Modeling of geochemical processes

Linear system of differential equations

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Dynamic models

Matrix **K** is diagonalized into $\mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^{-1}$. Then

$$\frac{d\mathbf{x}}{dt} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^{-1}\,\mathbf{x}$$

Multiplying by $\mathbf{U}^{-1}$ from left side gives $\mathbf{U}^{-1}\frac{d\mathbf{x}}{dt} = \mathbf{\Lambda}\,\mathbf{U}^{-1}\,\mathbf{x}$

Because $\mathbf{U}^{-1}$ is a matrix of constants, it is $\frac{d\mathbf{U}^{-1}\mathbf{x}}{dt} = \mathbf{\Lambda}\,\mathbf{U}^{-1}\,\mathbf{x}$

Let us substitute for $\mathbf{U}^{-1}\mathbf{x} = \mathbf{y}$. Then $\frac{d\mathbf{y}}{dt} = \mathbf{\Lambda}\,\mathbf{y}$

This equation can be split into a set of individual equations, $\frac{d\,y_i}{dt} = \lambda_i\,y_i$,

which can be solved at initial conditions, t = 0, y = y_0 as $y_i = e^{\lambda_i t}\,y_{i0}$

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The set of the equations can be expressed in vectors as

$\mathbf{y} = e^{\mathbf{\Lambda} t}\, \mathbf{y_0}$ and, after re-substitution, as $\mathbf{U}^{-1}\mathbf{x} = e^{\mathbf{\Lambda} t}\, \mathbf{U}^{-1}\mathbf{x_0}$

Multiplying matrix **U** from left side gives the expression for vector **x**

$$\mathbf{x} = \mathbf{U}\, e^{\mathbf{\Lambda} t}\, \mathbf{U}^{-1}\mathbf{x_0}$$

$$\mathbf{x} = \sum_i e^{\lambda_i t}\, (i^{th}\text{column of } \mathbf{U})(i^{th} \text{ row of } \mathbf{U}^{-1})\, \mathbf{x_0}$$

$$\mathbf{x} = \sum_i e^{\lambda_i t}\, \mathbf{U}\, \mathbf{e}_i\, \mathbf{e}_i^T\, \mathbf{U}^{-1}\mathbf{x_0}$$

$$\boxed{\mathbf{x} = \sum_i e^{\lambda_i t}\, \mathbf{U}_i\, \mathbf{x_0}}$$

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Example:. system of differential equations

$$\frac{dx_1}{dt} = 2\,x_1$$

$$\frac{dx_2}{dt} = x_1 + x_2$$

$$\frac{d\mathbf{x}}{dt} = \begin{bmatrix} 2 & 0 \\ 1 & 1 \end{bmatrix} \mathbf{x}$$

Initial conditions: t = 0, $x_1 = 1$ $x_2 = -1$

$$\mathbf{x}_0 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\,\mathbf{x}$$

$$\mathbf{A} = \begin{bmatrix} 2 & 0 \\ 1 & 1 \end{bmatrix} = \mathbf{U \Lambda U}^{-1} = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -\sqrt{2} & 0 \\ -1 & 1 \end{bmatrix}$$

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In general: $\mathbf{x} = e^{\lambda_i t}\, \mathbf{U}_1\, \mathbf{x}_0 \quad + \quad e^{\lambda_i t}\, \mathbf{U}_2\, \mathbf{x}_0$

$$\mathbf{x} = e^{2t} \begin{bmatrix} \sqrt{2}/2 \\ \sqrt{2}/2 \end{bmatrix} \begin{bmatrix} -\sqrt{2} & 0 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad + \quad e^{t} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\mathbf{x} = e^{2t} \begin{bmatrix} -1 \\ -1 \end{bmatrix} \quad + \quad e^{t} \begin{bmatrix} 0 \\ -2 \end{bmatrix}$$

$$x_1 = -e^{2t}$$

$$x_2 = -e^{2t} - 2e^{t}$$