{x}_k

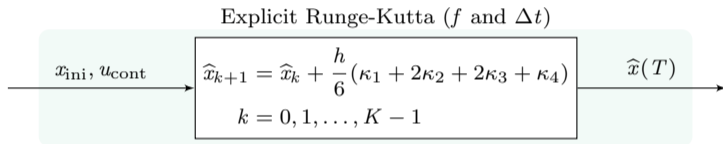
- The evaluations are stored as $\kappa_i \in \mathcal{R}^{N_x}$, $i \in \{1, 2, 3, 4\}$

The evaluations are then combined to construct the next approximation \hat{x}_{k+1} point

$$\hat{x}_{k+1} = \hat{x}_k + \frac{h}{6}(\kappa_1 + 2\kappa_2 + 2\kappa_3 + \kappa_4), \quad k = 0, 1, \dots, K - 1$$

Numerical simulations | Explicit Runge-Kutta (cont.)

The solution map obtained by using an explicit Runge-Kutta method of order-4, RK4



It can be understood as a continuous and differentiable nonlinear function

- The maximum order of differentiability depends on function f

Numerical simulations | Explicit Runge-Kutta (cont.)

Dynamical
models

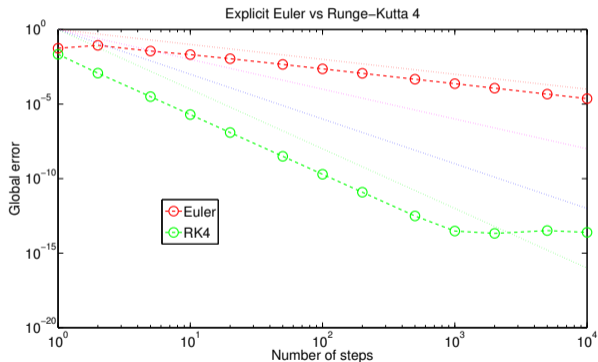
Continuous-time

Discrete-time

Numerical
simulations

One step of the RK4 method is as expensive as four Euler steps, though more accurate

- The accumulated approximation error has order $T(\Delta t)^4$



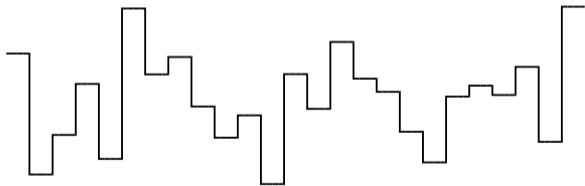
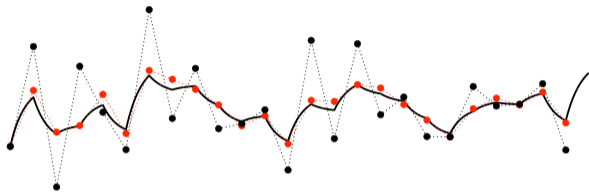
Numerical simulations | Explicit Runge-Kutta (cont.)

Dynamical
models

Continuous-time

Discrete-time

Numerical
simulations



Numerical simulations (cont.)

Summarising, consider a numerical simulation scheme over some time interval $[t_0, t_f]$

- The subintervals have a length $\Delta t = (t_0 - t_f)/K$

$$t_0 \cdots t_1 \cdots t_2 \cdots \cdots t_{k-1} \cdots \underbrace{t_k \cdots t_{k+1}}_{\Delta t} \cdots \cdots t_{K-1} \cdots t_K$$

- The nodes are indexed as $k = 0, 1, \dots, K$
- The position of the nodes

$$t_k := t_0 + k\Delta t, \quad k = 0, 1, \dots, K$$

The solution is approximated at nodes t_k by the values

$$\hat{x}_k \approx x(t_k | x(t_0), u_{\text{const}}; \theta_x) \quad (k = 0, 1, \dots, K)$$

Convergence

We define the order- p convergence of a method as worst-case local approximation error

$$\max_{k=0, \dots, K} \|\hat{x}_k - x(t_k)\| = \mathcal{O}((\Delta t)^p)$$

As $K \rightarrow \infty$, we expect that \hat{x}_k gets closer to $x(t_k)$