

CHEM-E7190
2021

Calculus, review

Intro to ODEs

Solution using a
Taylor expansion

Second- and
higher-order

From high to
first order ODEs



Aalto University

Ordinary differential equations

CHEM-E7190 (was E7140), 2021

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A brief review of calculus

Ordinary differential equation

Functions and their derivatives

Calculus, review

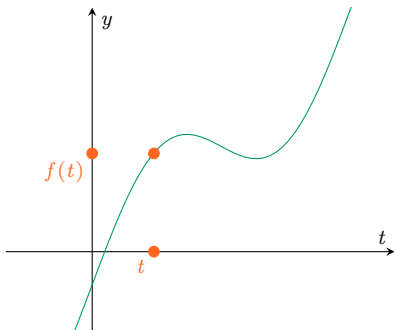
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A **function** $y = f(t)$ encodes the relation between two quantities or variables, y and t



Consider the **rate of change** of quantity y corresponding to a change in t

- It is the ratio between the differential change in y and the corresponding differential change in variable t

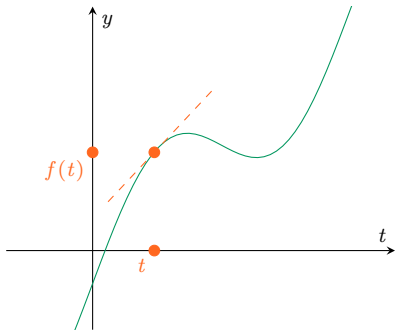
We conventionally call the **ratio of differential changes** the derivative of function f

Functions and their derivatives (cont.)

The **derivative** of a function $f(t)$ is the rate of change of the function, it is a number

- ↪ The derivative is defined with respect to the independent variable (here, t)
 - ↪ It can be computed at any point t of the domain of the function
-

We are given some function $f(t)$, we are interested in its derivative at some point t



Derivative of function f with respect to t

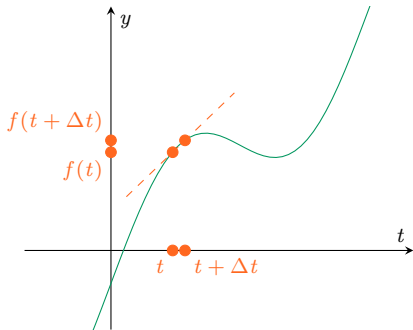
$$\rightsquigarrow \frac{df(t)}{dt}$$

The rate of change is understood as the slope of the tangent line to the function,

- ... at that specific point t

Functions and their derivatives (cont.)

The value of the derivative can be approximated by using small changes in t and $f(t)$



Consider the small change $t \rightarrow t + \Delta t$
and the associated $f(t) \rightarrow f(t + \Delta t)$

$$\frac{df(t)}{dt} \approx \frac{f(t + \Delta t) - f(t)}{\Delta t}$$

$$\rightsquigarrow \frac{\Delta y}{\Delta t}$$

The tangent line will be approximated

- By the secant line to the function
- Its slope is the approximation

Remember the equation of a line $y = mx + c$ through two points (x_1, y_1) and (x_2, y_2)

$$y = \frac{y_2 - y_1}{x_2 - x_1}(x - x_1) + y_1 = \underbrace{\left(\frac{y_2 - y_1}{x_2 - x_1}\right)}_{\Delta y / \Delta x} x + \underbrace{\frac{y_2 - y_1}{x_2 - x_1}x_1 + y_1}_{\text{constant}}$$

Functions and their derivatives (cont.)

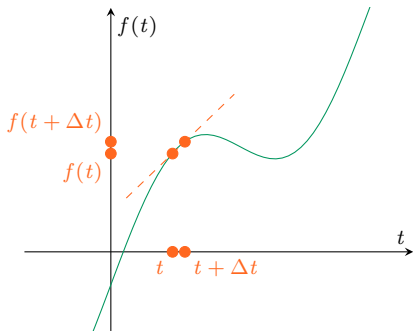
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We can improve the quality of this approximation, by letting Δt become smaller

- As $\Delta t \rightarrow 0$, the approximation will converge to the true derivative
- (Because the secant line will get closer to the tangent line)



$$\rightsquigarrow \frac{df(t)}{dt} = \lim_{\Delta t \rightarrow 0} \frac{f(t + \Delta t) - f(t)}{\Delta t}$$

Functions and their derivatives (cont.)

Calculus, review

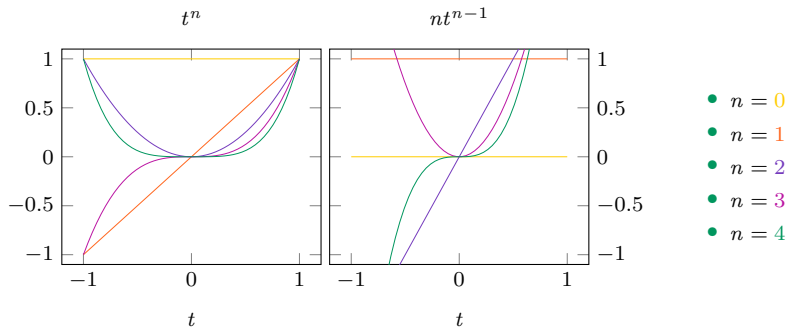
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Example

Power law

Consider the function $f(t) = t^n$ (the power law) and its derivative $\frac{df(t)}{dt} = nt^{n-1}$



- The derivative is commonly known (remembered), but we can derive it
- We will be using the approximation of derivative that we defined

Functions and their derivatives (cont.)

$$f(t) = t^n$$

By definition of derivative, we have

$$\begin{aligned} \frac{df(t)}{dt} &\approx \frac{f(t + \Delta t) - f(t)}{\Delta t} = \frac{1}{\Delta t} \left[\underbrace{(t + \Delta t)^n}_{\text{Powers of a binomial}} - t^n \right] \\ &= \frac{1}{\Delta t} \left[\underbrace{t^n + nt^{n-1}(\Delta t) + \frac{n(n-1)}{2}t^{n-2}(\Delta t)^2 + \dots - t^n}_{\text{Powers of a binomial} \rightsquigarrow \text{Binomial theorem}} \right] \\ &= \frac{1}{\Delta t} \left[\cancel{t^n} + nt^{n-1}(\Delta t) + \frac{n(n-1)}{2}t^{n-2}(\Delta t)^2 + \dots - \cancel{t^n} \right] \\ &= \frac{1}{\Delta t} \left[nt^{n-1}(\Delta t) + \frac{n(n-1)}{2}t^{n-2}(\Delta t)^2 + \underbrace{\mathcal{O}((\Delta t)^3)}_{\text{H.O. terms}} \right] \\ &= nt^{n-1} + \frac{n(n-1)}{2}t^{n-2}(\Delta t) + \mathcal{O}((\Delta t)^2) \\ &= nt^{n-1} + \mathcal{O}(\Delta t) \\ &\approx nt^{n-1} \end{aligned}$$

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Functions and their derivatives (cont.)

The first order derivative $df(t)/dt$ is the ratio of two distinct quantities $df(t)$ and dt

↪ The ratio can be manipulated by conventional algebraic procedures

Thus, we can have multiplication by some quantity

$$dt \frac{df}{dt} = df$$

And, multiplication and division by some quantity

$$\frac{df}{dt} \frac{dt}{dz} = \frac{df}{dz}$$

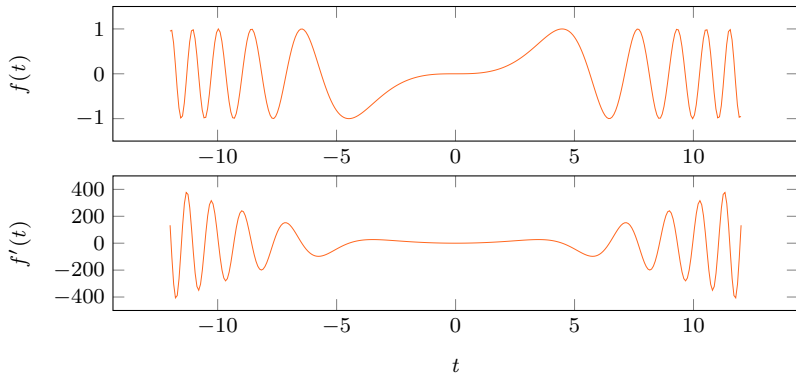
As an application, we get the **chain law** of derivation

$$\frac{df(g(t))}{dt} = \underbrace{\frac{df(g(t))}{dg(t)}}_{f'(g(t))} \underbrace{\frac{dg(t)}{dt}}_{g'(t)} = f'(t)$$

Functions and their derivatives (cont.)

Example

Consider the function $f(t) = \sin(t^3)$, compute its first derivative with respect to t



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A brief introduction to ODEs

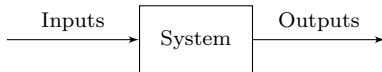
Ordinary differential equation

Introduction to ODEs

Ordinary differential equations (ODEs) are probably our most useful modelling tool

↪ (Together with probability)

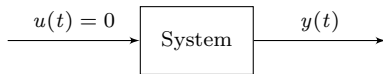
↪ (Not used in this course)



First some motivating and yet simple examples of ODEs (understood as system models)

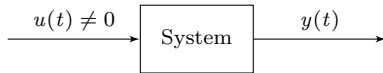
Systems for which the input is identically null over time

- Non-zero initial conditions
- **Force-free response**
- $y(t)$, when $u(t) = 0$



Systems for which the input is not identically null over time

- Zero initial conditions
- **Forced response**
- $y(t)$, when $u(t) \neq 0$



Calculus, review

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Example

Consider the problem of modelling the number of bacteria in some bacterial colony

- We assume that each bacterium in the colony gives rise to new individuals
- We also assume that we know the birth-rate, let us denote it by $\lambda > 0$

We assume that, on average, each bacterium will produce λ offsprings per unit time

- ↪ The size y of the colony varies (grows) in time proportionally to its size
- ↪ (That is, the larger the population, the larger the rate of growth)

$$\underbrace{\frac{dy(t)}{dt}}_{\dot{y}(t)} = \lambda y(t) \quad (\text{This identity is an ODE})$$

We are interested in knowing (determining) the size $y(t)$ of the population, over time

- The function $y(t)$ is the solution to the ordinary differential equation
- This is the function that satisfies the model $\dot{y}(t) = \lambda y(t)$

Introduction to ODEs (cont.)

The solution to the ODE is a (family of) function(s) $y(t)$ that satisfies the identity

$$\frac{dy(t)}{dt} = \dot{y}(t) = \lambda y(t)$$

There are many techniques that can be used to solve ordinary differential equations

- For the simple growth model we can separate the variables, then integrate

$$\frac{dy(t)}{dt} = \lambda y(t) \quad \rightsquigarrow \quad \int_{y_0}^y \frac{1}{y(t)} dy = \int_{t_0}^t \lambda dt$$

- 1 Move all terms in y to one side
- 2 Move all terms in t to the other side
- 3 Integrate both sides over appropriate intervals
- 4 The intervals are set in terms of initial conditions
- 5 (The initial, at time t_0 , size of the population , $y_0 = y(t = t_0)$)

Introduction to ODEs (cont.)

We have,

$$\begin{aligned} \rightsquigarrow \int_{y_0}^y \frac{1}{y(t)} dy &= \int_{t_0}^t \lambda dt \\ \rightsquigarrow \ln [y(t)]_{y_0}^y &= \lambda [t]_{t_0}^t \\ \rightsquigarrow \ln [y(t)] - \ln (y_0) &= \lambda t - \lambda t_0 \\ \rightsquigarrow \ln [y(t)] &= \lambda t - \underbrace{\lambda t_0 + \ln (y_0)}_{\text{constant}} \end{aligned}$$

Taking the exponential of both sides, we have

$$\begin{aligned} \rightsquigarrow y(t) &= \underbrace{e^{(\lambda t + \text{constant})}}_{e^{(\alpha + \beta)} = e^\alpha e^\beta} \\ &= e^{\lambda t} \cdot e^{\text{constant}} \\ &= e^{\lambda t} \cdot \text{constant} \end{aligned}$$

The bacteria population $y(t)$ evolves in time as an exponential function, it grows

- The exponential growth ($\lambda > 0$) is weighted by some constant
- The constant must be determined, we use initial conditions

Introduction to ODEs (cont.)

$$y(t) = e^{\lambda t} \cdot \text{constant}$$

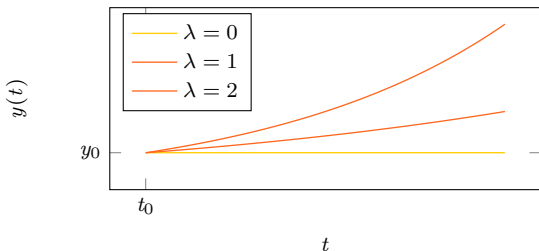
Suppose that at time $t = 0$, the population size is known to be $y(t = 0) = y_0 = y(0)$

$$y_0 = \underbrace{e^{\lambda \cdot 0}}_1 \cdot \text{constant} \quad \rightsquigarrow \quad \text{constant} = y_0$$

That is, the solution to the ordinary differential equation is given by $y(t) = (e^{\lambda t})y_0$

- We can solve this ODE analytically (We have a closed-form solution)
- Function $e^{\lambda t}$ is very important (The state transition function)

The system evolution, starting from an initial bacterial population size y_0 at time t_0



$$\rightsquigarrow y(t) = e^{\lambda t} y_0$$

$$\rightsquigarrow y_0 = 10$$

For $\lambda = 0$ the population size remains constant

- Zero birth-rate

Introduction to ODEs (cont.)

```
1 y0 = 10; % Set initial condition
2 lambda = 2; % Set model parameter
3
4 tMin = 00; tMax = 01; deltaT=0.1; % Define time range
5 tRange = tMin:deltaT:tMax; % Min, max, delta
6
7 y_clf = @(t) exp(lambda*t)*y0; % Set analytical solution
8
9 [timeR,y_num] = ode45(@(t,y) lambda*y,tRange,y0); % Compute the numerical
% solution using ODE45
10
11
12 figure(1); % Plotting stuff
13 hold on %
14 %
15 fplot(y_clf,[tMin,tMax],'k'); % Analytical
16 plot(timeR,y_num,'.-k'); % Numerical
17 %
18 stairs(timeR,y_num,'--r'); % Numerical
19 hold off %
20 %
21 xlabel('Time','FontSize',24) %
22 ylabel('N. of bacteria','FontSize',24) %
23 %
24 xlim([tMin,tMax]); %
25 ylim([0,max(y_num)]); %
26 % Could set a legend, ...
```



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Example

Reconsider the problem of modelling the number of bacteria in some bacterial colony

- We assume that bacteria procreate, at rate λ_1
- We assume that bacteria die, at rate λ_2

$$\begin{aligned}\dot{y}(t) &= \lambda_1 y(t) - \lambda_2 y(t) \\ &= \underbrace{(\lambda_1 - \lambda_2)}_{\lambda} y(t) \\ &= \lambda y(t)\end{aligned}$$

Formally, the resulting model (ODE) has not changed

- We know the solution for some initial condition

$$y(t) = (e^{\lambda t}) y_0$$

- λ is no longer restricted to be non-negative

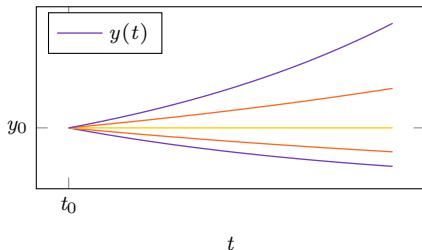
Introduction to ODEs (cont.)

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Suppose that at time $t = 0$, the population size is known to be $y(t = 0) = y_0 = y(0)$



$$\rightsquigarrow \lambda = \{-2, -1, 0, 1, 2\}$$

$$\rightsquigarrow y_0 = 10$$

We cannot discriminate between the effect of birth λ_1 and death λ_2 any longer (!)



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**Solution using a
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Solution by Taylor expansion

Ordinary differential equations

Solution by Taylor series expansion

Consider ODE $\dot{y}(t) = \lambda y(t)$, but suppose that we want approximate the solution $y(t)$

- Suppose we express the solution $y(t)$ by its Taylor series expansion

$$y(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + \dots$$

↪ This is a parametric representation of function $y(t)$

↪ The parameters $\{c_0, c_1, c_2, c_3, \dots\}$ are constants

We are interested in determining the actual solution $y(t)$, from this approximation

- To characterise a specific $y(t)$ we must set the parameters
- (We must determine the constants in the expansion)

In general, the Taylor series expansion of some function $f(x)$ around some point x_0

$$f(x) = f(x_0) + \left. \frac{df}{dx} \right|_{x_0} \frac{(x - x_0)}{1!} + \left. \frac{d^2 f}{dx^2} \right|_{x_0} \frac{(x - x_0)^2}{2!} + \left. \frac{d^3 f}{dx^3} \right|_{x_0} \frac{(x - x_0)^3}{3!} + \dots$$

Solution by Taylor series expansion (cont.)

Consider the ODE $\dot{y}(t) = \lambda y(t)$, we could compute its solution by variable separation

↪ We considered some value of λ and some initial condition $y(t=0) = y(0)$

↪ Then, we calculated the closed-form solution $y(t) = e^{\lambda t} y(0)$

By expressing the solution $y(t)$ in terms of its Taylor series expansion, we have

$$y(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + \mathcal{O}(t^5)$$

Given this expression of $y(t)$, we could also calculate its first derivative $\dot{y}(t)$

$$\rightsquigarrow \dot{y}(t) = 0 + c_1 + 2c_2 t + 3c_3 t^2 + 4c_4 t^3 + \mathcal{O}(t^4)$$

We substitute $\dot{y}(t)$ and $y(t)$ into the ordinary differential equation, $\dot{y}(t) = \lambda y(t)$

Solution by Taylor series expansion (cont.)

We substitute $\dot{y}(t)$ and $y(t)$ into the given ordinary differential equation, $\dot{y}(t) = \lambda y(t)$

$$\underbrace{0 + c_1 + 2c_2t + 3c_3t^2 + 4c_4t^3 + \mathcal{O}(t^4)}_{\dot{y}(t)} = \underbrace{\lambda c_0 + \lambda c_1t + \lambda c_2t^2 + \lambda c_3t^3 + \mathcal{O}(t^4)}_{\lambda y(t)}$$

The identity is satisfied when the coefficients of the powers of t in both sides match

$$\rightsquigarrow (t^0) \quad 1c_1 = \lambda c_0$$

$$\rightsquigarrow (t^1) \quad 2c_2 = \lambda c_1$$

$$\rightsquigarrow (t^2) \quad 3c_3 = \lambda c_2$$

$$\rightsquigarrow (t^3) \quad 4c_4 = \lambda c_3$$

$$\rightsquigarrow \dots$$

If we knew c_0 , we could calculate c_1 , then given c_1 we could calculate c_2 , from c_2 we could calculate c_3 , then given c_3 we could calculate c_4 , ...

$\rightsquigarrow c_0$ can be determined

Using the initial condition y_0 , we know that at $t = 0$, we have

$$y_0 = c_0 + \cancel{c_1t} + \cancel{c_2t^2} + \cancel{c_3t^3} + \dots$$

Solution by Taylor series expansion (cont.)

$$\rightsquigarrow c_0 = y_0$$

$$\rightsquigarrow c_1 = \lambda c_0 = \lambda y_0$$

$$\rightsquigarrow c_2 = \frac{1}{2}\lambda c_1 = \frac{1}{2}\lambda^2 y_0$$

$$\rightsquigarrow c_3 = \frac{1}{3}\lambda c_2 = \frac{1}{3!}\lambda^3 y_0$$

$$\rightsquigarrow c_4 = \frac{1}{4}\lambda c_3 = \frac{1}{4!}\lambda^4 y_0$$

$$\rightsquigarrow \dots$$

By substituting the coefficients $\{c_0, c_1, c_2, \dots\}$ in the series expansion of $y(t)$, we obtain

$$\begin{aligned} y(t) &= c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + \dots \\ &= y_0 + \lambda y_0 t + \frac{1}{2}\lambda^2 y_0 t^2 + \frac{1}{3!}\lambda^3 y_0 t^3 + \frac{1}{4!}\lambda^4 y_0 t^4 + \mathcal{O}(t^5) \\ &= \underbrace{\left[1 + \lambda t + \frac{1}{2}\lambda^2 t^2 + \frac{1}{3!}\lambda^3 t^3 + \frac{1}{4!}\lambda^4 t^4 + \mathcal{O}(t^5) \right]}_{\text{Exponential function } e^{\lambda t}} y_0 = e^{\lambda t} y_0 \end{aligned}$$



Solution by Taylor series expansion (cont.)

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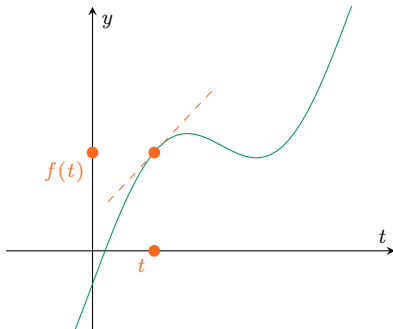
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Taylor series expansion

Any smooth function $f(t + \Delta t)$ can be expanded as a Taylor series at some point t

$$f(t \pm \Delta t) = f(t) + \frac{df(t)}{dt} \Delta t + \frac{d^2f(t)}{dt^2} \frac{(\Delta t)^2}{2!} + \frac{d^3f(t)}{dt^3} \frac{(\Delta t)^3}{3!} + \dots + \frac{d^n f(t)}{dt^n} \frac{(\Delta t)^n}{n!} + \dots$$



If we know the function, its first derivative, its second order derivative, ... at point t , we can approximate f near that point

↪ The more derivatives we add, the more accurate the approximation

$$\rightsquigarrow \text{Also, } f(t) = f(t_0) + \frac{df(t_0)}{dt}(t - t_0) + \frac{d^2f(t_0)}{dt^2} \frac{(t - t_0)^2}{2!} + \frac{d^3f(t_0)}{dt^3} \frac{(t - t_0)^3}{3!} + \dots$$

Solution by Taylor series expansion (cont.)

Example

Consider functions $f(t) = \sin(t)$ and $f(t) = \cos(t)$, compute the Taylor expansions

- Expand them about point $t_0 = 0$ (MacLaurin series expansions)

In general, we can write the expansion

$$f(t) = f(t_0) + \frac{df(t_0)}{dt}(t - t_0) + \frac{d^2f(t_0)}{dt^2}(t - t_0)^2 + \frac{d^3f(t_0)}{dt^3}(t - t_0)^3 + \dots$$

For the sine function, we have

$$\begin{aligned} \sin(t) &= \sin(0) + \cos(0)t - \frac{1}{2!}\sin(0)t^2 - \frac{1}{3!}\cos(0)t^3 + \frac{1}{4!}\sin(0)t^4 - \frac{1}{5!}\cos(0)t^5 + \dots \\ &= \cancel{\sin(0)} + \cos(0)t - \cancel{\frac{1}{2!}\sin(0)t^2} - \frac{1}{3!}\cos(0)t^3 + \cancel{\frac{1}{4!}\sin(0)t^4} - \frac{1}{5!}\cos(0)t^5 + \dots \\ &= t - \frac{t^3}{3!} + \frac{t^5}{5!} - \frac{t^7}{7!} + \dots = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} t^{2k+1} \end{aligned}$$

Solution by Taylor series expansion (cont.)

Calculus, review

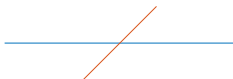
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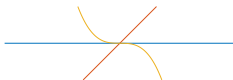
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$k = 0$



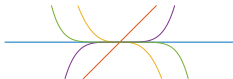
$k = 1$



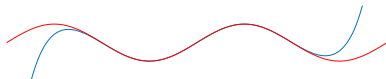
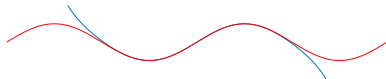
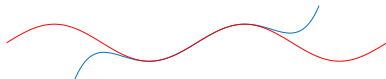
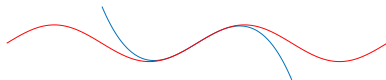
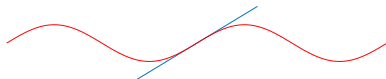
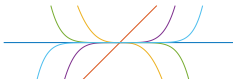
$k = 2$



$k = 3$



$k = 4$



Solution by Taylor series expansion (cont.)

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$$f(t) = f(t_0) + \frac{df(t_0)}{dt}(t - t_0) + \frac{d^2f(t_0)}{dt^2}(t - t_0)^2 + \frac{d^3f(t_0)}{dt^3}(t - t_0)^3 + \dots$$

For the cosine function, we have

$$\begin{aligned}\cos(t) &= \cos(0) - \cancel{\sin(0)t} - \frac{1}{2!}\cos(0)t^2 + \cancel{\frac{1}{3!}\sin(0)t^3} + \frac{1}{4!}\cos(0)t^4 - \cancel{\frac{1}{5!}\sin(0)t^5} + \dots \\ &= 1 - \frac{t^2}{2!} + \frac{t^4}{4!} - \frac{t^6}{6!} + \dots \\ &= \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} t^{2k}\end{aligned}$$

Solution by Taylor series expansion (cont.)

$$\cos(t) = 1 + 0t - \frac{t^2}{2!} + 0t^3 + \frac{t^4}{4!} + 0t^5 - \frac{t^6}{6!} + \dots = \sum_{k=0}^{\infty} \frac{(-1)^n}{(2n)!} t^{2n}$$

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1 tRange = -2*pi:0.01:+2*pi;           # Define the t-range
2
3 Fcos = @(t) cos(t);                  # Define functional variable
4                                       # Fcos of t
5
6 Ccos_1 = [0 1];                      # Set coefficients of a 1st
7   Tcos_1 = polyval(Ccos_1,xRange);   # order expansion, evaluation
8
9 Ccos_3 = [-1/factorial(2) 0 1];       # Set coefficients of a 2nd
10  Tcos_3 = polyval(Ccos_3,xRange);   # order expansion, evaluation
11
12 Ccos_5 = [1/factorial(4) 0 -1/factorial(2) 0 1]; # Set coefficients of a 3rd
13  Tcos_5 = polyval(Ccos_5,xRange);   # order expansion, evaluation
14
15 figure(1); hold on                   # Some plotting
16
17 fplot(Fcos);                          # Plots function Fcos
18
19 plot(xRange, Tcos_1);                  # Plots 1st approximation
20 plot(xRange, Tcos_3);                  # Plots 2nd approximation
21 plot(xRange, Tcos_5);                  # Plots 3rd approximation
22
23 hold off

```



Solution by Taylor series expansion (cont.)

We can consider the Taylor series expansion of the exponential function e^t (important)

$$\rightsquigarrow e^t = 1 + t + \frac{t^2}{2!} + \frac{t^3}{3!} + \frac{t^4}{4!} + \dots$$

We can consider the Taylor series expansion of the function $e^{\lambda t}$ (this is also important)

- By replacing t with λt , we obtain

$$\rightsquigarrow e^{\lambda t} = 1 + (\lambda t) + \frac{(\lambda t)^2}{2!} + \frac{(\lambda t)^3}{3!} + \frac{(\lambda t)^4}{4!} + \dots$$

We may want to write the Taylor series expansion of function e^{it} , with $i = \sqrt{-1}$

$$\begin{aligned} \rightsquigarrow e^{it} &= 1 + it + \frac{(it)^2}{2!} + \frac{(it)^3}{3!} + \frac{(it)^4}{4!} + \dots \\ &= 1 + it - \frac{t^2}{2!} - i\frac{t^3}{3!} + \frac{t^4}{4!} + i\frac{t^5}{5!} + \dots \\ &= \underbrace{1 - \frac{t^2}{2!} + \frac{t^4}{4!} + \dots}_{\cos(t)} + i \underbrace{\left(t - \frac{t^3}{3!} + \frac{t^5}{5!} + \dots\right)}_{\sin(t)} \\ &= \cos(t) + i \sin(t) \end{aligned}$$

Again, by replacing t with it

\rightsquigarrow (Euler's formula)

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Second- and higher-order systems

Ordinary differential equation

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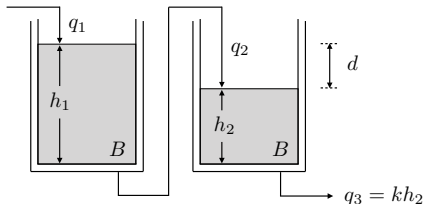
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Example

Two tanks (SS to IO representation and return)

Consider a system consisting of two cylindric liquid tanks, same cross section B [m²]

- A main inflow to tank 1, a main outflow from tank 2
- The outflow from tank 1 is the inflow to tank 2



First liquid tank

- Inflow, rate q_1 [m³s⁻¹]
- Outflow, rate q_2 [m³s⁻¹]
- h_1 is the liquid level [m]

Second liquid tank

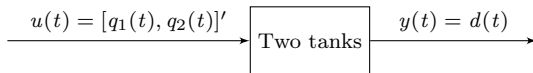
- Inflow, rate q_2 [m³s⁻¹]
- Outflow, rate q_3 [m³s⁻¹]
- h_2 is the liquid level [m]

Second- and higher-order systems (cont.)

Suppose that flow-rates q_1 and q_2 can be set to some desired value (pumps)

Also, suppose that q_3 depends linearly on the liquid level in the tank, h_2

- $q_3 = k \cdot h_2$ [m^3s^{-1}], with k [m^2s^{-1}] some appropriate constant



Inputs, q_1 and q_2 , both measurable and manipulable

↪ They influence the liquid levels in the tanks

Output, $d = h_1 - h_2$, measurable, not manipulable

↪ It is influenced by the inputs

State variables, V_1 and V_2 , not measurable and not manipulable

↪ They evolve according to own dynamics

↪ They are also influenced by the inputs

Second- and higher-order systems (cont.)

For an incompressible fluid, by mass conservation

$$\begin{cases} \frac{dV_1(t)}{dt} = q_1(t) - q_2(t) \\ \frac{dV_2(t)}{dt} = q_2(t) - q_3(t) \end{cases} \rightsquigarrow \begin{cases} \dot{h}_1(t) = \frac{1}{B}q_1(t) - \frac{1}{B}q_2(t) \\ \dot{h}_2(t) = \frac{1}{B}q_2(t) - \frac{k}{B}h_2(t) \end{cases}$$

By taking the first derivative of $y(t) = h_1(t) - h_2(t)$ and rearranging, we obtained

$$\dot{y}(t) = \dot{h}_1(t) - \dot{h}_2(t) = \frac{1}{B}u_1(t) - \frac{2}{B}u_2(t) + \frac{k}{B}[h_1(t) - y(t)]$$

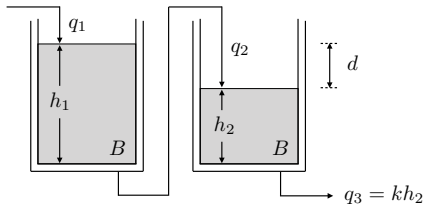
By taking the second derivative of $y(t)$ and rearranging, we obtained

$$\begin{aligned} \ddot{y}(t) &= \frac{1}{B}\dot{u}_1(t) - \frac{2}{B}\dot{u}_2(t) + \frac{k}{B}\dot{h}_1(t) - \frac{k}{B}\dot{y}(t) \\ &= \frac{1}{B}\dot{u}_1(t) - \frac{2}{B}\dot{u}_2(t) + \underbrace{\frac{k}{B^2}u_1(t) - \frac{k}{B^2}u_2(t)}_{\frac{k}{B}\dot{h}_1(t)} - \frac{k}{B}\dot{y}(t) \end{aligned}$$

Second- and higher-order systems (cont.)

Rearranging terms, the IO system's representation is an ordinary differential equation

$$\rightsquigarrow \ddot{y}(t) + \frac{k}{B}\dot{y}(t) - \frac{1}{B}\dot{u}_1(t) + \frac{2}{B}\dot{u}_2(t) - \frac{k}{B^2}u_1(t) + \frac{k}{B}u_2(t) = 0$$



Suppose that the inputs are zero

$$\rightsquigarrow u_1(t) = q_1(t) = 0$$

$$\rightsquigarrow u_2(t) = q_2(t) = 0$$

Also their derivatives are zero

$$\ddot{y}(t) + \frac{k}{B}\dot{y}(t) = +\cancel{\frac{1}{B}\dot{u}_1(t)} - \cancel{\frac{2}{B}\dot{u}_2(t)} + \cancel{\frac{k}{B^2}u_1(t)} - \cancel{\frac{k}{B}u_2(t)} \rightsquigarrow \ddot{y}(t) + \frac{k}{B}\dot{y}(t) = 0$$

What's $y(t)$, for some $y(0)$ and $\dot{y}(0)$?

Second- and higher-order systems (cont.)

Calculus, review

Intro to ODEs

Solution using a
Taylor expansionSecond- and
higher-orderFrom high to
first order ODEs**Homogeneous equation**

Consider the ordinary differential equation of a IO model (linear and time invariant)

$$\alpha_n \frac{d^n y(t)}{dt^n} + \dots + \alpha_1 \frac{dy(t)}{dt} + \alpha_0 y(t) = \beta_m \frac{d^m u(t)}{dt^m} + \dots + \beta_1 \frac{du(t)}{dt} + \beta_0 u(t)$$

Let the RHS of be zero, define the **homogenous equation** associated to the model

$$\rightsquigarrow a_n \frac{d^n y(t)}{dt^n} + \dots + a_1 \frac{dy(t)}{dt} + a_0 y(t) = 0$$

The solution $y(t)$ to the homogeneous equation can be defined as the system response (the output) for an input $u(t)$ that is null for $t \geq t_0$ and for given initial conditions**Input- or force-free response**

- We may denote it as $h(t)$



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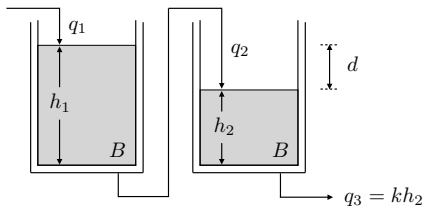
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Example

$$\ddot{y}(t) + \frac{k}{B}\dot{y}(t) = 0$$

Interest is in $y(t)$ for some given initial conditions $y(0)$ and $\dot{y}(0)$ (assuming $u(t) = 0$)

- We want to use the Taylor expansion of the solution $y(t)$
 - For simplicity, let $k/B = 1$
- ↪ We solve $\ddot{y}(t) + \dot{y}(t) = 0$



The differential equation is second-order

↪ Initial *position*

$$y(t=0) = y(0)$$

↪ Initial *velocity*

$$\dot{y}(t=0) = \dot{y}(0)$$

Second- and higher-order systems (cont.)

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$$\ddot{y}(t) + \dot{y}(t) = 0$$

- We assume that $y(t)$ can be expressed by using a Taylor series expansion

$$y(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + \dots$$

- We can compute the first derivative of the assumed solution $y(t)$, $\dot{y}(t)$

$$\dot{y}(t) = c_1 + 2c_2 t + 3c_3 t^2 + 4c_4 t^3 + 5c_5 t^4 + \dots$$

- We compute the second derivative of the assumed solution $y(t)$, $\ddot{y}(t)$

$$\ddot{y}(t) = 2c_2 + 2 \cdot 3c_3 t + 3 \cdot 4c_4 t^2 + 4 \cdot 5c_5 t^3 + \dots$$

- Then, proceed by substituting function and derivatives into the ODEs

Second- and higher-order systems (cont.)

$$y(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + \dots$$

After considering initial conditions $y(t=0) = y(0)$ and $\dot{y}(t=0) = \dot{y}(0)$, we have

$$y(t=0) = c_0 + \cancel{c_1 t} + \cancel{c_2 t^2} + \cancel{c_3 t^3} + \cancel{c_4 t^4} + \dots = y(0)$$

$$\rightsquigarrow c_0 = y(0)$$

$$\dot{y}(t=0) = c_1 + \cancel{2c_2 t} + \cancel{3c_3 t^2} + \cancel{4c_4 t^3} + \cancel{5c_5 t^4} + \dots = \dot{y}(0)$$

$$\rightsquigarrow c_1 = \dot{y}(0)$$

- Then, from the ordinary differential equation $\ddot{y}(t) + \dot{y}(t) = 0$ we have

$$\underbrace{2c_2 + 2 \cdot 3c_3 t + 3 \cdot 4c_4 t^2 + 4 \cdot 5c_5 t^3 + \dots}_{\ddot{y}(t)} = - \underbrace{(c_1 + 2c_2 t + 3c_3 t^2 + 4c_4 t^3 + 5c_5 t^4 + \dots)}_{\dot{y}(t)}$$

Second- and higher-order systems (cont.)

$$\underbrace{2c_2 + 2 \cdot 3c_3t + 3 \cdot 4c_4t^2 + 4 \cdot 5c_5t^3 + \dots}_{\ddot{y}(t)} = \underbrace{(-c_1 - 2c_2t - 3c_3t^2 - 4c_4t^3 - 5c_5t^4 - \dots)}_{\dot{y}(t)}$$

By equating the coefficients to satisfy the identity and rearranging, we obtain

$$\rightsquigarrow 2c_2 = -c_1$$

$$\rightsquigarrow 2 \cdot 3c_3 = -2c_2$$

$$\rightsquigarrow 3 \cdot 4c_4 = -3c_3$$

$$\rightsquigarrow 4 \cdot 5c_5 = -4c_4$$

$$\rightsquigarrow \dots$$

- $c_0 = y(0)$

- $c_1 = \dot{y}(0)$

- $c_2 = -\frac{1}{2}\dot{y}(0)$

- $c_3 = +\frac{1}{3!}\dot{y}(0)$

- $c_4 = -\frac{1}{4!}\dot{y}(0)$

- $c_5 = +\frac{1}{5!}\dot{y}(0)$

- \dots

Second- and higher-order systems (cont.)

$$y(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + \dots$$

Substituting the coefficients in the assumed (Taylor's) solution form, we obtain

$$\begin{aligned} y(t) &= y(0) + \dot{y}(0)t - \frac{1}{2}\dot{y}(0)t^2 + \frac{1}{3!}\dot{y}(0)t^3 - \frac{1}{4!}\dot{y}(0)t^4 + \frac{1}{5!}\dot{y}(0)t^5 - \dots \\ &= y(0) - \dot{y}(0) \underbrace{\left(-t + \frac{1}{2}t^2 - \frac{1}{3!}t^3 - \frac{1}{4!}t^4 + \frac{1}{5!}t^5 - \dots \right)}_{-1+e^{-t}} \\ &= \underbrace{y(0) + \dot{y}(0)}_{k_1} \underbrace{-\dot{y}(0)}_{k_2} e^{-t} \\ &= k_1 + k_2 e^{-t} \end{aligned}$$

With k_1 and k_2 constant values depending on the initial conditions

$$\rightsquigarrow k_1 = y(0) + \dot{y}(0)$$

$$\rightsquigarrow k_2 = -\dot{y}(0)$$

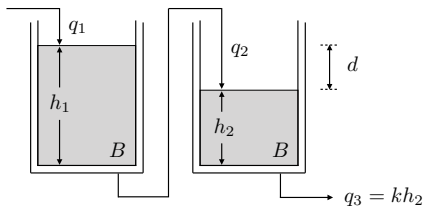
We used $e^{-t} = 1 + (-t) + \frac{(-t)^2}{2} + \frac{(-t)^3}{3!} + \dots$

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Example



$$\ddot{y}(t) + \dot{y}(t) = 0$$

For simplicity, we let $\frac{k}{B} = 1$ and obtained the system evolution by solving the ODE

$$y(t) = y(0) + \dot{y}(0) - \dot{y}(0)e^{-t}$$

```

1 y0 = ?; % Initial position, set me!
2 yd0 = ?; % Initial velocity, set me!
3
4 tMin = 0; % Initial time is zero,
5 tMax = ?; % Final time, set me!
6 tRnage = [tMin, tMax] % Define the time interval
7
8 yt = @(t) y0 + yd0 - yd0*exp(-t) % Define the solution function
9
10 fplot(yt, tRange) % Plot solution over time

```



Second- and higher-order systems (cont.)

Higher-order systems

Consider the general linear time-invariant system and homogeneous (with no inputs)

$$\alpha_n \frac{d^n y}{dt^n} + \alpha_{n-1} \frac{d^{n-1} y}{dt^{n-1}} + \cdots + \alpha_2 \frac{d^2 y}{dt^2} + \alpha_1 \frac{dy}{dt} + \alpha_0 y = 0$$

Or, equivalently

$$\alpha_n y^{(n)} + \alpha_{n-1} y^{(n-1)} + \cdots + \alpha_1 \ddot{y} + \alpha_0 y = 0$$

We consider an alternative to assuming that the solution is written as Taylor expansion

Instead of using Taylor expansions, we assume that the solution is given by $y(t) = e^{\lambda t}$

- (Which is not very different, in practice)

$$y(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + \cdots$$

$$e^{\lambda t} = 1 + \lambda t + \frac{(\lambda t)^2}{2!} + \frac{(\lambda t)^3}{3!} + \cdots$$

Second- and higher-order systems (cont.)

If we set the solution to be $y(t) = e^{\lambda t}$, then we can easily compute its derivatives

$$\rightsquigarrow \dot{y}(t) = \lambda e^{\lambda t}$$

$$\rightsquigarrow \ddot{y}(t) = \lambda^2 e^{\lambda t}$$

$$\rightsquigarrow \dots$$

$$\rightsquigarrow y^{(n)}(t) = \lambda^n e^{\lambda t}$$

These functions can be substituted into homogeneous linear time-invariant ODEs

$$\alpha_n y^{(n)} + \alpha_{n-1} y^{(n-1)} + \dots + \alpha_1 \dot{y} + \alpha_0 y = 0$$

By substituting the assumed solution and derivatives into the differential equation

$$\rightsquigarrow [\alpha_n \lambda^n + \alpha_{n-1} \lambda^{n-1} + \dots + \alpha_2 \lambda^2 + \alpha_1 \lambda + \alpha_0] e^{\lambda t} = 0$$

The identity is verified for all n values of λ solving the **characteristic equation**

$$\underbrace{\alpha_n \lambda^n + \alpha_{n-1} \lambda^{n-1} + \dots + \alpha_2 \lambda^2 + \alpha_1 \lambda + \alpha_0}_{\text{Characteristic polynomial}} = 0$$

Characteristic equation

Second- and higher-order systems (cont.)

$$\alpha_n \lambda^n + \alpha_{n-1} \lambda^{n-1} + \cdots + \alpha_2 \lambda^2 + \alpha_1 \lambda + \alpha_0 = 0$$

The characteristic equation has n solutions, or roots, collected in set $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$

- They can be real and/or complex (and associated complex-conjugate) numbers
 - They can be positive and/or negative, distinct and repeated (multiplicity)
-

$$\alpha_n y^{(n)} + \alpha_{n-1} y^{(n-1)} + \cdots + \alpha_1 \dot{y} + \alpha_0 y = 0$$

For distinct (real and complex) roots, the ODE solution has the simple form

$$\begin{aligned} y(t) &= c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t} + \cdots + c_n e^{\lambda_n t} \\ &= \sum_{i=1}^n c_i e^{\lambda_i t} \end{aligned}$$

The solution is a sum of exponential functions, each weighted by coefficients

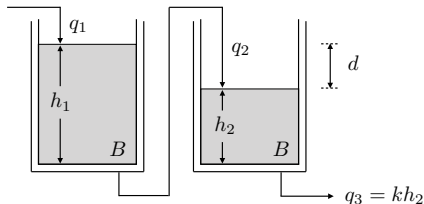
- The coefficients are determined from the n initial conditions

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Example



$$\ddot{y}(t) + \frac{k}{B}\dot{y}(t) = 0$$

For simplicity, let $\frac{k}{B} = 1$ and obtained the system evolution of $\ddot{y}(t) + \dot{y}(t) = 0$

$$y(t) = y(0) + \dot{y}(0) - \dot{y}(0)e^{-t}$$

Start by assuming a solution $y(t) = e^{\lambda t}$ and computing its derivatives $\dot{y}(t)$ and $\ddot{y}(t)$

- ↪ Substitute then in the original system ODE
- ↪ Compute the characteristic equation
- ↪ Solve the characteristic equation



Second- and higher-order systems (cont.)

Definition

Characteristic polynomial

Consider the homogeneous part of the linear and time-invariant differential equation

$$\alpha_n \frac{d^n y(t)}{dt^n} + \dots + \alpha_1 \frac{dy(t)}{dt} + \alpha_0 y(t) = 0$$

The **characteristic polynomial** is a n -order polynomial in the variable λ whose coefficients correspond to the coefficients $\{\alpha_0, \alpha_1, \dots, \alpha_n\}$ of the homogeneous equation

$$\begin{aligned} \rightsquigarrow P(\lambda) &= \alpha_n \lambda^n + \alpha_{n-1} \lambda^{n-1} + \dots + \alpha_1 \lambda + \alpha_0 \\ &= \sum_{i=0}^n \alpha_i \lambda^i \end{aligned}$$

Any polynomial of order n with real coefficients has n real or complex-conjugate roots

- The roots are solutions of the **characteristic equation**

$$\rightsquigarrow P(\lambda) = \sum_{i=0}^n \alpha_i \lambda^i = 0$$

Second- and higher-order systems (cont.)

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In general, there are $r \leq n$ **distinct roots** p_i , each with **multiplicity** ν_i

$$\rightsquigarrow \overbrace{p_1 \cdots p_1}^{\nu_1} \overbrace{p_2 \cdots p_2}^{\nu_2} \cdots \overbrace{p_r \cdots p_r}^{\nu_r}$$

\rightsquigarrow If $i \neq j$, then $p_i \neq p_j$

$$\rightsquigarrow \sum_{i=1}^r \nu_i = n$$

Consider the case in which all roots have multiplicity equal one (no repetitions)

$$\rightsquigarrow \overbrace{p_1 \ p_2 \ \cdots \ p_{n-1} \ p_n}^n$$

\rightsquigarrow If $i \neq j$, then $p_i \neq p_j$

$$\rightsquigarrow \nu_i = 1, \text{ for every } i$$

Second- and higher-order systems (cont.)

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Definition

Modes

Let p be one of the roots with multiplicity ν of the characteristic polynomial

The **modes** associated to that root are the ν functions of time

$$\rightsquigarrow e^{pt}, te^{pt}, t^2 e^{pt}, \dots, t^{\nu-1} e^{pt}$$

A system with a n -order characteristic polynomial has n modes

Let $p = 1$ and $\nu = 4$

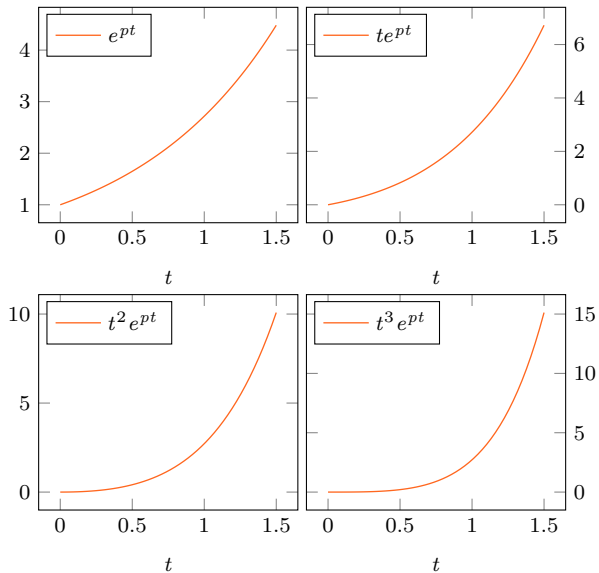
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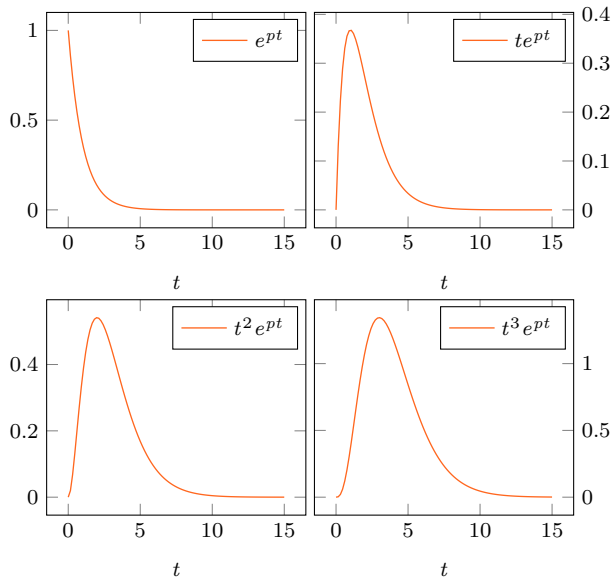
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Let $p = -1$ and $\nu = 4$



Second- and higher-order systems (cont.)

The modes from the characteristic polynomial, the mixing coefficients are parameters

$$h(t) = \sum_{i=1}^r \left(\sum_{k=0}^{\nu_i-1} A_{i,k} t^k e^{p_i t} \right)$$

The coefficients determine the force-free evolution, from every possible initial condition

Theorem

Solution of the homogeneous equation

Consider the homogeneous equation

$$a_n \frac{d^n y(t)}{dt^n} + \cdots + a_1 \frac{dy(t)}{dt} + a_0 y(t) = 0$$

A real function $h(t)$ is the solution of a homogeneous linear time-invariant differential equation if and only if $h(t)$ can be written as a linear combination of the modes

$$\rightsquigarrow h(t) = \sum_{i=1}^r \left(\sum_{k=0}^{\nu_i-1} A_{i,k} t^k e^{p_i t} \right)$$

Second- and higher-order systems (cont.)

Modes are functions of time, their linear combinations are a family of functions of time

- The family is parameterised by the coefficients of the combination
- (Different coefficients correspond to different family members)

Definition

Linear combinations of modes

A linear combination of the n modes is a function $h(t)$, a weighted sum of the modes

- Each mode is weighted by some coefficient

Each individual root p_i with multiplicity ν_i is associated to a combination of ν_i terms

$$A_{i,0} e^{p_i t} + A_{i,1} t e^{p_i t} + \cdots + A_{i,\nu_i-1} t^{\nu_i-1} e^{p_i t} = \underbrace{\sum_{k=0}^{\nu_i-1} A_{i,k} t^k e^{p_i t}}_{\text{root } p_i}$$

There is a total of r distinct roots, $i = 1, \dots, r$

Second- and higher-order systems (cont.)

$$A_{i,0}e^{p_i t} + A_{i,1}te^{p_i t} + \cdots + A_{i,\nu_i-1}t^{\nu_i-1}e^{p_i t} = \underbrace{\sum_{k=0}^{\nu_i-1} A_{i,k}t^k e^{p_i t}}_{\text{root } p_i}$$

As there are r distinct roots, $i = 1, \dots, r$, the complete linear combination of modes

$$h(t) = \underbrace{\sum_{k=0}^{\nu_1-1} A_{1,k}t^k e^{p_1 t}}_{\text{root } p_1} + \underbrace{\sum_{k=0}^{\nu_2-1} A_{2,k}t^k e^{p_2 t}}_{\text{root } p_2} + \cdots + \underbrace{\sum_{k=0}^{\nu_r-1} A_{r,k}t^k e^{p_r t}}_{\text{root } p_r}$$

$$\rightsquigarrow = \sum_{i=1}^r \left(\sum_{k=0}^{\nu_i-1} A_{i,k}t^k e^{p_i t} \right)$$

Consider the case in which all roots (n) have multiplicity equal to one (no repetitions)

$$\rightsquigarrow h(t) = A_1 e^{p_1 t} + A_2 e^{p_2 t} + \cdots + A_n e^{p_n t} = \sum_{i=1}^n A_i e^{p_i t}$$

(We have omitted the second subscript of coefficients A)

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Second- and higher-order systems (cont.)

Example

Consider the following homogenous differential equation

$$3\frac{d^4y(t)}{dt^4} + 21\frac{d^3y(t)}{dt^3} + 45\frac{d^2y(t)}{dt^2} + 39\frac{dy(t)}{dt} + 12y(t) = 0$$

The associated characteristic polynomial

$$P(\lambda) = 3\lambda^4 + 21\lambda^3 + 45\lambda^2 + 39\lambda + 12 = 3(\lambda + 1)^3(\lambda + 4)$$

The characteristic equation has four roots

↪ The system has four modes

$$p_1 = -1, \quad (\nu_1 = 3) \quad \rightsquigarrow \quad \begin{cases} e^{-t} \\ te^{-t} \\ t^2e^{-t} \end{cases}$$

$$p_2 = -4, \quad (\nu_2 = 1) \quad \rightsquigarrow \quad \begin{cases} e^{-4t} \end{cases}$$

The family of functions $h(t)$ is given as a linear combination of the modes

$$h(t) = \underbrace{A_{1,0}e^{-t} + A_{1,1}te^{-t} + A_{1,2}t^2e^{-t}}_{\text{root } p_1} + \underbrace{A_2e^{-4t}}_{\text{root } p_2}$$

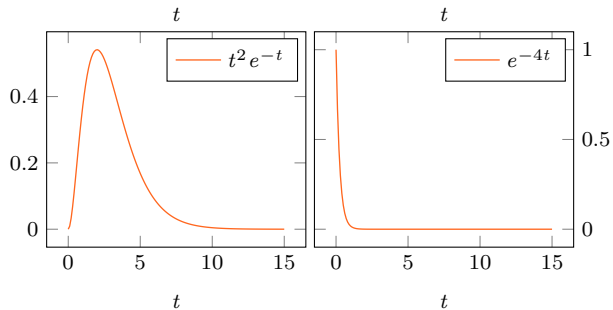
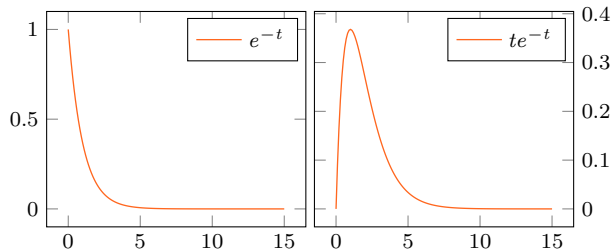
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Second- and higher-order systems (cont.)

Complex and conjugate roots

A characteristic polynomial $P(s)$ with complex roots will have complex signal modes

$$h(t) = \sum_{i=1}^r \left(\sum_{k=0}^{\nu_i-1} A_{i,k} t^k e^{p_i t} \right) \quad (\text{Yet, their combination must be a real function})$$

Let $P(s)$ be a characteristic polynomial with roots $p_i = \alpha_i + j\omega_i$ of multiplicity ν_i

- Let $p'_i = \alpha_i - j\omega_i$ with multiplicity $\nu'_i = \nu_i$ be the conjugate complex root

The contribution of each pair (p_i, p'_i) to the linear combination can be re-written

$$\sum_{k=0}^{\nu_i-1} M_{i,k} t^k e^{\alpha_i t} \cos(\omega_i t + \phi_{i,k}) \quad (\text{Coefficients } M_{i,k} \text{ and } \phi_{i,k})$$

Or, equivalently

$$\sum_{k=0}^{\nu_i-1} \left[B_{i,k} t^k e^{\alpha_i t} \cos(\omega_i t) + C_{i,k} t^k e^{\alpha_i t} \sin(\omega_i t) \right] \quad (\text{Coefficients } B_{i,k} \text{ and } C_{i,k})$$

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The solution equations

$$h(t) = \sum_{i=1}^R \sum_{k=0}^{\nu_i-1} A_{i,k} t^k e^{p_i t} + \sum_{i=R+1}^{R+S} \sum_{k=0}^{\nu_i-1} M_{i,k} t^k e^{\alpha_i t} \cos(\omega_i t + \phi_{i,k})$$

$$\left(\rightsquigarrow \sum_{i=1}^R A_i e^{p_i t} + \sum_{i=R+1}^{R+S} M_i e^{\alpha_i t} \cos(\omega_i t + \phi_i) \right)$$

The solution equations

$$h(t) = \sum_{i=1}^R \sum_{k=0}^{\nu_i-1} A_{i,k} t^k e^{p_i t} + \sum_{i=R+1}^{R+S} \sum_{k=0}^{\nu_i-1} \left[B_{i,k} t^k e^{\alpha_i t} \cos(\omega_i t) + C_{i,k} t^k e^{\alpha_i t} \sin(\omega_i t) \right]$$

$$\left(\rightsquigarrow \sum_{i=1}^R A_i e^{p_i t} + \sum_{i=R+1}^{R+S} \left[B_i e^{\alpha_i t} \cos(\omega_i t) + C_i e^{\alpha_i t} \sin(\omega_i t) \right] \right)$$

They provide the parametric structure of the linear combination and are all equivalent

Second- and higher-order systems (cont.)

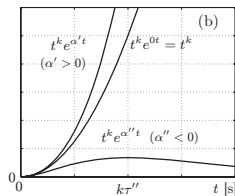
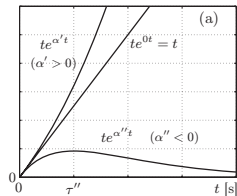
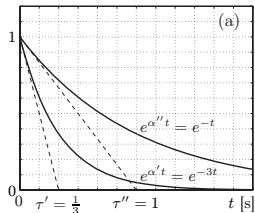
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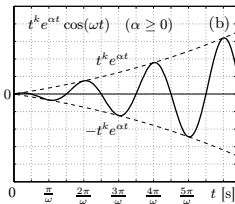
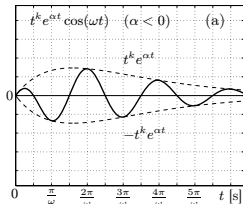
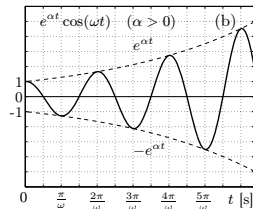
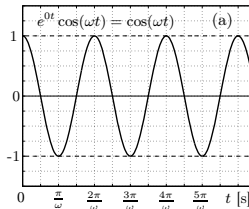
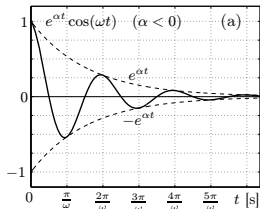
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From high to first order ODEs

Ordinary differential equation

From high-order ODEs to systems of first-order ODEs

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Consider the general linear time-invariant n -order system and homogeneous (no inputs)

$$\alpha_n \frac{d^n y}{dt^n} + \alpha_{n-1} \frac{d^{n-1} y}{dt^{n-1}} + \cdots + \alpha_2 \frac{d^2 y}{dt^2} + \alpha_1 \frac{dy}{dt} + \alpha_0 y = 0$$

Or, equivalently

$$\alpha_n y^{(n)} + \alpha_{n-1} y^{(n-1)} + \cdots + \alpha_1 \ddot{y} + \alpha_0 y = 0$$

We can convert the n -order equation into a set of n first order equations, and solve it

As a preprocessing step, we start by dividing all the coefficients by α_n

$$y^{(n)}(t) + \underbrace{\alpha_{n-1}}_{\alpha_{n-1}/\alpha_n} y^{(n-1)}(t) + \cdots + \underbrace{\alpha_2}_{\alpha_2/\alpha_n} \ddot{y}(t) + \underbrace{\alpha_1}_{\alpha_1/\alpha_n} \dot{y}(t) + \underbrace{\alpha_0}_{\alpha_0/\alpha_n} y = 0$$

From high-order ODEs to first-order ODEs (cont.)

$$y^{(n)}(t) + a_{n-1}y^{(n-1)}(t) + \cdots + a_2\ddot{y}(t) + a_1\dot{y}(t) + a_0y = 0$$

Firstly, we introduce a set of n new variables $x(t) = [x_1(t), x_2(t), \dots, x_n(t)]'$

$$x_1(t) = y(t)$$

$$x_2(t) = \dot{y}(t)$$

$$x_3(t) = \ddot{y}(t)$$

$$\dots = \dots$$

$$x_{n-1}(t) = y^{(n-2)}(t)$$

$$x_n(t) = y^{(n-1)}(t)$$

Then, we introduce their first-order derivatives $\dot{x}(t) = [\dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t)]'$

$$\dot{x}_1(t) = \dot{y}(t) = x_2(t)$$

$$\dot{x}_2(t) = \ddot{y}(t) = x_3(t)$$

$$\dot{x}_3(t) = \dddot{y}(t) = x_4(t)$$

$$\dots = \dots$$

$$\dot{x}_{n-1}(t) = y^{(n-1)}(t) = x_n(t)$$

$$\dot{x}_n(t) = y^{(n)}(t) = -a_{n-1}x_n(t) - a_{n-1}x_{n-1}(t) - \cdots - a_2x_3(t) - a_1x_2(t) - a_0x_1(t)$$

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From high-order ODEs to first-order ODEs (cont.)

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$$\dot{x}_1(t) = \dot{y}(t) = x_2(t)$$

$$\dot{x}_2(t) = \ddot{y}(t) = x_3(t)$$

$$\dot{x}_3(t) = \dddot{y}(t) = x_4(t)$$

$$\dots = \dots$$

$$\dot{x}_{n-1}(t) = y^{(n-1)}(t) = x_n(t)$$

$$\dot{x}_n(t) = y^{(n)}(t) = -a_{n-1}x_n(t) - a_{n-1}x_{n-1}(t) - \dots - a_2x_3(t) - a_1x_2(t) - a_0x_1(t)$$

That is, we get the set of linear equations with explicit dependences between terms

$$\dot{x}_1 = 0x_1 + 1x_2 + 0x_3 + 0x_4 + \dots + 0x_n$$

$$\dot{x}_2 = 0x_1 + 0x_2 + 1x_3 + 0x_4 + \dots + 0x_n$$

$$\dot{x}_3 = 0x_1 + 0x_2 + 0x_3 + 1x_4 + \dots + 0x_n$$

$$\dots = \dots$$

$$\dot{x}_{n-1} = 0x_1 + 0x_2 + 0x_3 + 0x_4 + \dots + 1x_n$$

$$\dot{x}_n = -a_0x_1 - a_1x_2 - a_2x_3 - a_3x_4 - \dots - a_{n-1}x_n$$

From high-order ODEs to first-order ODEs (cont.)

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$$\dot{x}_1 = 0x_1 + 1x_2 + 0x_3 + 0x_4 + \cdots + 0x_n$$

$$\dot{x}_2 = 0x_1 + 0x_2 + 1x_3 + 0x_4 + \cdots + 0x_n$$

$$\dot{x}_3 = 0x_1 + 0x_2 + 0x_3 + 1x_4 + \cdots + 0x_n$$

$$\dots = \dots$$

$$\dot{x}_{n-1} = 0x_1 + 0x_2 + 0x_3 + 0x_4 + \cdots + 1x_n$$

$$\dot{x}_n = -a_0x_1 - a_1x_2 - a_2x_3 - a_3x_4 - \cdots - a_{n-1}x_n$$

We can write a $\dot{x}(t)$ as a matrix-vector multiplication $Ax(t)$, a system of equations

$$\underbrace{\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \vdots \\ \dot{x}_{n-1} \\ \dot{x}_n \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ -a_0 & -a_1 & -a_2 & -a_3 & \cdots & -a_{n-1} \end{bmatrix}}_A \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix}}_{x(t)}$$

From high-order ODEs to first-order ODEs (cont.)

Example

Consider a linear and time-invariant homogeneous system representation

$$\ddot{y} + a_2\dot{y} + a_1y + a_0y = 0$$

- The system in IO representation is a third-order ODE

We are interested in formulating the system as a matrix system

- The system is third-order (max derivative of y)
- A system of 3 first-order ODEs

We first introduce three dummy variables $x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix}$

Then, we get

$$x_1(t) = y(t)$$

$$x_2(t) = \dot{y}(t)$$

$$x_3(t) = \ddot{y}(t)$$

From high-order ODEs to first-order ODEs (cont.)

$$\ddot{y} + a_2\dot{y} + a_1y + a_0y = 0$$

We compute the derivatives of the $x(t)$ variables with respect to time $\dot{x}(t) = \begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \dot{x}_3(t) \end{bmatrix}$

- Remember that we defined them as $x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix} = \begin{bmatrix} y(t) \\ \dot{y}(t) \\ \ddot{y}(t) \end{bmatrix}$

That is,

$$\begin{aligned} \dot{x}_1(t) &= \dot{y}(t) \\ &= x_2(t) \\ \dot{x}_2(t) &= \ddot{y}(t) \\ &= x_3(t) \\ \dot{x}_3(t) &= \dddot{y}(t) \\ &= -a_2x_3(t) - a_1x_2(t) - a_0x_1(t) \end{aligned}$$

In matrix form, we can write

$$\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \dot{x}_3(t) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix}$$

From high-order ODEs to first-order ODEs (cont.)

Example

Consider the following linear and time-invariant homogeneous system

$$3 \frac{d^4 y(t)}{dt^4} + 21 \frac{d^3 y(t)}{dt^3} + 45 \frac{d^2 y(t)}{dt^2} + 39 \frac{dy(t)}{dt} + 12y(t) = 0$$

The system in IO representation is a fourth-order ODE

↪ A system of 4 first-order ODEs

We first divide by the leading coefficient ($a_4 = 3$)

$$\frac{d^4 y(t)}{dt^4} + \underbrace{7}_{a_3} \frac{d^3 y(t)}{dt^3} + \underbrace{15}_{a_2} \frac{d^2 y(t)}{dt^2} + \underbrace{13}_{a_1} \frac{dy(t)}{dt} + \underbrace{4}_{a_0} y(t) = 0$$

By using the general expression derived earlier,

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 & -a_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

From high-order ODEs to first-order ODEs (cont.)

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$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 & -a_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -4 & -13 & -15 & -7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

```

1 A = [ 0  1  0  0; ...           % The state matrix
2       0  0  1  0; ...
3       0  0  0  1; ...
4       -4 -13 -15 -7 ];
5
6
7 x0 = randn(4,1);                % The initial condition (randomly chosen)
8
9 f = @(t,x) A*x;                  % The vector field (the dynamics)
10
11 tRange = 0:0.1:10;              % Time interval of interest (0 to 10, step
12     0.1)
13 [t,x_num] = ode45(f,tRange,x0); % Numerical solution

```



From high-order ODEs to first-order ODEs (cont.)

Example

Consider the second-order linear and homogeneous differential equation

$$\ddot{y}(t) + 3\dot{y}(t) + 2y(t) = 0$$

The initial conditions (at $t = 0$),

$$\begin{cases} y(0) = 2 \\ \dot{y}(0) = -3 \end{cases}$$

We want to determine its solution

We start by assuming that its solution is given by function $y(t) = e^{\lambda t}$

Then, we compute the derivatives of the assumed solution

- Up to order $n = 2$

Then, we have

$$\dot{y}(t) = \lambda e^{\lambda t}$$

$$\ddot{y}(t) = \lambda^2 e^{\lambda t}$$

From high-order ODEs to first-order ODEs (cont.)

Now we substitute the solution and its derivatives into the original equation, to get

$$\underbrace{\ddot{y}(t)}_{\lambda^2 e^{\lambda t}} + 3 \underbrace{\dot{y}(t)}_{\lambda e^{\lambda t}} + 2 \underbrace{y(t)}_{e^{\lambda t}} = 0$$

Rearranging, we have

$$\begin{aligned}\lambda^2 e^{\lambda t} + 3\lambda e^{\lambda t} + 2e^{\lambda t} &= 0 \\ e^{\lambda t} (\lambda^2 + 3\lambda + 2) &= 0\end{aligned}$$

The roots of the characteristic polynomial $\lambda^2 + 3\lambda + 2 = (\lambda + 2)(\lambda + 1) = 0$,

$$\begin{cases} \lambda_1 = -1 \\ \lambda_2 = -2 \end{cases} \quad (\text{Real, with negative real part})$$

We formulate the general solution,

$$\begin{aligned}y(t) &= C_1 e^{\lambda_1 t} + C_2 e^{\lambda_2 t} \\ &= C_1 e^{(-1)t} + C_2 e^{(-2)t}\end{aligned}$$

From high-order ODEs to first-order ODEs (cont.)

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$$y(t) = C_1 e^{(-1)t} + C_2 e^{(-2)t}$$

By using the initial conditions, we determine the unknown coefficients,

$$\begin{cases} y(t=0) = C_1 \underbrace{e^{-t}}_{=1} + C_2 \underbrace{e^{-2t}}_{=1} = 2 \\ \dot{y}(t=0) = -C_1 \underbrace{e^{-t}}_{=1} - 2C_2 \underbrace{e^{-2t}}_{=1} = -3 \end{cases}$$

We can then solve for C_1 and C_2 , to get the pair of coefficients

$$\rightsquigarrow C_1 = 1$$

$$\rightsquigarrow C_2 = 1$$

The solution is stable, as it is the sum of stable exponentials

$$y(t) = e^{-t} + e^{-2t}$$

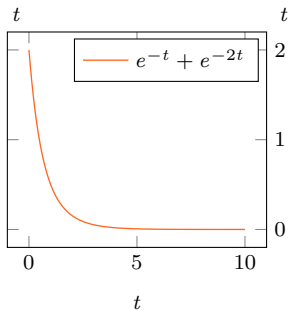
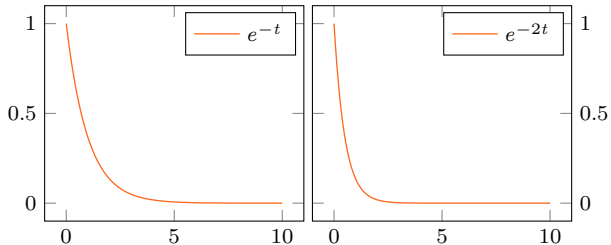
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From high-order ODEs to first-order ODEs (cont.)

We can reformulate $\ddot{y}(t) + 3\dot{y}(t) + 2y(t) = 0$ as a system of 2 first-order equations

- 1 We start by introducing two dummy variables

$$\begin{cases} x_1 = y^{(0)} \\ x_2 = y^{(1)} \end{cases}$$

- 2 We compute the time derivatives

$$\begin{cases} \dot{x}_1 = y^{(1)} = x_2 \\ \dot{x}_2 = y^{(2)} = -3x_2 - 2x_1 \end{cases}$$

- 3 Rewriting in matrix form

$$\underbrace{\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix}}_A \underbrace{\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}}_{x(t)}$$

Note how the two eigenvalues of A equal the roots of the characteristic polynomial



From high-order ODEs to first-order ODEs (cont.)

Example

Consider the second-order linear and homogeneous differential equation

$$\ddot{y}(t) - \underbrace{3\dot{y}(t)}_{\text{flipped sign}} + 2y(t) = 0$$

The same initial conditions (at $t = 0$),

$$\begin{cases} y(0) = 2 \\ \dot{y}(0) = -3 \end{cases}$$

We want to determine its solution

We start by assuming that its solution is given by function $y(t) = e^{\lambda t}$

Then, we compute the derivatives up to order $n = 2$, to get

$$\begin{aligned} \dot{y}(t) &= \lambda e^{\lambda t} \\ \ddot{y}(t) &= \lambda^2 e^{\lambda t} \end{aligned}$$

From high-order ODEs to first-order ODEs (cont.)

Now we substitute the solution and its derivatives into the original equation, to get

$$\underbrace{\ddot{y}(t)}_{\lambda^2 e^{\lambda t}} - 3 \underbrace{\dot{y}(t)}_{\lambda e^{\lambda t}} + 2 \underbrace{y(t)}_{e^{\lambda t}} = 0$$

Rearranging, we have

$$\begin{aligned}\lambda^2 e^{\lambda t} - 3\lambda e^{\lambda t} + 2e^{\lambda t} &= 0 \\ e^{\lambda t} (\lambda^2 - 3\lambda + 2) &= 0\end{aligned}$$

The roots of the characteristic polynomial $\lambda^2 - 3\lambda + 2 = (\lambda - 2)(\lambda - 1) = 0$,

$$\begin{cases} \lambda_1 = 1 \\ \lambda_2 = 2 \end{cases} \quad (\text{Real, with positive real part})$$

We formulate the general solution,

$$\begin{aligned}y(t) &= C_1 e^{\lambda_1 t} + C_2 e^{\lambda_2 t} \\ &= C_1 e^{(+1)t} + C_2 e^{(+2)t}\end{aligned}$$

From high-order ODEs to first-order ODEs (cont.)

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$$y(t) = C_1 e^t + C_2 e^{2t}$$

The solution is unstable because at least one of the exponentials in the sum is unstable

By using the initial conditions, we can still determine the unknown coefficients,

$$\begin{cases} y(t=0) = C_1 \underbrace{e^t}_{=1} + C_2 \underbrace{e^{2t}}_{=1} = 2 \\ \dot{y}(t=0) = C_1 \underbrace{e^t}_{=1} + 2C_2 \underbrace{e^{2t}}_{=1} = -3 \end{cases}$$

We can then solve for C_1 and C_2 , to get the pair of coefficients

$$\rightsquigarrow C_1 = 7$$

$$\rightsquigarrow C_2 = -5$$

The solution,

$$y(t) = 7e^t + 5e^{2t}$$

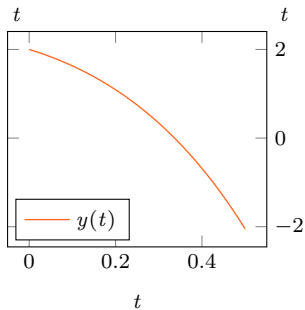
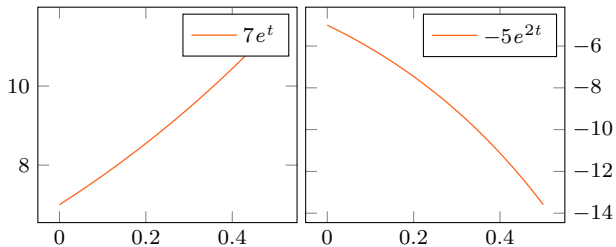
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Example

Consider the second-order linear and homogeneous differential equation

$$\ddot{y}(t) + 1\dot{y}(t) - 2y(t) = 0$$

The initial conditions (at $t = 0$),

$$\begin{cases} y(0) = 2 \\ \dot{y}(0) = -3 \end{cases}$$

We want to determine its solution



From high-order ODEs to first-order ODEs (cont.)

The roots of the characteristics polynomial and the eigenvalues of the state matrix

- The two are closely connected

This fact can be easily checked for small-size systems

Consider the general linear and homogeneous equation $y^{(3)} + a_2 y^{(2)} + a_1 y^{(1)} + a_0 y = 0$

- A third-order ordinary differential equation
- Its characteristic polynomial $P(\lambda)$

$$\lambda^3 + a_2 \lambda^2 + a_1 \lambda + a_0$$

The system as three first-order differential equations

$$\underbrace{\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \dot{x}_3(t) \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 \end{bmatrix}}_A \underbrace{\begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix}}_{x(t)},$$

(After we defined the dummy variables $x_1(t) = y(t)$, $x_2(t) = \dot{y}(t)$, and $x_3(t) = \ddot{y}(t)$)

From high-order ODEs to first-order ODEs (cont.)

The eigenvalues of matrix A are given by the values of λ such that $\det(A - \lambda I) = 0$

We have,

$$\begin{aligned} A - \lambda I &= \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 \end{bmatrix} - \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix} \\ &= \begin{bmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ -a_0 & -a_1 & -a_2 - \lambda \end{bmatrix} \end{aligned}$$

The determinant,

$$\begin{aligned} \det \begin{bmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ -a_0 & -a_1 & -a_2 - \lambda \end{bmatrix} &= -\lambda [\lambda(\lambda + a_2) + a_1] - a_0 \\ &= -\lambda [\lambda^2 + a_2\lambda + a_1] - a_0 \\ &= -\lambda^3 - a_2\lambda^2 - a_1\lambda - a_0 \end{aligned}$$

The determinant is zero for values of λ that are roots of the characteristic polynomial

The eigenvalues of A correspond to the roots of the characteristic polynomial $P(\lambda)$

\rightsquigarrow This is because $\det(A - \lambda I) = 0$ equals $P(\lambda)$

Calculus, review

Intro to ODEs

Solution using a
Taylor expansionSecond- and
higher-orderFrom high to
first order ODEs

Example

Consider a linear and time-invariant homogeneous ODE $\ddot{y} + a_2\dot{y} + a_1y + a_0y = 0$

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\begin{aligned} A - \lambda I &= \underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 \end{bmatrix}}_A - \lambda \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_I = \begin{bmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ -a_0 & -a_1 & -a_2 - \lambda \end{bmatrix} \\ &= -\lambda \left[-\lambda(-\lambda - a_2) + a_1 \right] + 1 \left[-a_0 \right] + 0 \\ &= -\lambda^3 - \lambda^2 a_2 - \lambda a_1 - a_0 \\ &\rightsquigarrow \lambda^3 + a_2 \lambda^2 + a_1 \lambda + a_0 = 0 \end{aligned}$$



From high-order ODEs to first-order ODEs (cont.)

When we convert a N_x -order ordinary differential equation that is linear and homogeneous, we obtain a system of n first-order ordinary differential equations (unforced)

The general form of the system,

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

We will look more closely at it

Case 1: The dynamics of the state variables are decoupled

Let $x(t) = (x_1(t), x_2(t), \dots, x_{N_x}(t))'$ be the set of state variables

- The evolution of state variable x_i is not affected by x_j
- For all pairs (i, j) , with $i, j \in \{1, \dots, N_x\}$
- We say, the dynamics are decoupled

This condition corresponds to a special structure of matrix A

- Matrix A is diagonal

$$\underbrace{\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \vdots \\ \dot{x}_n(t) \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}}_A \underbrace{\begin{bmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_n(t) \end{bmatrix}}_{x(t)}$$

From high-order ODEs to first-order ODEs (cont.)

$$\underbrace{\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \vdots \\ \dot{x}_n(t) \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}}_A \underbrace{\begin{bmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_n(t) \end{bmatrix}}_{x(t)}$$

The dynamics of the individual state variables have this simple structure

$$\begin{cases} \dot{x}_1 = \lambda_1 x_1(t) \\ \dot{x}_2 = \lambda_2 x_2(t) \\ \vdots \\ \dot{x}_n = \lambda_n x_n(t) \end{cases}$$

We can solve them for a initial condition $x(0) = (x_1(0), x_2(0), \dots, x_{N_x}(0))'$

$$\begin{cases} x_1(t) = e^{\lambda_1 t} x_1(0) \\ x_2(t) = e^{\lambda_2 t} x_2(0) \\ \vdots \\ x_n(t) = e^{\lambda_n t} x_n(0) \end{cases}$$

From high-order ODEs to first-order ODEs (cont.)

When we re-write the system of solutions in vector form, we obtain the general solution

$$\underbrace{\begin{bmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_n(t) \end{bmatrix}}_{x(t)} = \underbrace{\begin{bmatrix} e^{\lambda_1 t} & 0 & \cdots & 0 \\ 0 & e^{\lambda_2 t} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{\lambda_n t} \end{bmatrix}}_{e^{At}} \underbrace{\begin{bmatrix} x_1(0) \\ x_2(0) \\ \vdots \\ x_n(0) \end{bmatrix}}_{x(0)}$$

The matrix exponential of the state matrix A is a matrix, e^{At} , and it has size $N_x \times N_x$

- Its computation is generally difficult for an arbitrary matrix A
- But, it is very easy to compute when matrix A is diagonal

Matrix e^{At} is called the **state transition matrix**

- It makes state variables transition in time
- From an initial condition $x(0)$, to $x(t)$
- According to $x(t) = e^{At}x(0)$
- (Remember $y(t) = e^{\lambda t}y_0$)

From high-order ODEs to first-order ODEs (cont.)

Case 2: The dynamics of the state variables are not decoupled

The standard form of the state-space model $\dot{x}(t) = Ax(t)$ characterises the (unforced) dynamics in a coordinate system whose components are physically meaningful, typically

- The components $x = (x_1, x_2, \dots, x_{N_x})'$ often correspond to physical variables
- Because our state-space models are usually derived from conservation laws

Though interpretable from a process viewpoint, this representation is however arbitrary and not necessarily convenient in terms of solving for the time evolution of the system

- The solution to systems with decoupled dynamics is much easier to compute
- Simplicity is merely due to the difficulty to compute matrix exponentials

However, the vast majority of process systems do not present decoupled dynamics

- Composition of compounds affect each other
- Temperature affects compositions
- ...