# Dynamical models and numerical simulations CHEM-E7225 (was E7195), 2024 

Francesco Corona ( $\neg-\neg$ )
Chemical and Metallurgical Engineering
School of Chemical Engineering

# Dynamical models 

Dynamical models and numerical simulations

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 continuos-time systems

- How to convert them to discrete-time systems

Continuous-time systems are often described by ordinary differential equations (ODE)
$\rightsquigarrow$ Other common forms of ODEs (delayed ODE)
$\rightsquigarrow$ Differential-algebraic equations (DAE)
$\rightsquigarrow$ Partial differential equations (PDE)

## Continuous-time models (cont.)

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

$$
\dot{x}(t)=f\left(t, x(t), u(t) \mid \theta_{x}\right)
$$

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

Nonlinear time-varying systems

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

$$
\rightsquigarrow \theta_{x} \in \mathcal{R}^{N_{\theta_{x}}}
$$


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

Function $f$ is a general map from time $t$, state $x(t)$, controls $u(t)$ and parameters $\theta_{x}$ - $f:[0, T] \times \mathcal{R}^{N_{x}} \times \mathcal{R}^{N_{u}} \mapsto \mathcal{R}^{N_{x}}$, to the rate of change of the state

- Because $t$ is an explicit argument, function $f$ is time-varying

$$
\left[\begin{array}{c}
\dot{x_{1}}(t) \\
\dot{x_{2}}(t) \\
\vdots \\
\dot{x_{N_{x}}}(t)
\end{array}\right]=\left[\begin{array}{c}
f_{1}\left(x_{1}(t), x_{2}(t), \ldots, x_{N_{x}}(t), u_{1}(t), u_{2}(t), \ldots, u_{N_{u}}(t), t \mid \theta_{x}\right) \\
f_{2}\left(x_{1}(t), x_{2}(t), \ldots, x_{N_{x}}(t), u_{1}(t), u_{2}(t), \ldots, u_{N_{u}}(t), t \mid \theta_{x}\right) \\
\vdots \\
f_{N_{x}}\left(x_{1}(t), x_{2}(t), \ldots, x_{N_{x}}(t), u_{1}(t), u_{2}(t), \ldots, u_{N_{u}}(t), t \mid \theta_{x}\right)
\end{array}\right]
$$

$$
\underbrace{\left[\begin{array}{c}
\dot{x_{1}}(t) \\
\dot{x_{2}}(t) \\
\vdots \\
x_{N_{x}}(t)
\end{array}\right]}_{\dot{x}(t)}=\underbrace{\left[\begin{array}{c}
f_{1}\left(x_{1}(t), x_{2}(t), \ldots, x_{N_{x}}(t), u_{1}(t), u_{2}(t), \ldots, u_{N_{u}}(t), t \mid \theta_{x}\right) \\
f_{2}\left(x_{1}(t), x_{2}(t), \ldots, x_{N_{x}}(t), u_{1}(t), u_{2}(t), \ldots, u_{N_{u}}(t), t \mid \theta_{x}\right) \\
\vdots \\
f_{N_{x}}\left(x_{1}(t), x_{2}(t), \ldots, x_{N_{x}}(t), u_{1}(t), u_{2}(t), \ldots, u_{N_{u}}(t), t \mid \theta_{x}\right)
\end{array}\right]}_{f\left(x(t), u(t), t \mid \theta_{x}\right)}
$$

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

$$
\begin{aligned}
\dot{x}(t) & =f\left(x(t), u(t), t \mid \theta_{x}\right) \\
& :=\bar{f}\left(x(t), t \mid \bar{\theta}_{x}\right)
\end{aligned}
$$

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

Continuous-time models (cont.)

$$
\dot{x}(t)=f\left(x(t), t \mid \bar{\theta}_{x}\right)
$$

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 $\dot{x}(t)=\bar{f}\left(x(t), t \mid \bar{\theta}_{x}\right)$

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

$$
x(t)=x_{0}+\int_{0}^{t} f\left(x(\tau), \tau \mid \bar{\theta}_{x}\right) d \tau
$$

## 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 $\theta_{x}$
- (The initial condition, $x(t=0)=x_{0}$, is also fixed)

Then, we have the uncontrolled dynamical system

$$
\begin{aligned}
& \dot{x}(t)=f\left(t, x(t) \mid \theta_{x}\right), \quad t \in[0, T] \\
& x(0)=x_{0}
\end{aligned}
$$

The solution,

$$
x(t)=x_{0}+\int_{0}^{t} f\left(x(\tau), \tau \mid \theta_{x}\right) d \tau
$$

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


## Theorem

## Existence and uniqueness

Let $f:\left[t_{\mathrm{ini}}, t_{\mathrm{fin}}\right] \times \mathcal{R}^{N_{x}} \rightarrow \mathcal{R}^{N_{x}}$ be some continuous function in $x(t)$ and $t$
Consider the initial value problem with initial value

$$
\begin{aligned}
\dot{x}(t) & =f\left(t, x(t) \mid \theta_{x}\right), \quad t \in\left[t_{\mathrm{ini}}, t_{\mathrm{fin}}\right] \\
x\left(t_{\mathrm{ini}}\right) & =x_{0}
\end{aligned}
$$

The IVP has a solution $x:\left[t_{\text {ini }}, t_{\text {fin }}\right] \rightarrow \mathcal{R}^{N_{x}}$ 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 $\left(x(t), x^{\prime}(t)\right)$,

$$
\left\|f\left(x(t), t \mid \theta_{x}\right)-f\left(x^{\prime}(t), t \mid \theta_{x}\right)\right\| \leq L\left\|x(t)-x^{\prime}(t)\right\|, \quad \forall t \in\left[t_{\mathrm{ini}}, t_{\mathrm{fin}}\right]
$$

Or, equivalently, for any pair $\left(x(t), x^{\prime}(t)\right)$

$$
\frac{\left\|f\left(x(t), t \mid \theta_{x}\right)-f\left(x^{\prime}(t), t \mid \theta_{x}\right)\right\|}{\left\|x(t)-x^{\prime}(t)\right\|} \leq L, \quad \forall t \in\left[t_{\mathrm{ini}}, t_{\mathrm{fin}}\right]
$$

## Continuous-time models (cont.)

$$
\frac{\left\|f\left(x(t), t \mid \theta_{x}\right)-f\left(x^{\prime}(t), t \mid \theta_{x}\right)\right\|}{\left\|x(t)-x^{\prime}(t)\right\|} \leq L, \quad \forall t \in\left[t_{\mathrm{ini}}, t_{\mathrm{fin}}\right]
$$

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

## Theorem

## Local existence and uniqueness

Let $f:\left[t_{\mathrm{ini}}, t_{\mathrm{fin}}\right] \times \mathcal{R}^{N_{x}} \rightarrow \mathcal{R}^{N_{x}}$ be some continuous function in $x(t)$ and $t$
Consider the initial value problem with initial value

$$
\begin{aligned}
\dot{x}(t) & =f\left(t, x(t) \mid \theta_{x}\right), \quad t \in\left[t_{\mathrm{ini}}, t_{\mathrm{fin}}\right] \\
x\left(t_{\mathrm{ini}}\right) & =x_{0}
\end{aligned}
$$

If $f$ is continuously differentiable with respect to $x(t)$ for all $t \in\left[t_{\mathrm{ini}}, t_{\text {fin }}^{\prime}\right]$, there exists a non-empty interval $\left[t_{\mathrm{ini}}, t_{\text {fin }}^{\prime}\right]$ with $t_{\text {fin }}^{\prime} \in\left(t_{\mathrm{ini}}, t_{\text {fin }}\right]$ 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 $\left[0, T^{\prime}\right]$ with $T^{\prime}<1$, the solution exists and it is also unique


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

$$
\frac{\left\|f\left(x^{\boldsymbol{\omega}}(t)\right)-f\left(x^{\boldsymbol{\omega}}(t)\right)\right\|}{\left\|x^{\boldsymbol{\omega}}(t)-x^{\boldsymbol{\omega}}(t)\right\|} \not \leq L
$$

There is no single $L$ that satisfies the inequality for all pairs $\left(x^{\boldsymbol{\omega}}(t), x^{\boldsymbol{\omega}}(t)\right)$

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

## Continuous-time models (cont.)



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

$$
\begin{equation*}
\frac{\| f(x)(t))-f(x)(t)) \|}{\|x \leftarrow(t)-x(t)\|} \leq L \tag{?}
\end{equation*}
$$

If not, is it at least locally Lipschitz?

## Continuous-time models (cont.)

## Dynamical

## Example



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

$$
\begin{equation*}
\frac{\left\|f\left(x^{\boldsymbol{\omega}}(t)\right)-f\left(x^{\boldsymbol{\omega}}(t)\right)\right\|}{\left\|x^{\boldsymbol{\omega}}(t)-x(t)\right\|} \leq L \tag{?}
\end{equation*}
$$

If not, is it at least locally Lipschitz?

## Continuous-time models (cont.)

## Example



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

$$
\begin{equation*}
\frac{\| f\left(x^{\boldsymbol{\omega}}(t)\right)-f(x \text { (t) }) \|}{\|x \uparrow(t)-x \uparrow(t)\|} \leq L \tag{?}
\end{equation*}
$$

If not, is it at least locally Lipschitz?

## Continuous-time models (cont.)

## Dynamical

## Example

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

$$
\begin{equation*}
\frac{\left\|f\left(x^{\boldsymbol{\omega}}(t)\right)-f\left(x^{\boldsymbol{\omega}}(t)\right)\right\|}{\left\|x^{\boldsymbol{\omega}}(t)-x(t)\right\|} \leq L \tag{?}
\end{equation*}
$$

If not, is it at least locally Lipschitz?

## Continuous-time models (cont.)

## Dynamical

## Example

Is $f(x(t))=\|x(t)\|_{2}$ a globally Lipschitz continuous function?

$$
\begin{equation*}
\frac{\left\|f\left(x^{\boldsymbol{\omega}}(t)\right)-f\left(x^{\boldsymbol{\omega}}(t)\right)\right\|}{\left\|x^{\boldsymbol{\omega}}(t)-x(t)\right\|} \leq L \tag{?}
\end{equation*}
$$

If not, is it at least locally Lipschitz?

$$
x_{1}(t)
$$

$$
x_{2}(t)
$$

## Example

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

$$
\begin{equation*}
\frac{\left\|f\left(x^{\boldsymbol{\omega}}(t)\right)-f\left(x^{\boldsymbol{\omega}}(t)\right)\right\|}{\left\|x^{\boldsymbol{\omega}}(t)-x^{\boldsymbol{\omega}}(t)\right\|} \leq L \tag{?}
\end{equation*}
$$

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)


## Steady-state, stationary, equilibrium, or fixed points

- Values of $x$ (fixed $\theta_{x}$ and $u$ ) such that $f\left(x(t) \mid \theta_{x}\right)=0$

$$
\begin{aligned}
\frac{d x(t)}{d t} & =f\left(x(t) \mid \theta_{x}\right) \\
& =0
\end{aligned}
$$

## Stability

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

- At some point in time, the system is perturbed, some change occurs
$\rightsquigarrow$ 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)
$\rightsquigarrow$ 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)


## Dynamical

Continuous-time models (cont.)
Stable


Time ( $t$ )
Unstable


Time ( $t$ )

## Continuous-time models | LTIs

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

Linear time-invariant systems, LTI
$\xrightarrow{u(t)} \begin{aligned} & \dot{x}(t)=A x(t)+B u(t) \\ & y(t)=C x(t)+D u(t)\end{aligned} \quad y(t)$

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

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

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

$$
\rightsquigarrow A \in \mathcal{R}^{N_{x} \times N_{x}}
$$

$$
\rightsquigarrow B \in \mathcal{R}^{N_{x} \times N_{u}}
$$

$$
\rightsquigarrow\{A, B\}=\theta_{x} \in \mathcal{R}^{\left(N_{x} \times N_{x}\right)+\left(N_{x} \times N_{u}\right)}
$$

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

$$
\rightsquigarrow C \in \mathcal{R}^{N_{y} \times N_{x}}
$$

$$
\rightsquigarrow D \in \mathcal{R}^{N_{y} \times N_{u}}
$$

$$
\rightsquigarrow\{C, D\}=\theta_{y} \in \mathcal{R}^{\left(N_{y} \times N_{x}\right)+\left(N_{y} \times N_{u}\right)}
$$

Linear time-invariant systems $f=A x+B u$ are Lipschitz continuous with respect to $x$

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


## Continuous-time models | LTIs (cont.)

## Dynamical

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

$$
\begin{aligned}
& x(t)=\underbrace{e^{A\left(t-t_{\mathrm{ini}}\right)} x\left(t_{\mathrm{ini}}\right)+\int_{t_{\mathrm{ini}}}^{t} e^{A(t-\tau)} B u(\tau) \mathrm{d} \tau} \\
& y(t)=\underbrace{C e^{A\left(t-t_{\mathrm{ini}}\right)} x\left(t_{\mathrm{ini}}\right)+C \int_{t_{\mathrm{ini}}}^{t} e^{A(t-\tau)} B u(\tau) \mathrm{d} \tau}_{C x(t)}+D u(t)
\end{aligned}
$$

The solution is known as the Lagrange formula
$\rightsquigarrow$ Based on the state transition matrix, $e^{A t}$

## 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 $u(t) \in \mathcal{R}^{N_{u}}$

$$
x(t)=A x(t)+B u(t)
$$

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 $x_{f}=x\left(t_{f}\right)$

- ..., 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


## Definition

## Controllability gramian

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

$$
x(t)=A x(t)+B u(t)
$$

The system's controllability gramian is a $\left(N_{x} \times N_{x}\right)$ matrix, real and symmetric

$$
W_{c}(t)=\int_{0}^{t} e^{A \tau} B B^{T} e^{A^{T} \tau} \mathrm{~d} \tau
$$

## Theorem

## Controllability test (I)

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

$$
x(t)=A x(t)+B u(t)
$$

Let $W_{c}(t)=\int_{0}^{t} e^{A \tau} B B^{T} e^{A^{T}} \tau \mathrm{~d} \tau$ be the controllability gramian of the system

- The system is controllable iff $W_{c}(t)$ is non-singular, for all $t>0$

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


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

$$
\rightsquigarrow \quad u(t)=-K x(t)
$$

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

$$
K=\left(B^{\prime} Q_{f} B+R\right)^{-1} B^{\prime} Q_{f} A
$$

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

Observability of linear-time-invariant systems
Consider a linear and time-invariant system $(A, C)$ with $x(t) \in \mathcal{R}^{N_{x}}$ and $u(t) \in \mathcal{R}^{N_{y}}$

$$
\begin{aligned}
\dot{x}(t) & =A x(t) \\
y(t) & =C x(t)
\end{aligned}
$$

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 $\left(t_{f}<\infty\right)$

- ..., from any arbitrary initial state $x\left(t_{0}\right)$


## Continuous-time models | LTIs (cont.)

## Definition

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

$$
\left\{\begin{array}{l}
\dot{x}(t)=A x(t) \\
y(t)=C x(t)
\end{array}\right.
$$

The system's observability gramian is a $\left(N_{x} \times N_{x}\right)$ matrix, real and symmetric

$$
W_{o}(t)=\int_{0}^{t} e^{A^{T} \tau} C^{T} C e^{A \tau} \mathrm{~d} \tau
$$

## Theorem

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

$$
\left\{\begin{array}{l}
\dot{x}(t)=A x(t) \\
y(t)=C x(t)
\end{array}\right.
$$

Let $W_{o}(t)=\int_{0}^{t} e^{A^{T}} \tau C^{T} C e^{A \tau} \mathrm{~d} \tau$ 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

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

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

$$
\begin{aligned}
\int_{0}^{t_{f}} e^{A^{T} \tau} y(\tau) \mathrm{d} \tau & =\int_{0}^{t_{f}} e^{A^{T} \tau} C e^{A \tau} x(0) \mathrm{d} \tau \\
& =W_{o}\left(t_{f}\right) x(0)
\end{aligned}
$$

Thus, we have

$$
x(0)=W_{o}^{-1}(t f) \int_{0}^{t_{f}} e^{A^{T} \tau} C y(\tau) \mathrm{d} \tau
$$

The initial state is given as a function of the inverse of the observability gramian $W_{o}(t f)$ and the integral $\int_{0}^{t_{f}} e^{A^{T} \tau} C e^{A \tau} y(\tau) \mathrm{d} \tau$ which can be computed from measurements $y(\tau)$

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


## 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 $y(t) \in \mathcal{R}^{N_{y}}$

$$
\left\{\begin{array}{l}
\dot{x}(t)=A x(t)+B u(t) \\
y(t)=C x(t)
\end{array}\right.
$$

The linear and time-invariant dynamical system

$$
\left\{\begin{array}{l}
\dot{\hat{x}}(t)=A \widehat{x}(t)+B u(t)+K_{L}(y(t)-\widehat{y}(t)) \\
\widehat{y}(t)=C \widehat{x}(t)
\end{array}\right.
$$

with $\widehat{x} \in \mathcal{R}^{N_{x}}, \widehat{y}(t) \in \mathcal{R}^{N_{y}}$ 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

System


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


$$
\begin{aligned}
\dot{x}(t) & =f\left(x(t), u(t), z(t) \mid \theta_{x}\right) \\
0 & =h\left(x(t), u(t), z(t) \mid \theta_{z}\right) \\
y(t) & =g\left(x(t), z(t), u(t) \mid \theta_{y}\right)
\end{aligned} \quad \xrightarrow{ }
$$

$$
\begin{aligned}
& \rightsquigarrow x(t) \in \mathcal{R}^{N_{x}} \\
& \rightsquigarrow u(t) \in \mathcal{R}^{N_{u}} \\
& \rightsquigarrow \\
& \rightsquigarrow z(t) \in \mathcal{R}^{N_{z}} \\
& \rightsquigarrow \theta_{x} \in \mathcal{R}^{N_{\theta_{x}}} \\
& \rightsquigarrow \theta_{z} \in \mathcal{R}^{N_{\theta_{z}}} \\
& \rightsquigarrow t \in \mathcal{R}
\end{aligned}
$$

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

$$
\rightsquigarrow \theta_{y} \in \mathcal{R}^{N_{\theta_{y}}}
$$

The algebraic equations cannot be solved independently of the differential equations

$$
\left[\begin{array}{c}
\dot{x_{1}}(t) \\
\dot{x_{2}}(t) \\
\vdots \\
\dot{x_{N_{x}}}(t) \\
0 \\
0 \\
\vdots \\
0
\end{array}\right]=\left[\begin{array}{c}
f_{1}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{x}\right) \\
f_{2}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{x}\right) \\
\vdots \\
f_{N_{x}}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{x}\right) \\
h_{1}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{z}\right) \\
h_{2}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{z}\right) \\
\vdots \\
h_{N_{z}}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{z}\right)
\end{array}\right]
$$

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

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

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

## Continuous-time models | DAE (cont.)

Function $h: \mathcal{R}^{N_{x}} \times \mathcal{R}^{N_{u}} \times \mathcal{R}^{N_{z}} \rightarrow \mathcal{R}^{N_{z}}$,

$$
\begin{aligned}
& h(x(t), u(t), z(t) \mid \\
& \left.\theta_{x}\right)= \\
& \qquad\left[\begin{array}{c}
h_{1}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{z}\right) \\
h_{2}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{z}\right) \\
\vdots \\
\\
h_{N_{z}}\left(x_{1}(t), \ldots, x_{N_{x}}(t), u_{1}(t), \ldots, u_{N_{u}}(t), z_{1}(t), \ldots, z_{N_{z}}(t) \mid \theta_{z}\right)
\end{array}\right]
\end{aligned}
$$

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

$$
\begin{align*}
& \frac{\partial h(x(t), u(t), z(t))}{\partial z}= \\
& \underbrace{\left[\begin{array}{cccc}
{\left[\partial h_{2}(x, u, z) / \partial z_{1}\right.} & \cdots & \partial h_{2}(x, u, z) / \partial z_{n_{z}} & \cdots \\
& & \left.\partial h_{2}(x, u, z) / \partial z_{N_{z}}\right] \\
{\left[\partial h_{n_{z}}(x, u, z) / \partial z_{1}\right.} & \cdots & \partial h_{n_{z}}(x, u, z) / \partial z_{n_{z}} & \cdots \\
\vdots & & \vdots & \left.\partial h_{n_{z}}(x, u, z) / \partial z_{N_{z}}\right] \\
{\left[\partial h_{N_{z}}(x, u, z) / \partial z_{1}\right.} & \cdots & \partial h_{N_{z}}(x, u, z) / \partial z_{n_{z}} & \cdots \\
N_{z} \times N_{z}
\end{array} \partial h_{N_{z}}(x, u, z) / \partial z_{N_{z}}\right]}_{\begin{array}{cccc}
{\left[\partial h_{1}(x, u, z) / \partial z_{1}\right.} & \cdots & \partial h_{1}(x, u, z) / \partial z_{n_{z}} & \cdots
\end{array}}]
\end{align*}
$$

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

$$
\frac{d h(x(t), z(t))}{d t}=0
$$

For the total derivative of the algebraic equations, we have

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

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

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

## Continuous-time models (cont.)

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

- That is, the motion of the state in an infinitesimal time period

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

$$
\begin{aligned}
x(\Delta t) & =x_{0}+\int_{0}^{\Delta t} f(x(t)) d t \\
& \approx x_{0}+f\left(x_{0}\right) \int_{0}^{\Delta t} d t \\
& =x_{0}+f\left(x_{0}\right)[t]_{0}^{\Delta t} \\
& =x_{0}+f\left(x_{0}\right) \Delta t
\end{aligned}
$$

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 $t=0$

$$
\begin{aligned}
x(1 \Delta t) & =x(0)+f(x(0)) \Delta t \\
x(2 \Delta t) & =x(1 \Delta t)+f(x(1 \Delta t)) \Delta t \\
\cdots & =\cdots \\
x(k \Delta t) & =x((k-1) \Delta t)+f(x((k-1) \Delta t)) \Delta t \\
\cdots & =\cdots \\
x(\underbrace{(K-1) \Delta t}_{T-\Delta t}) & =x(\underbrace{(K-1) \Delta t}_{T-2 \Delta t})+f(x(\underbrace{(K-1) \Delta t}_{T-2 \Delta t})) \Delta t \\
x(\underbrace{K \Delta t}_{T}) & =x(\underbrace{(K-1) \Delta t}_{T-\Delta t})+f(x(\underbrace{(K-1) \Delta t}_{T-\Delta t})) \Delta t
\end{aligned}
$$

Continuous-time models (cont.)

$$
x(t)=x_{0}+\int_{0}^{t} f(x(\tau), u(\tau)) d \tau
$$

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

$$
\begin{aligned}
x(\Delta t) & =x_{0}+\int_{0}^{\Delta t} f(x(t), u(t)) d t \\
& \approx x_{0}+f\left(x_{0}, u_{0}\right) \int_{0}^{\Delta t} d t \\
& =x_{0}+f\left(x_{0}, u_{0}\right) \Delta t
\end{aligned}
$$

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 $(x(t))_{t=0}^{T}$

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

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 $\left\{t_{k}=k \Delta t\right\}_{k=0}^{K}$
- $\Delta t$ denotes the (common) duration

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

$$
\left\{x\left(t_{k}=k \Delta t\right)\right\}_{k=0}^{K}
$$

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

## Continuous-time models (cont.)

Suppose that $\dot{x}(t)=f\left(x(t), u(t) \mid \theta_{x}\right)$ 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 $t \in\left[t_{k}, t_{k+1}\right)$

We can treat the transition from state $x\left(t_{k}\right)$ to $x\left(t_{k+1}\right)$ 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 $\left(t_{k}, t_{k+1}\right]$, the solution to the individual IVP exists and it is unique

- With initial value $x\left(t_{k}\right)=x_{\text {init }}$


## Continuous-time models (cont.)

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

$$
\begin{aligned}
& \dot{x}(t)=f\left(x(t), u_{\text {const }} \mid \theta_{x}\right), \quad t \in[0, \Delta t] \\
& x(0)=x_{\mathrm{ini}}
\end{aligned}
$$

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

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

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

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

The map from pair $\left(x_{\text {init }}, u_{\text {const }}\right)$ to process $(x(t))_{0}^{\Delta t}$ is denoted as the solution map

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

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

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

We define the transition function which returns that final value $x\left(\Delta t \mid x_{\text {ini }}, u_{\text {const }} ; \theta_{x}\right)$

$$
f_{\Delta t}: \mathcal{R}^{N_{x}} \times \mathcal{R}^{N_{u}} \rightarrow \mathcal{R}^{N_{x}}
$$

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

$$
x\left(\Delta t \mid x_{\mathrm{ini}}, u_{\mathrm{const}} ; \theta_{x}\right)=f_{\Delta t}\left(x_{\mathrm{ini}}, u_{\mathrm{const}} \mid \theta_{x}\right)
$$

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

$$
x\left(t_{k+1}\right)=f_{\Delta t}\left(x\left(t_{k}\right), u_{k} \mid \theta_{x}\right) \quad(k=0,1, \ldots K)
$$

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.)

For linear and time-invariant dynamical systems $\dot{x}(t)=A x(t)+B u(t)$ with $x(0)=x_{\text {init }}$ and constant input $u_{\text {const }}$, the solution map $x\left(t \mid x_{\mathrm{ini}}, u_{\mathrm{ini}}, \theta_{x}\right)$ is explicitly known

$$
\begin{aligned}
x\left(t \mid x_{\mathrm{ini}}, u_{\mathrm{ini}}, \theta_{x}\right) & =\underbrace{e^{A t} x_{\mathrm{ini}}+\int_{0}^{t} e^{A(t-\tau)} B u_{\mathrm{const}} d \tau}_{f_{\Delta t}\left(x_{\mathrm{ini}}, u_{\mathrm{const}} \mid \theta_{x}\right)} \\
& =\underbrace{e^{A t} x_{\mathrm{ini}}+\left(\int_{0}^{t} e^{A(t-\tau)} d \tau\right) B u_{\mathrm{const}}}_{f_{\Delta t}\left(x_{\mathrm{ini}}, u_{\mathrm{const}} \mid \theta_{x}\right)}
\end{aligned}
$$

The corresponding discrete-time system with sampling time $\Delta t$ is linear time-invariant

$$
\begin{gathered}
x\left(t_{k+1}\right)=\underbrace{A_{\Delta t} x\left(t_{k}\right)+B_{\Delta t} u_{k}}_{f_{\Delta t}\left(x\left(t_{k}\right), u_{k} \mid \theta_{x}\right)}, \quad(k=0,1, \ldots, K-1) \\
\rightsquigarrow A_{\Delta t}=e^{A \Delta t} \text { and } B_{\Delta t}=\left(\int_{0}^{\Delta t} e^{A(\Delta t-\tau)} d \tau\right) B
\end{gathered}
$$

Since $\Delta t$ 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 $\left(A_{\Delta t}, B_{\Delta t}\right)$

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

$$
x_{k+1}=f_{k}\left(x_{k}, u_{k} \mid \theta_{x}\right), \quad k \in \mathcal{N}_{0 \rightsquigarrow K-1}
$$

$\rightsquigarrow K+1$ state vectors, $x_{0}, x_{1}, \ldots, x_{k}, \ldots, x_{K} \in \mathcal{R}^{N_{x}}$
$\rightsquigarrow K$ input vectors, $u_{0}, u_{1}, \ldots, u_{k}, \ldots, u_{K-1} \in \mathcal{R}^{N_{u}}$
$\rightsquigarrow$ Some time-horizon of length $K$
$\rightsquigarrow$ Parameter vector $\theta_{x} \in \mathcal{R}^{N_{\theta_{x}}}$
$\rightsquigarrow$ (Time-varying dynamics)
Given the initial state $x_{0}$ and all the controls $u_{0}, u_{1}, \ldots, u_{K-1}$, we could recursively call the functions $f_{k}\left(x_{k}, u_{k} \mid \theta_{x}\right)$ and sequentially obtain all the other states $x_{1}, x_{2}, \ldots, x_{K}$

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


## Definition

## Forward simulation

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

- The argument are $x_{0}$ and the collection $u_{0}, u_{1}, \ldots, u_{K-1}$
- The image is the collection $x_{0}, x_{1}, \ldots, x_{K}$

That is, we have

$$
\begin{aligned}
f_{\mathrm{sim}} & : \mathcal{R}^{N_{x}+\left(K \times N_{u}\right)} \rightarrow \mathcal{R}^{(K+1) N_{x}} \\
& :\left(x_{0}, u_{0}, u_{1}, \ldots, u_{K-1}\right) \mapsto\left(x_{0}, x_{1}, \ldots, x_{K}\right)
\end{aligned}
$$

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

$$
x_{k+1}=f_{k}\left(x_{k}, u_{k} \mid \theta_{x}\right) \quad\left(\text { for all } k \in \mathcal{N}_{0 \rightsquigarrow K-1}\right)
$$

## Discrete-time models | LTI

- $x_{0}, x_{1}, \ldots, x-K, \ldots, x_{K} \in \mathcal{R}^{N_{x}}$

Linear time-invariant systems, LTI

$$
x_{k+1}=A x_{k}+B u_{k}, \quad k \in \mathcal{N}_{0 \rightsquigarrow K-1}
$$

- $u_{0}, u_{1}, \ldots, u_{k}, \ldots, u_{K-1} \in \mathcal{R}^{N_{u}}$
- $A \in \mathcal{R}^{N_{x} \times N_{x}}$
- $B \in \mathcal{R}^{N_{x} \times N_{u}}$
- $\{A, B\}=\theta_{x} \in \mathcal{R}^{\left(N_{x} \times N_{x}\right)+\left(N_{x} \times N_{u}\right)}$

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

$$
\begin{aligned}
f_{\mathrm{sim}}\left(x_{0}, u_{0}, \ldots, u_{K-1}\right) & =\left[\begin{array}{c}
x_{0} \\
x_{1} \\
x_{2} \\
\vdots \\
x_{K}
\end{array}\right] \\
& =\left[\begin{array}{c}
x_{0} \\
A x_{0}+B u_{0} \\
A^{2} x_{0}+A B u_{0}+B u_{1} \\
\vdots \\
A^{K} x_{0}+\sum_{k=0}^{K-1} A^{K-1-k} B u_{k}
\end{array}\right]
\end{aligned}
$$

$$
\left[\begin{array}{c}
x_{0} \\
x_{1} \\
x_{2} \\
\vdots \\
x_{K}
\end{array}\right]=\underbrace{\left[\begin{array}{c}
x_{0} \\
A x_{0}+B u_{0} \\
A^{2} x_{0}+A B u_{0}+B u_{1} \\
\vdots \\
A^{K} x_{0}+\sum_{k=0}^{K-1} A^{K-1-k} B u_{k}
\end{array}\right]}_{x_{\mathrm{sim}}\left(x_{0}, u_{0}, \ldots, u_{K-1}\right)}
$$

Consider the terminal value $x_{K}$ after $K$ steps from $x_{0}$ and subjected to $u_{0} \rightsquigarrow u_{K-1}$,

$$
x_{K}=A^{K} x_{0}+\underbrace{\left[\begin{array}{llll}
A^{K-1} B & A^{K-2} B & \cdots & B
\end{array}\right]}_{\mathcal{C}_{K}}\left[\begin{array}{c}
u_{0} \\
u_{1} \\
\vdots \\
u_{K-1}
\end{array}\right]
$$

Matrix $\mathcal{C}_{K}$ is the discrete-time controllability matrix of the linear time-invariant system

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

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

- $x_{0}, x_{1}, \ldots, x_{k}, \ldots, x_{K} \in \mathcal{R}^{N_{x}}$


## Affine time-varying systems

$x_{k+1}=A_{k} x_{k}+B_{k} u_{k}+c_{k}, \quad k \in \mathcal{N}_{0 \rightsquigarrow K-1}$

- $u_{0}, u_{1}, \ldots, u_{k}, \ldots, u_{K-1} \in \mathcal{R}^{N_{u}}$
- $A_{0}, A_{1}, \ldots, A_{k}, \ldots, A_{K} \in \mathcal{R}^{N_{x} \times N_{x}}$
- $B_{0}, B_{1}, \ldots, B_{k}, \ldots, B_{K} \in \mathcal{R}^{N_{x} \times N_{u}}$
- $\left\{A_{k}, B_{k}\right\}=\theta_{x} \in \mathcal{R}^{\left(N_{x} \times N_{x}\right)+\left(N_{x} \times N_{u}\right)}$

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

$$
x_{k+1}=f_{k}\left(x_{k}, u_{k} \mid \theta_{x}\right)
$$

- Linearisation of nonlinear (and time-varying) dynamics around point ( $\bar{x}_{k}, \bar{u}_{k}$ )
- We assume the that point $\left(\bar{x}_{k}, \bar{u}_{k}\right)$ is a term in a trajectory $\left\{\left(x_{k}, u_{k}\right)\right\}$
- (For example, $\left\{\bar{x}_{0}, \bar{x}_{1}, \ldots, \bar{x}_{K}\right\}$ and $\left\{\bar{u}_{0}, \bar{u}_{1}, \ldots, \bar{u}_{K-1}\right\}$ )

$$
\dot{x}(t)=f_{f}\left(x(t), u(t) \mid \theta_{x}\right)
$$

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 $x^{\prime}(t)=x(t)-\bar{x}(t)$ and $u^{\prime}(t)=u(t)-\bar{u}(t)$,
$\underbrace{\left[\begin{array}{c}x_{1}^{\prime}(t) \\ \vdots \\ x_{N_{x}}^{\prime}(t)\end{array}\right]}_{x^{\prime}(t)}=\underbrace{\left[\begin{array}{ccc}\frac{\partial f_{1}^{t}}{\partial x_{1}} & \cdots & \frac{\partial f_{1}^{t}}{\partial x_{N_{x}}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_{N_{x}}^{t}}{\partial x_{1}} & \cdots & \frac{\partial f_{N_{x}}^{t}}{\partial x_{N_{x}}}\end{array}\right]}_{A^{t}} \underbrace{\left[\begin{array}{c}x_{1}^{\prime}(t) \\ \vdots \\ x_{N_{x}}^{\prime}(t)\end{array}\right]}_{(\bar{x}(t), \bar{u}(t))}+\underbrace{\left[\begin{array}{ccc}\frac{\partial f_{1}^{t}}{\partial u_{1}} & \cdots & \frac{\partial f_{1}^{t}}{\partial u_{N_{u}}} \\ \vdots & \ddots & \vdots \\ \vdots \\ \frac{\partial f_{N_{x}}^{t}}{\partial u_{1}} & \cdots & \frac{\partial f_{N_{x}}^{t}}{\partial u_{N_{u}}}\end{array}\right]_{(\bar{x}(t), \bar{u}(t))} \underbrace{\left[\begin{array}{c}u_{1}^{\prime}(t) \\ \vdots \\ u_{N_{u}}^{\prime}(t)\end{array}\right]}_{u^{\prime}(t)}}_{x^{\prime}(t)}$ $+\underbrace{\left[\begin{array}{c}f_{1}^{t} \\ f_{2}^{t} \\ \vdots \\ f_{N_{x}}^{t}\end{array}\right]_{(\bar{x}(t), \bar{u}(t))}}_{c^{t}}$

- $A^{t}$ 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 $(\bar{x}(t), \bar{u}(t))$


## Dynamical

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

$$
\begin{aligned}
\underbrace{\left[\begin{array}{c}
x_{1}^{\prime}(t) \\
\vdots \\
x_{N_{x}}^{\prime}(t)
\end{array}\right]}_{x^{\prime}(t)}= & \underbrace{\left[\begin{array}{ccc}
a_{1,1}^{t} & \cdots & a_{1, N_{x}}^{t} \\
\vdots & \ddots & \vdots \\
a_{N_{x}, 1}^{t} & \cdots & a_{N_{x}, N_{x}}^{t}
\end{array}\right]}_{\left(N_{x} \times N_{x}\right)} \underbrace{\left[\begin{array}{c}
x_{1}^{\prime}(t) \\
\vdots \\
x_{N_{x}}^{\prime}(t)
\end{array}\right]}_{\left(N_{x} \times 1\right)}+\underbrace{\left[\begin{array}{ccc}
b_{1,1}^{t} & \cdots & b_{1, N_{u}}^{t} \\
\vdots & \ddots & \vdots \\
b_{N_{x}, 1}^{t} & \cdots & b_{N_{x}, N_{u}}^{t}
\end{array}\right]}_{\left(N_{x} \times N_{u}\right)} \underbrace{\left[\begin{array}{c}
u_{1}^{\prime}(t) \\
\vdots \\
u_{N_{u}}^{\prime}(t)
\end{array}\right]}_{\left(N_{u} \times 1\right)} \\
& +\underbrace{\left[\begin{array}{c}
c_{1}^{t} \\
c_{2}^{t} \\
\vdots \\
c_{N_{x}}^{t}
\end{array}\right]}_{N_{x} \times 1}
\end{aligned}
$$

Discrete-time models | Affine (cont.)

$$
x_{k+1}=f_{k}\left(x_{k}, u_{k} \mid \theta\right)
$$

Similarly, we can approximate nonlinear and time-varying dynamics in discrete-time We have the affine time-varying system,

$$
\begin{aligned}
\underbrace{x_{k+1}-\bar{x}_{k+1}}_{x_{k+1}^{\prime}} & =f_{k}\left(x_{k}, u_{k}\right)-\bar{x}_{k+1} \\
& \approx \underbrace{\left.\frac{\partial f}{\partial x}\right|_{\left(\bar{x}_{k}, \bar{u}_{k}\right)}}_{A_{k} \in \mathcal{R}^{N_{x} \times N_{x}}} \underbrace{\left(x_{k}-\bar{x}_{k}\right)}_{x_{k}^{\prime}}+\underbrace{\left.\frac{\partial f}{\partial u}\right|_{\left(\bar{x}_{k}, \bar{u}_{k}\right)}}_{B_{k} \in \mathcal{R}^{N_{x} \times N_{u}}} \underbrace{\left(u_{k}-\bar{u}_{k}\right)}_{u_{k}^{\prime}}+\underbrace{f_{k}\left(\bar{x}_{k}, \bar{u}_{k}\right)-\bar{x}_{k+1}}_{c_{k} \in \mathcal{R}^{N_{x} \times 1}}
\end{aligned}
$$

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

$$
x_{K}=\left(A_{K-1} \cdots A_{0}\right) x_{0}+\sum_{k=0}^{K-1}\left(\prod_{j=k+1}^{K-1} A_{j}\right)\left(B_{k} u_{k}+c_{k}\right)
$$

# Numerical simulations 

Dynamical models and 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 $\dot{x}(t)=f\left(x(t), u(t) \mid \theta_{x}\right)$ with $x(0)=x_{0}$ has a unique solution when $f$ is Lipschitz continuous with respect to $x(t)$ and continuous with respect to $t$
$\rightsquigarrow$ 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

The idea of a numerical simulation method is to compute an approximation to a solution map $x\left(t \mid x_{\mathrm{ini}}, u_{\text {const }} ; \theta_{x}\right)$ for $t \in[0, T]$, the computation is known as an integrator
$\rightsquigarrow$ Remember, the function from pair $\left(x_{\text {ini }}, u_{\text {const }}\right)$ to process $\{x(t)\}_{0}^{T}$
An intuitive way to compute an approximation for $x\left(t \mid x_{\text {init }}, u_{\text {const }} ; \theta_{x}\right)$ when $t \in[0, T]$

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


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

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

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

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 $\left\{t_{k}\right\}$ as nodes in the time grid

Starting from $\widehat{x}_{0}=x_{\text {init }}$, we then perform $K$ sequential linear extrapolation steps

$$
\widehat{x}_{k+1}=\widehat{x}_{k}+f\left(\widehat{x}_{k}, u_{\text {const }} \mid \theta_{x}\right) \Delta t, \quad k=0,1, \ldots, K-1
$$

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

- This allows us to start the sequence with $\widehat{x}_{0}=x_{\text {ini }}$


Sequentially, the individual integration steps
$\rightsquigarrow k=0$

$$
\widehat{x}_{1}=\widehat{x}_{0}+f\left(\widehat{x}_{0}, u_{\mathrm{const}} \mid \theta_{x}\right) \Delta t
$$

$\rightsquigarrow k=1$

$$
\widehat{x}_{2}=\widehat{x}_{1}+f\left(\widehat{x}_{1}, u_{\text {const }} \mid \theta_{x}\right) \Delta t
$$

$\rightsquigarrow k=K-1$

$$
\widehat{x}_{K}=\widehat{x}_{K-1}+f\left(\widehat{x}_{K-1}, u_{\text {const }} \mid \theta_{x}\right) \Delta t
$$



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

- (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

$$
\underbrace{\left\|\widehat{x}\left(T \mid x_{\text {init }}, u_{\text {const }}, \theta_{x}\right)-x\left(T \mid x_{\mathrm{init}}, u_{\text {const }}, \theta_{x}\right)\right\|}
$$

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

This would suggest running integration procedures with many small-sized subintervals
$\rightsquigarrow$ The scheme requires the evaluation of function $f\left(x_{\text {ini }}, u_{\text {const }} \mid \theta_{x}\right)$ at each step
$\rightsquigarrow$ Good approximations with many steps require many function evaluations
(Other methods can achieve the desired accuracy levels with lower computational cost)

The order-4 Runge-Kutta integration method, RK4 generates a sequence of values $\widehat{x}_{k}$, by evaluating (and store) function $f$ four times at each node $k$, from $\widehat{x}_{0}=x_{\text {init }}$

From approximation $\widehat{x}_{k}$ and with constant input $u_{\text {const }}$, at each node $k$ we have

$$
\begin{aligned}
\kappa_{1} & =f\left(\widehat{x}_{k}, u_{\text {const }} \mid \theta_{x}\right) \\
\kappa_{2} & =f\left(\widehat{x}_{k}+\frac{\Delta t}{2} \kappa_{1}, u_{\text {const }} \mid \theta_{x}\right) \\
\kappa_{3} & =f\left(\widehat{x}_{k}+\frac{\Delta t}{2} \kappa_{2}, u_{\text {const }} \mid \theta_{x}\right) \\
\kappa_{4} & =f\left(\widehat{x}_{k}+\Delta t \kappa_{3}, u_{\text {const }} \mid \theta_{x}\right)
\end{aligned}
$$

Each function evaluation is explicit and performed around the approximation point $\widehat{x}_{k}$

- 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 $\widehat{x}_{k+1}$ point

$$
\widehat{x}_{k+1}=\widehat{x}_{k}+\frac{h}{6}\left(\kappa_{1}+2 \kappa_{2}+2 \kappa_{3}+\kappa_{4}\right), \quad k=0,1, \ldots, K-1
$$

The solution map obtained by using an explicit Runge-Kutta method of order-4, RK4
Explicit Runge-Kutta ( $f$ and $\Delta t$ )


It can be understood as a continuous and differentiable nonlinear function

- The maximum order of differentiability depends on function $f$

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.)


$$
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$$

Summarising, consider a numerical simulation scheme over some time interval $\left[t_{0}, t_{f}\right]$

- The subintervals have a length $\Delta t=\left(t_{0}-t_{f}\right) / K$

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

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

$$
t_{k}:=t_{0}+k \Delta t, \quad k=0,1, \ldots, K
$$

The solution is approximated at nodes $t_{k}$ by the values

$$
\widehat{x}_{k} \approx x\left(t_{k} \mid x\left(t_{0}\right), u_{\text {const }} ; \theta_{x}\right) \quad(k=0,1, \ldots, K)
$$

## Convergence

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

$$
\max _{k=0, \ldots, K}\left\|\widehat{x}_{k}-x\left(t_{k}\right)\right\|=\mathcal{O}\left((\Delta t)^{p}\right)
$$

As $K \rightarrow \infty$, we expect that $\widehat{x}_{k}$ gets closer to $x\left(t_{k}\right)$

