Ordinary Differential Equation Systems

1. Matrix representation of ODE systems
2. Linear ODE systems
3. Linear ODE systems with constant coefficients
4. In-class exercise

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Ordinary Differential Equation Systems

Matrix Representation of ODE Systems

Introduction

- Sets of coupled ordinary differential equations (ODEs) are most conveniently represented and analyzed as ODE systems
- Unique solutions of ODE systems are guaranteed to exist under reasonably mild assumptions
- Systems of linear ODEs can be solved analytically using eigenvalues and eigenvectors
- Systems of nonlinear ODEs usually require numerical solution using tools such as MATLAB

ODE System Representation

- 2-dimensional nonlinear system

$$\frac{dy_1}{dx} = f_1(x, y_1, y_2) \qquad \mathbf{f}(x,\mathbf{y}) = \begin{bmatrix} f_1(x, y_1, y_2) \\ f_2(x, y_1, y_2) \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad \frac{d\mathbf{y}}{dx} = \mathbf{f}(x,\mathbf{y})$$

$$\frac{dy_2}{dx} = f_2(x, y_1, y_2)$$

- *n*-dimensional nonlinear system

$$\begin{aligned} \frac{dy_1}{dx} &= f_1(x, y_1, \ldots, y_n) \\ &\vdots \\ \frac{dy_n}{dx} &= f_n(x, y_1, \ldots, y_n) \end{aligned} \qquad \mathbf{f}(x,\mathbf{y}) = \begin{bmatrix} f_1(x, y_1, \ldots, y_n) \\ \vdots \\ f_n(x, y_1, \ldots, y_n) \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \quad \frac{d\mathbf{y}}{dx} = \mathbf{f}(x,\mathbf{y})$$

Nonlinear System Example

- Batch chemical reactor

$$\frac{dC_A}{dt} = -2k_1 C_A^2 C_B - k_2 C_A C_C \quad C_A(0) = C_{A0}$$

$$\frac{dC_B}{dt} = -k_1 C_A^2 C_B - k_3 C_B C_C^3 \quad C_B(0) = C_{B0}$$

$$\frac{dC_C}{dt} = k_1 C_A^2 C_B - k_2 C_A C_C - 3k_3 C_B C_C^3 \quad C_C(0) = 0$$

- Nonlinear system representation

$$\mathbf{y} = \begin{bmatrix} C_A \\ C_B \\ C_C \end{bmatrix} \quad \mathbf{y}_0 = \begin{bmatrix} C_{A0} \\ C_{B0} \\ 0 \end{bmatrix}$$

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}) = \begin{bmatrix} -2k_1 C_A^2 C_B - k_2 C_A C_C \\ -k_1 C_A^2 C_B - k_3 C_B C_C^3 \\ k_1 C_A^2 C_B - k_2 C_A C_C - 3k_3 C_B C_C^3 \end{bmatrix}$$

Existence and Uniqueness of Solutions

- Initial value problem (IVP)

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x,\mathbf{y}) \quad \mathbf{y}(x_0) = \mathbf{y}_0$$

- Jacobian matrix

$$J(x,\mathbf{y}) = \frac{\partial \mathbf{f}(x,\mathbf{y})}{\partial \mathbf{y}} = \begin{bmatrix} \partial f_1(x,\mathbf{y})/\partial y_1 & \cdots & \partial f_1(x,\mathbf{y})/\partial y_n \\ \vdots & \ddots & \vdots \\ \partial f_n(x,\mathbf{y})/\partial y_1 & \cdots & \partial f_n(x,\mathbf{y})/\partial y_n \end{bmatrix}$$

- Theorem
  - » A solution is a differentiable vector function $\mathbf{y} = \mathbf{h}(x)$ defined on some interval $a < x < b$ containing $\boldsymbol{x}_0$ that satisfies the IVP
  - » Let $\mathbf{f}(x,\mathbf{y})$ be a continuous function with a continuous Jacobian matrix in some domain containing the initial condition, then the IVP has a unique solution on some interval containing $\boldsymbol{x}_0$

Conversion to ODE System

- Second-order nonlinear ODE

$$\frac{d^2y}{dx^2} = F\left(x, \frac{dy}{dx}, y\right)$$

- State variable definition

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} y \\ \dfrac{dy}{dx} \end{bmatrix}$$

- System of 1st-order ODEs

$$\frac{dy_1}{dx} = y_2$$

$$\frac{dy_2}{dx} = F(x, y_1, y_2)$$

$$\mathbf{f}(x, \mathbf{y}) = \begin{bmatrix} y_2 \\ F(x, y_1, y_2) \end{bmatrix} \qquad \frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y})$$

Ordinary Differential Equation Systems

Linear ODE Systems

ODE System Representation

- 2-dimensional linear system

$$\frac{dy_1}{dx} = a_{11}(x)y_1 + a_{12}(x)y_2$$
$$\frac{dy_2}{dx} = a_{21}(x)y_1 + a_{22}(x)y_2$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad \frac{d\mathbf{y}}{dx} = \begin{bmatrix} a_{11}(x) & a_{12}(x) \\ a_{21}(x) & a_{22}(x) \end{bmatrix} \mathbf{y} = \mathbf{A}(x)\mathbf{y}$$

- *n*-dimensional linear system

$$\frac{dy_1}{dx} = a_{11}(x)y_1 + \cdots + a_{1n}(x)y_n$$
$$\vdots$$
$$\frac{dy_n}{dx} = a_{n1}(x)y_1 + \cdots + a_{nn}(x)y_n$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \quad \mathbf{A}(x) = \begin{bmatrix} a_{11}(x) & \cdots & a_{1n}(x) \\ \vdots & \ddots & \vdots \\ a_{n1}(x) & \cdots & a_{nn}(x) \end{bmatrix} \quad \frac{d\mathbf{y}}{dx} = \mathbf{A}(x)\mathbf{y}$$

Homogeneous Linear Systems

- Initial value problem (IVP)

$$\frac{d\mathbf{y}}{dx} = \mathbf{A}(x)\mathbf{y} \quad \mathbf{y}(x_0) = \mathbf{y}_0$$

  - » Let $\mathbf{A}(x)$ be a continuous function in some domain containing the initial condition, then the IVP has a unique solution on some interval containing x_0

- Solution form
  - » Given two solutions $\mathbf{y}^{(1)}(x)$ and $\mathbf{y}^{(2)}(x)$, any linear combination of these two solutions is also a solution: $\boldsymbol{y}(x) = c_1 \mathbf{y}^{(1)}(x) + c_2\mathbf{y}^{(2)}(x)$
  - » The n linearly independent solutions $\mathbf{y}^{(1)}(x)$, $\mathbf{y}^{(2)}(x)$,…, $\mathbf{y}^{(n)}(x)$ form a basis for the general solution
  - » General solution:

$$\mathbf{y}(x) = c_1\mathbf{y}^{(1)}(x) + c_2\mathbf{y}^{(2)}(x) + \cdots + c_n\mathbf{y}^{(n)}(x)$$

Non-Homogeneous Linear Systems

- Initial value problem (IVP)

$$\frac{d\mathbf{y}}{dx} = \mathbf{A}(x)\mathbf{y} + \mathbf{g}(x) \quad \mathbf{y}(x_0) = \mathbf{y}_0$$

  » Let $\mathbf{A}(x)$ and $\mathbf{g}(x)$ be continuous functions in some domain containing the initial condition, then the IVP has a unique solution on some interval containing x_0

- Solution form

  » The general solution has the following form where $\mathbf{y}^{(h)}(x)$ is the solution of the homogeneous equation and $\mathbf{y}^{(p)}(x)$ is a particular solution of the nonhomogeneous equation:

$$\mathbf{y}(x) = \mathbf{y}^{(h)}(x) + \mathbf{y}^{(p)}(x)$$

  » The particular solution can be obtained using the method of variation of parameters (see text)

Ordinary Differential Equation Systems

Linear ODE Systems with Constant Coefficients

ODE System Representation

- 2-dimensional linear system with constant coefficients

$$\frac{dy_1}{dx} = a_{11}y_1 + a_{12}y_2 \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \qquad \frac{d\mathbf{y}}{dx} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\mathbf{y} = \mathbf{A}\mathbf{y}$$

$$\frac{dy_2}{dx} = a_{21}y_1 + a_{22}y_2$$

- n-dimensional linear system with constant coefficients

$$\frac{dy_1}{dx} = a_{11}y_1 + \cdots + a_{1n}y_n$$

$$\vdots$$

$$\frac{dy_n}{dx} = a_{n1}y_1 + \cdots + a_{nn}y_n$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad \mathbf{A} = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} \qquad \frac{d\mathbf{y}}{dx} = \mathbf{A}\mathbf{y}$$

Linear System Example

- Two storage tanks in series

$$\frac{dh_1}{dt} = \frac{w_i - C_{v1}h_1}{\rho A_1} \quad h_1(0) = h_{10}$$

$$\frac{dh_2}{dt} = \frac{C_{v1}h_1 - C_{v2}h}{\rho A_2} \quad h_2(0) = h_{20}$$

- Linear ODE system representation

$$\mathbf{y} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} \quad \mathbf{y}_0 = \begin{bmatrix} h_{10} \\ h_{20} \end{bmatrix}$$

$$\frac{d\mathbf{y}}{dt} = \begin{bmatrix} -\frac{C_{v1}}{\rho A_1} & 0 \\ \frac{C_{v1}}{\rho A_2} & -\frac{C_{v2}}{\rho A_2} \end{bmatrix} \mathbf{y} + \begin{bmatrix} \frac{w_i}{\rho A_1} \\ 0 \end{bmatrix} = \mathbf{A}\mathbf{y} + \mathbf{b} \quad \mathbf{y}(0) = \mathbf{y}_0$$

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Conversion to Homogeneous System

- Non-homogeneous linear system

$$\frac{d\mathbf{y}}{dt} = \mathbf{A}\mathbf{y} + \mathbf{b} \quad \mathbf{0} = \mathbf{A}\overline{\mathbf{y}} + \mathbf{b} \quad \Rightarrow \quad \overline{\mathbf{y}} = -\mathbf{A}^{-1}\mathbf{b}$$

- Homogeneous linear system

$$\mathbf{y}'(t) = \mathbf{y}(t) - \overline{\mathbf{y}} \qquad \frac{d\mathbf{y}'}{dt} = \frac{d\mathbf{y}}{dt} = \mathbf{A}(\mathbf{y}' + \overline{\mathbf{y}}) + \mathbf{b}$$

$$\frac{d\mathbf{y}'}{dt} = \mathbf{A}\mathbf{y}' + \mathbf{A}(-\mathbf{A}^{-1}\mathbf{b}) + \mathbf{b} = \mathbf{A}\mathbf{y}' \qquad \mathbf{y}'(0) = \mathbf{y}(0) - \overline{\mathbf{y}}$$

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Matrix Diagonalization

- Initial value problem (IVP)

$$\frac{d\mathbf{y}}{dx} = \mathbf{A}\mathbf{y} \qquad \mathbf{y}(x_0) = \mathbf{y}_0$$

- Matrix diagonalization
  - » If the *n*x*n* matrix **A** has *n* distinct eigenvalues, the eigenvectors $\mathbf{x}^{(1)}$, $\mathbf{x}^{(2)}$, …, $\mathbf{x}^{(n)}$ are linearly independent
  - » The *n*x*n* modal matrix **X** is formed with these eigenvectors as column vectors
  - » The similarity transformation $\mathbf{D} = \mathbf{X}^{-1}\mathbf{A}\mathbf{X}$ diagonalizes the matrix **A**

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{12} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \quad \Rightarrow \quad \mathbf{D} = \mathbf{X}^{-1}\mathbf{A}\mathbf{X} = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}$$

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Solution of the Diagonalized System

- Variable transformation

$$\mathbf{z}(x) = \mathbf{X}^{-1}\mathbf{y}(x) \quad \Rightarrow \quad \mathbf{y}(x) = \mathbf{X}z(x)$$

- Transformed equations

$$\mathbf{X}\frac{d\mathbf{z}}{dx} = \mathbf{AXz} \quad \Rightarrow \quad \frac{d\mathbf{z}}{dx} = \mathbf{X}^{-1}\mathbf{AXz} = \mathbf{Dz} = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}\mathbf{z}$$

$$\mathbf{y}(0) = \mathbf{Xz}(0) = \mathbf{y}_0 \quad \Rightarrow \quad \mathbf{z}(0) = \mathbf{X}^{-1}\mathbf{y}_0$$

- Solution of the decoupled equations

$$\frac{dz_j}{dx} = \lambda_j z_j \quad \Rightarrow \quad z_j(x) = z_j(0)e^{\lambda_j x} \qquad j = 1,2,\ldots,n$$

Solution of the Original System

- Variable transformation

$$\mathbf{y}(x) = \mathbf{X}\mathbf{z}(x) = \left[\mathbf{x}^{(1)} \quad \mathbf{x}^{(2)} \quad \cdots \quad \mathbf{x}^{(n)}\right]\mathbf{z}(x)$$

- Solution form

$$\mathbf{y}(x) = \mathbf{x}^{(1)} z_1(x) + \mathbf{x}^{(2)} z_2(x) + \cdots + \mathbf{x}^{(n)} z_n(x)$$

$$\mathbf{y}(x) = z_1(0)\mathbf{x}^{(1)} e^{\lambda_1 x} + z_2(0)\mathbf{x}^{(2)} e^{\lambda_2 x} + \cdots + z_n(0)\mathbf{x}^{(n)} e^{\lambda_n x}$$

- If the eigenvectors $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(n)}$ of the constant matrix $\mathbf{A}$ are linearly independent, then the general solution of the IVP is:

$$\mathbf{y}(x) = c_1 \mathbf{x}^{(1)} e^{\lambda_1 x} + \cdots + c_n \mathbf{x}^{(n)} e^{\lambda_n x}$$

Isothermal Batch Reactor

- Chemical reactor model: A → B → C

$$\frac{dC_A}{dt} = -k_1 C_A \quad \frac{dC_B}{dt} = k_1 C_A - k_2 C_B \quad C_A(0) = 10, C_B(0) = 0$$

- Eigenvalue calculation: $k_1 = 1$, $k_2 = 2$

$$\mathbf{y}(t) = \begin{bmatrix} C_A(t) \\ C_B(t) \end{bmatrix} \quad \frac{d\mathbf{y}}{dt} = \begin{bmatrix} -1 & 0 \\ 1 & -2 \end{bmatrix} \mathbf{y} = \mathbf{A}\mathbf{y}$$

$$\lambda_1 = -2 \quad \mathbf{x}^{(1)} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \lambda_2 = -1 \quad \mathbf{x}^{(2)} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

- Linear ODE solution

$$\mathbf{y}(t) = \begin{bmatrix} C_A(t) \\ C_B(t) \end{bmatrix} = c_1 \mathbf{x}^{(1)} e^{\lambda_1 t} + c_2 \mathbf{x}^{(2)} e^{\lambda_2 t} = c_1 \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{-2t} + c_2 \begin{bmatrix} 1 \\ 1 \end{bmatrix} e^{-t}$$

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Isothermal Batch Reactor

- Linear ODE solution

$$\mathbf{y}(t) = \begin{bmatrix} C_A(t) \\ C_B(t) \end{bmatrix} = c_1 \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{-2t} + c_2 \begin{bmatrix} 1 \\ 1 \end{bmatrix} e^{-t}$$

- Apply initial conditions

$$\mathbf{y}(0) = \begin{bmatrix} C_A(0) \\ C_B(0) \end{bmatrix} = c_1 \begin{bmatrix} 0 \\ 1 \end{bmatrix} + c_2 \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 10 \\ 0 \end{bmatrix}$$

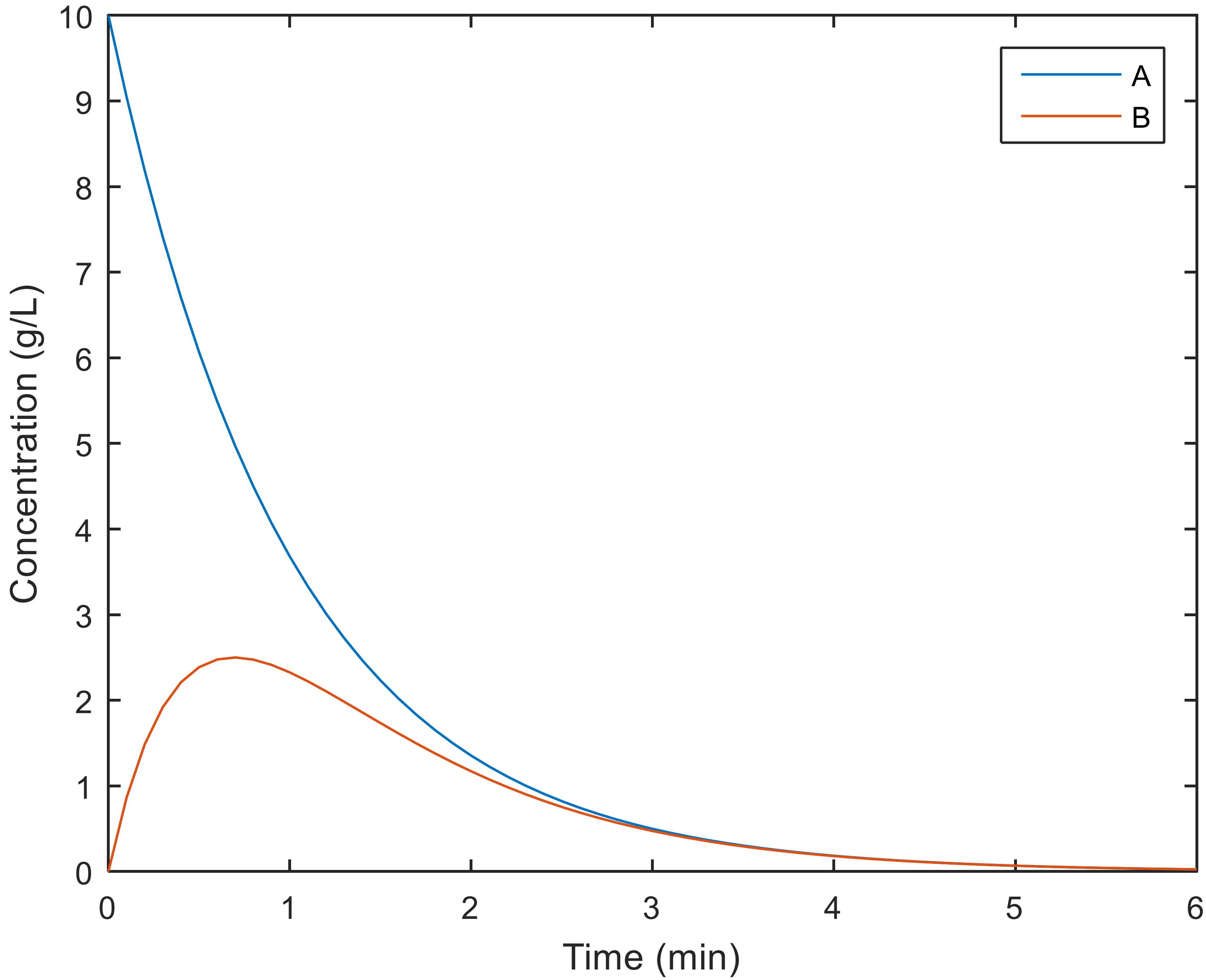
- Formulate matrix problem

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 10 \\ 0 \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} -10 \\ 10 \end{bmatrix}$$

- Solution

$$\begin{bmatrix} C_A(t) \\ C_B(t) \end{bmatrix} = -10 \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{-2t} + 10 \begin{bmatrix} 1 \\ 1 \end{bmatrix} e^{-t} = \begin{bmatrix} 10e^{-t} \\ -10e^{-2t} + 10e^{-t} \end{bmatrix}$$

Plot of Solution



Ordinary Differential Equation Systems

In-class Exercise