(Systems of) Differential Equations [DEs]

Chemical reactions:

Example 1 $\quad A \xrightarrow{k_1>0} B$ ← reaction rate (given)

can be modelled by two DEs:

$' = \frac{d}{dt}$

$$\begin{cases} [A]' = -k_1[A] \,, & [A](0) = A_0 \\ [B]' = k_1[B] \,, & [B](0) = B_0 \end{cases}$$ ← initial values (given)

define $\begin{cases} x = [A] \\ y = [B] \end{cases} \Rightarrow \begin{cases} x' = -k_1 x \,, & x(0) = A_0 \\ y' = k_1 y \,, & y(0) = B_0 \end{cases}$

$$\Leftrightarrow \begin{cases} \begin{pmatrix} x \\ y \end{pmatrix}' = \begin{pmatrix} -k_1 & 0 \\ 0 & k_1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \\ \begin{pmatrix} x \\ y \end{pmatrix}(0) = \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \end{cases}$$ ← 2 by 2 matrix

$$\Leftrightarrow \begin{cases} \vec{x}' = A\vec{x} \\ \vec{x}(0) = \vec{A}_0 \end{cases}$$

linear system of ODEs ↕ ordinary

Example 2 $\quad A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$

$$\begin{cases} [A]' = -k_1[A] + k_2[B] \\ [B]' = k_1[A] - k_2[B] \end{cases}$$

linear system of ODEs

Example 3

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} AB$$

$$\begin{cases} [A]' = -k_1 \cdot [A] \cdot [B] + k_2 \cdot [AB] \\ [B]' = -k_1 \cdot [A] \cdot [B] + k_2 \cdot [AB] \\ [AB]' = k_1 \cdot [A] \cdot [B] - k_2 \cdot [AB] \end{cases}$$

non-linear

(matrix)

Example 4

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} AB$$

$$2A + C \underset{k_4}{\overset{k_3}{\rightleftharpoons}} A_2C$$

$$\begin{cases} [A]' = -k_1 \cdot [A] \cdot [B] + k_2 [AB] - k_3 [A]^2 [C] + k_4 [A_2C] \\ [B]' = -k_1 \cdot [A] \cdot [B] + k_2 [AB] \\ [AB]' = k_1 \cdot [A] \cdot [B] - k_2 [AB] \\ [C]' = -k_3 \cdot [A]^2 [C] + k_4 [A_2C] \\ [A_2C]' = k_3 \cdot [A]^2 [C] - k_4 [A_2C] \end{cases}$$

nonlinear system of five DEs

A linear system of DEs (in general):

$$\vec{x}'(t) = A \cdot \vec{x}(t)$$

time-derivative (componentwise)

A: n by n matrix

$\vec{x}(t)$: vector $\begin{pmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_n(t) \end{pmatrix}$

$n=1$: $\begin{cases} x'(t) = a \cdot x(t) \\ x(0) = x_0 \end{cases}$ given

"1 by 1 matrix"

solution: $x(t) = e^{at} \cdot x_0$

check: $\begin{cases} x'(t) = a \cdot e^{at} \cdot x_0 \\ a \cdot x(t) = a \cdot e^{at} \cdot x_0 \end{cases}$))! ☺

$n > 1$: we "try" $\vec{x}(t) = e^{\lambda t} \cdot \vec{v}$ (to be determined)

substitute this trial function in: $\vec{x}'(t) = A\vec{x}(t)$ ⊙ (A: n by n matrix)

$\Rightarrow \vec{x}'(t) = (e^{\lambda t}\vec{v})' = (e^{\lambda t})' \cdot \vec{v} = \lambda e^{\lambda t} \cdot \vec{v}$ [*]

and $\vec{x}'(t) = A\vec{x}(t) = A e^{\lambda t}\vec{v}$ [**]

[*] must be equal to [**]: $A e^{\lambda t}\vec{v} = \lambda e^{\lambda t}\vec{v}$

divide by $e^{\lambda t}$ (which is $\neq 0$): $\boxed{A\vec{v} = \lambda\vec{v}}$

$\Leftrightarrow$ (!!) λ is an eigenvalue of the matrix A ("fingerprint") with eigenvector $\vec{v}$

given linear system ⊙: find λ and $\vec{v}$!

$\Rightarrow \vec{x}(t) = e^{\lambda t}\vec{v}$ solves ⊙

Suppose $\lambda_1, \lambda_2, \dots, \lambda_n$ are eigenvalues of the matrix A with accompanying eigenvectors $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_n$.

Then the solutions of the original linear system of DEs:

$$\vec{x}^{(1)}(t) = e^{\lambda_1 t}\vec{v}_1, \quad \vec{x}^{(2)}(t) = e^{\lambda_2 t}\vec{v}_2, \quad \dots, \quad \vec{x}^{(n)}(t) = e^{\lambda_n t}\vec{v}_n$$

solution(1) solution(2) solution(n)

The general solution (via the superposition principle for linear differential equations)

$$\Downarrow$$

$$\vec{x}(t) = C_1 e^{\lambda_1 t}\vec{v}_1 + C_2 e^{\lambda_2 t}\vec{v}_2 + \dots + C_n e^{\lambda_n t}\vec{v}_n$$

to be determined from n initial conditions: (at $t=0$)

$$\vec{x}(0) = \vec{x}_0 \leftarrow \text{given}$$

Example $n=2$: $\vec{x}'(t) = \underbrace{\begin{pmatrix} 3 & 6 \\ 6 & 3 \end{pmatrix}}_{=A}\vec{x}(t)$, $\vec{x}(0) = \underbrace{\begin{pmatrix} 3 \\ -1 \end{pmatrix}}_{=\vec{x}_0}$

eigenvalues of A: $\lambda_1 = 9$, $\lambda_2 = -3$ with $\vec{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\vec{v}_2 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$

$$\Rightarrow \vec{x}(t) = C_1 e^{9t}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + C_2 e^{-3t}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

apply initial conditions: $\vec{x}(0) = C_1 \underbrace{e^{0}}_{=1}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + C_2 \underbrace{e^{-0}}_{=1}\begin{pmatrix} -1 \\ 1 \end{pmatrix} \overset{\text{must be}}{=\!=} \begin{pmatrix} 3 \\ -1 \end{pmatrix}$

$\Longrightarrow$ find C_1 and C_2 from: $\begin{cases} C_1 - C_2 = 3 \\ C_1 + C_2 = -1 \end{cases} \Rightarrow \begin{cases} C_1 = 1 \\ C_2 = -2 \end{cases}$

$$\Longrightarrow \vec{x}(t) = 1.\begin{pmatrix} 1 \\ 1 \end{pmatrix}e^{9t} - 2\begin{pmatrix} 1 \\ -1 \end{pmatrix}e^{-3t} \Rightarrow \begin{cases} x_1(t) = e^{9t} + 2e^{-3t} \\ x_2(t) = e^{9t} - 2e^{-3t} \end{cases}$$

A special form of DEs:

"separable equations"

$$y'(t) = f(t) \cdot g(y(t))$$

given functions

⇕ re-write

$$\frac{dy}{dt} = f(t) \cdot g(y)$$

⇕ "divide"

$$\frac{dy}{g(y)} = f(t)\,dt$$

⇕ integrate (both sides)

$$\int \frac{dy}{g(y)} = \int f(t)\,dt$$

find "primitives" ("anti-derivates")

$$\Leftrightarrow \quad G(y) = F(t) + C$$

integration constant

!!!

G=?, F=?

→! note that we define G as the primitive of $\frac{1}{g}$!

"solve", "take G^{-1} on both sides"

$$y = G^{-1}(F(t) + C)$$

$y(t)$

comes from the initial condition

$$y(t_0) = y_0$$

given (mostly = 0)

given value

will be clear in examples

Example 1

$$\begin{cases} y' = \lambda y \\ y(0) = 1 \end{cases}$$

λ: given constant

$$\Leftrightarrow \frac{dy}{dt} = \lambda y \Leftrightarrow \frac{dy}{y} = \lambda\, dt \Leftrightarrow \int \frac{dy}{y} = \int \lambda\, dt \Leftrightarrow \int \frac{dy}{y} = \lambda \cdot \int 1\, dt$$

$$\Longleftrightarrow \ln(y) = \lambda t + C$$

$\ln$: natural logarithm

$$\Leftrightarrow y = e^{\lambda t + C}$$

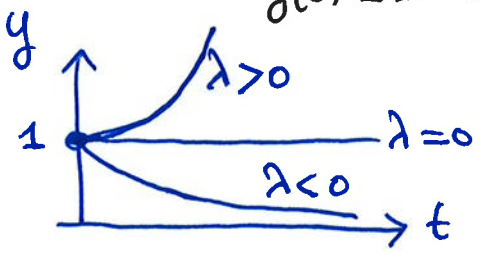
$$\Leftrightarrow y = e^{\lambda t} \cdot e^{C}$$

$$y(0) = 1 \Rightarrow 1 = e^{0} \cdot e^{C} \Rightarrow C = 0$$

$$\Downarrow$$

$$y = e^{\lambda t}$$

$=$ $y(t)$



Example 2

$$\begin{cases} y' = 3yt^2 \\ y(0) = 2 \end{cases}$$

$$\Leftrightarrow \frac{dy}{y} = 3t^2 dt \Leftrightarrow \int \frac{dy}{y} = 3\int t^2 dt \Leftrightarrow \ln(y) = 3 \cdot \frac{1}{3} t^3 + C$$

$$\Leftrightarrow \ln(y) = t^3 + C$$

$$\Leftrightarrow y = e^{t^3} \cdot e^{C}$$

$$y(0) = \underbrace{e^{0^3}}_{=1} \cdot e^{C} = 2 \Rightarrow C = \ln(2)$$

$$y = e^{t^3} \cdot e^{\ln(2)}$$

$$= 2 \cdot e^{t^3}$$

$=$ $y(t)$

Example 3

$$\begin{cases} y' = e^{t-y} \\ y(0) = 5 \end{cases}$$

$$\Leftrightarrow \frac{dy}{dt} = e^t \cdot e^{-y} \Leftrightarrow \frac{dy}{e^y} = e^t dt \Leftrightarrow e^y dy = e^t dt$$

$$\Leftrightarrow \int e^y dy = \int e^t dt$$

$$\Leftrightarrow e^y = e^t + C$$

$$\Leftrightarrow y = \ln(e^t + C)$$

$$y(0) = \ln(\underbrace{e^0}_{=1} + C) = 5 \Rightarrow \ln(1+C) = 5$$

$$\Downarrow C = -1 + e^5$$

$$y = \ln(e^t - 1 + e^5)$$

$\parallel$

$y(t)$

etcetera etcetera .....

BUT, be careful!

Example 4

$$\begin{cases} y' = 2\sqrt{y} \\ y(0) = 0 \end{cases}$$

$$\Leftrightarrow \int \frac{dy}{\sqrt{y}} = 2\int 1\, dt \Leftrightarrow 2\sqrt{y} = 2t + C \Leftrightarrow y = \left(t + \frac{C}{2}\right)^2$$

$$y(0) = \left(\frac{C}{2}\right)^2 = 0 \Rightarrow C = 0$$

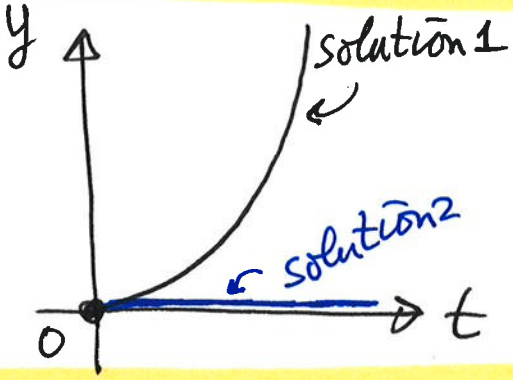
$$\Downarrow$$

$$y(t) = t^2$$

!?! $y(t) = 0$, for all values of t ("$\forall$")

also solves this DE! → check $0' = 2\sqrt{0}$ ✓ ($0' = 0$, $2\sqrt{0} = 0$) and $y(0) = 0$ ✓

in a picture:



Another (special) example

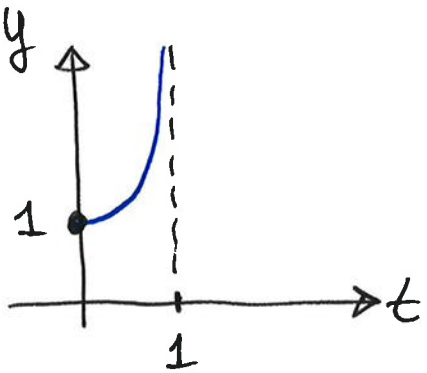
Example 5

$$\begin{cases} y' = y^2 \\ y(0) = 1 \end{cases}$$

$$\Leftrightarrow \int \frac{dy}{y^2} = \int 1\,dt \Leftrightarrow -\frac{1}{y} = t + c \Leftrightarrow y = -\frac{1}{t+c}$$

$y(0)=1$: $1 = -\frac{1}{0+c} \Rightarrow c = -1$

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

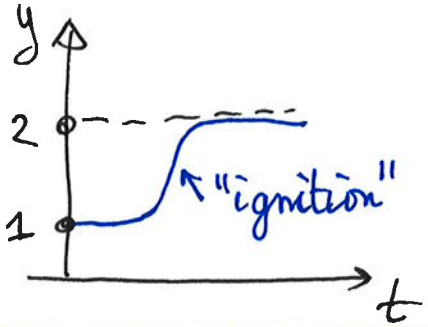


solution $y(t)$ exists only for $t \in [0,1)$! ← 1 excluded

Nonlinear example from chemistry: Example 6

$$\begin{cases} y' = (2-y)\,e^{-20/y} \\ y(0) = 1 \end{cases}$$

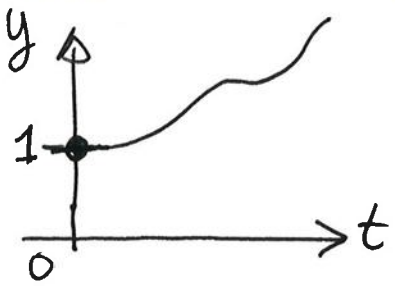
No formula for the solution $y(t)$ known!
($\Rightarrow$ need numerical solution)



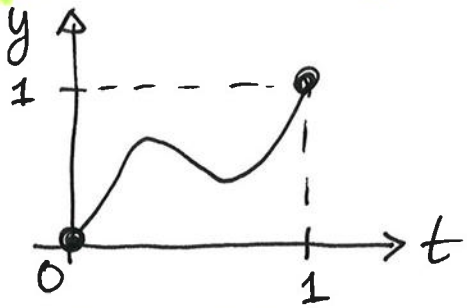
Initial-value problems $\longleftrightarrow$ Boundary-value problems

(second order DEs)

$$\begin{cases} y'' + y = 0 \\ y(0) = 1 \\ y'(0) = 0 \end{cases} \qquad y(t) = ?$$



$$\begin{cases} y'' + y = 0 \\ y(0) = 0 \\ y(1) = 1 \end{cases} \qquad y(t) = ?$$



A nonlinear boundary-value problem (from chemistry and also in astrophysics)

$$\begin{cases} y'' + \lambda e^{y} = 0 \\ y(0) = y(1) = 0 \end{cases}$$

parameter λ

* $\lambda \leq 0$: one solution $y(t)$
* $0 < \lambda < 3.5\ldots$: two solutions $y_1(t)$ and $y_2(t)$
* $\lambda = 3.5\ldots$: one solution $y(t)$
* $\lambda > 3.5\ldots$: NO solutions exist!

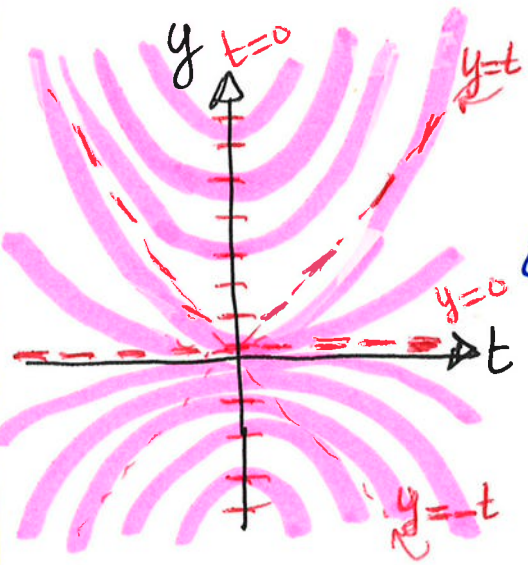
Direction field of a differential equation

* Draw/sketch in the t-y plane in "all" points (t,y), --- as many points as possible --, the "slope" (= richtingscoëfficiënt)
* all solutions of the DE must follow these directions
  ⇝ connect the points, while checking the slopes.
* Note: $y' = \frac{dy}{dt}$ is the slope of the solution $y(t)$, which is the solution of the DE $y' = f(t,y)$.
  ↑ known/given

example: $y' = ty$

$$\begin{cases} \text{in } t=0: y' = 0 \cdot y = 0 \Rightarrow \text{—} \\ \text{in } y=0: y' = t \cdot 0 = 0 \Rightarrow \text{—} \\ \text{in } y=t: y' = t^2 \Rightarrow \text{⟋} \\ \text{in } y=-t: y' = -t^2 \Rightarrow \text{⟍} \end{cases}$$

"et cetera" ---



check: $\int \frac{dy}{y} = \int t\,dt$

$\Leftrightarrow \ln(y) = \frac{1}{2}t^2 + c$

$\Leftrightarrow y = e^{\frac{1}{2}t^2} \cdot \text{constant}$ ("e^c")

← —curves

A linear second-order differential equation

$$y'' + p(t)\,y' + q(t)\,y = r(t) \qquad y(t) = ?$$

$p(t)$, $q(t)$: given functions of time t

$r(t)$: "inhomogeneous term" (given)

If $r(t) = 0$, then homogeneous DE

"Superposition-principle" for linear homogeneous DEs:

If $y_1(t)$ is a solution of DE (with $r \equiv 0$) AND $y_2(t)$ is another solution, then: every linear combination

$y(t) = c_1 y_1(t) + c_2 y_2(t)$ also solves this DE (!)

We can check this very easily:

$$y' = \frac{dy}{dt} = \frac{d}{dt}\left(c_1 y_1(t) + c_2 y_2(t)\right) = c_1 \frac{dy_1}{dt} + c_2 \frac{dy_2}{dt}$$

and $$y'' = \frac{d^2y}{dt^2} = \dots = c_1 \frac{d^2y_1}{dt^2} + c_2 \frac{d^2y_2}{dt^2}$$

substitute in DE:



$$\frac{d^2y}{dt^2} + p(t)\frac{dy}{dt} + q(t)y = c_1\frac{d^2y_1}{dt^2} + c_2\frac{d^2y_2}{dt^2} + p(t)\left[c_1\frac{dy_1}{dt} + c_2\frac{dy_2}{dt}\right] + q(t)\left[c_1y_1 + c_2y_2\right]$$

$$= c_1\left[\frac{d^2y_1}{dt^2} + p(t)\frac{dy_1}{dt} + q(t)y_1\right] + c_2\left[\frac{d^2y_2}{dt^2} + p(t)\frac{dy_2}{dt} + q(t)y_2\right]$$

y_1 and y_2 are solutions of DE

$$= c_1 \cdot 0 + c_2 \cdot 0 = 0 \quad \S$$

($y(t) = c_1y_1 + c_2y_2$ is a solution of DE)

Example: $y'' - y = 0$

$y_1(t) = e^t$ solves this DE AND $y_2(t) = e^{-t}$ also!

check: $\begin{cases} (e^t)'' - e^t = e^t - e^t = 0 \ \S \\ (e^{-t})'' - e^{-t} = e^{-t} - e^{-t} = 0 \ \S \end{cases}$

"two times $-$ = $+$"

$\Rightarrow y(t) = c_1e^t + c_2e^{-t}$ is a solution.

c_1, c_2 will be found by two extra conditions

For example: $y(0) = 4$ & $y'(0) = -2$

$y(0) = c_1e^0 + c_2e^{-0} = c_1 + c_2 = 4$

$y'(t) = c_1e^t - c_2e^{-t} \Rightarrow y'(0) = c_1 - c_2 = -2$

$\Rightarrow \begin{matrix} c_1 = 1 \\ c_2 = 3 \end{matrix}$

$\Rightarrow y(t) = e^t + 3e^{-t}$

Second-order linear homogeneous DE

with constant p and q

$$y'' + py' + qy = 0$$

(+ two extra conditions, to be specified in the exercise/model)

p, q: given constants

Try solutions of the form: $y(t) = e^{\lambda t}$

λ: yet unknown

Substitute in DE: $\lambda^2 e^{\lambda t} + p\lambda e^{\lambda t} + q e^{\lambda t} = 0$

Divide by $e^{\lambda t}$ (which is $\neq 0$)

$$\Rightarrow \quad \lambda^2 + p\lambda + q = 0 \qquad (p, q \text{ given numbers})$$

Apply "abc"-formule

$$\lambda_{1,2} = \frac{-p \pm \sqrt{p^2 - 4q}}{2}$$

$\Rightarrow$ Three possible situations:

1) $p^2 - 4q > 0$
2) $p^2 - 4q = 0$
3) $p^2 - 4q < 0$

Case I $p^2 > 4q \Rightarrow \lambda_1 \in \mathbb{R}, \lambda_2 \in \mathbb{R}$ and $\lambda_1 \neq \lambda_2$

solutions are: $e^{\lambda_1 t}$ and $e^{\lambda_2 t}$

$\Rightarrow$ "superposition principle" $y(t) = c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t}$

Case II $p^2 = 4q \Rightarrow \lambda_1 = \lambda_2 = \frac{-p}{2}$

solutions are: $e^{\lambda_1 t}$ and ~~$e^{\lambda_2 t} = e^{\lambda_1 t}$~~ (?) $\rightarrow t e^{\lambda_1 t}$

$\Rightarrow y(t) = c_1 e^{\lambda_1 t} + c_2 t e^{\lambda_1 t}$

$= (c_1 + c_2 t) e^{\lambda_1 t}$ $\quad (= (c_1 + c_2 t) e^{\lambda_2 t} \text{---})$

Case III $p^2 < 4q \Rightarrow \lambda_{1,2} = \frac{-p \pm \sqrt{4q - p^2} \cdot i}{2}$ ($\sqrt{-1}$)

note: $\lambda_2 = \overline{\lambda_1}$ (example: $\lambda_1 = 1+i$ and $\lambda_2 = 1-i$)

solutions are: $e^{(\alpha+\beta i)t}$ and $e^{(\alpha-\beta i)t}$

with $\alpha = \frac{-p}{2}$ and $\beta = \sqrt{q - \frac{p^2}{4}}$

making use of $e^{ix} = \cos(x) + i \cdot \sin(x)$

$\Rightarrow y(t) = e^{\frac{-p}{2}t} \cdot \left(c_1 \cos\left(\sqrt{q - \tfrac{1}{4}p^2}\, t\right) + c_2 \sin\left(\sqrt{q - \tfrac{1}{4}p^2}\, t\right)\right)$

the "i"'s "disappear" in the constants c_1 and c_2

Higher-order linear homogeneous DEs

Example 1: $y''' - y'' - 6y' = 0$ (we need three extra conditions because of y''')

y''': third order; homogeneous

$y = e^{\lambda t} \Rightarrow \lambda^3 - \lambda^2 - 6\lambda = 0 \Leftrightarrow \lambda(\lambda-3)(\lambda+2) = 0$

$\Rightarrow \lambda_1 = 0, \lambda_2 = 3, \lambda_3 = -2 \Rightarrow y_1 = 1, y_2 = e^{3t}, y_3 = e^{-2t}$

$\Rightarrow y(t) = c_1 + c_2 e^{3t} + c_3 e^{-2t}$

"*1"

Example 2: $y'''' - 16y = 0$ (we need four extra conditions because of y'''')

y'''': fourth order; homogeneous

$y = e^{\lambda t} \Rightarrow \lambda^4 - 16 = 0 \overset{!!!}{\Longrightarrow} \lambda_1 = 2, \lambda_2 = -2, \lambda_3 = 2i, \lambda_4 = -2i$

$2^4 = 16$ ✓

$(-2)^4 = 16$ ✓

$(2i)^4 = 2^4 \cdot i^4 = 2^4 (i^2)^2 = 2^4 (-1)^2 = 2^4 = 16$ ✓

$(-2i)^4 = (-2)^4 \cdot i^4 = -- = 2^4 = 16$ ✓

$y(t) = c_1 e^{2t} + c_2 e^{-2t} + c_3 \cos(2t) + c_4 \sin(2t)$

Inhomogeneous DEs

Example 1:

$$\begin{cases} y' + y = t \\ y(0) = 2 \end{cases} \quad (*)$$

1) first solve homogeneous DE: $y' + y = 0$

write $y_h' + y_h = 0$ (homogeneous) $\xrightarrow{\text{solve}} y_h(t) = c \cdot e^{-t}$ (keep c first)

2) try a so-called particular (special) solution of $(*)$:
call this solution $y_p(t)$.

$$y_p' + y_p = t \quad (**)$$

Try: $y_p(t) = At + B$ (because of t)

$\Rightarrow y_p' = A$ and substitute in $(**)$: $\underbrace{A}_{y_p'} + \underbrace{At + B}_{y_p} = 1 \cdot t + 0$ (must be and must hold for all t-values)

$$\Rightarrow \begin{cases} A + B = 0 \\ A = 1 \end{cases} \Rightarrow \begin{cases} A = 1 \\ B = -1 \end{cases}$$

$$\Rightarrow y_p(t) = t - 1$$

full solution $\Rightarrow$ $y(t) = y_h(t) + y_p(t) = ce^{-t} + t - 1$

3) Now use $y(0) = 2$: $2 = ce^{0} + 0 - 1 = c - 1 \Rightarrow c = 3$

$$\Rightarrow y(t) = 3e^{-t} + t - 1$$

Example 2: $y'' - 4y' + 5y = e^t$

$p = -4 \quad q = 5 \quad r(t)$

1) $y_h'' - 4y_h' + 5y_h = 0$ (first solve DV with $r \equiv 0$)

$\Longrightarrow \lambda_1 = 2+i, \lambda_2 = 2-i \Rightarrow y_h(t) = c_1 e^{2t}\cos(t) + c_2 e^{2t}\sin(t)$

check earlier calculation

2) $y_p'' - 4y_p' + 5y_p = e^t$ (find one solution of DV with $r = e^t$)

Try (because of e^t): $y_p(t) = Ae^t$

Substitute: $\underbrace{Ae^t}_{=y_p''} \underbrace{-4Ae^t}_{=-4y_p'} + \underbrace{5Ae^t}_{=5y_p} \overset{\text{must be}}{=\!=} \underbrace{e^t}_{=r(t)}$

$\Longrightarrow A - 4A + 5A = 1 \Rightarrow 2A = 1 \Rightarrow A = \frac{1}{2} \Rightarrow y_p(t) = \frac{1}{2}e^t$

$\Longrightarrow y(t) = y_h(t) + y_p(t) = c_1 e^{2t}\cos(t) + c_2 e^{2t}\sin(t) + \frac{1}{2}e^t$

c_1, c_2: from two extra conditions (not specified in this example)

Why does this work?

$$y'' + py' + qy = (y_h'' + y_p'') + p(y_h' + y_p') + q(y_h + y_p)$$

$$= \underbrace{[y_h'' + py_h' + qy_h]}_{=0} + \underbrace{[y_p'' + py_p' + qy_p]}_{=r(t)}$$

$$=\!= r(t)$$