Modeling of geochemical processes

Linear Algebra Refreshing

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Modeling of geochemical processes
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Eigen Values and Eigen Vectors of Matrix

The square matrix $\mathbf{A}_{nxn}$ can be decomposed (factorized) into a product of three matrix

$$\mathbf{A}_{nxn} = \mathbf{U}_{nxn}\mathbf{\Lambda}_{nxn}\mathbf{U}^{-1}_{nxn}$$

$\mathbf{\Lambda}_{nxn}$ is diagonal matrix with diagonal components λ_i called eigen values of matrix **A**

$\mathbf{U}_{nxn}$ is a square matrix that comprises column vectors $\mathbf{u_i}$ called eigen vectors of matrix **A**

An example:

$$\begin{bmatrix} -1 & -6 \\ 1 & 4 \end{bmatrix} = \begin{bmatrix} 3 & 2 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ -1 & -3 \end{bmatrix}$$

$$\lambda_1 = 1 \qquad \lambda_2 = 2 \qquad \mathbf{u}_1 = \begin{bmatrix} 3 \\ -1 \end{bmatrix} \qquad \mathbf{u}_2 = \begin{bmatrix} 2 \\ -1 \end{bmatrix}$$

Modeling of geochemical processes
Dynamic models

The eigencomponents (every eigen value and eigen vector) are connected by linear equation (in vectors): $\mathbf{A}\,\mathbf{u}_i = \lambda_i\,\mathbf{u}_i$

the example $\begin{bmatrix} -1 & -6 \\ 1 & 4 \end{bmatrix}\begin{bmatrix} 3 \\ -1 \end{bmatrix} = 1\begin{bmatrix} 3 \\ -1 \end{bmatrix}$, and $\begin{bmatrix} -1 & -6 \\ 1 & 4 \end{bmatrix}\begin{bmatrix} 2 \\ -1 \end{bmatrix} = 2\begin{bmatrix} 2 \\ -1 \end{bmatrix}$

Determination λ_i and $\mathbf{u}_i$

It results from the former equation that $\det\left(\mathbf{A} - \lambda_i\,\mathbf{I}\right) = 0$; it is

$$\det\begin{bmatrix} a_{11} - \lambda & a_{12} & a_{13} \\ a_{21} & a_{22} - \lambda & a_{23} \\ a_{31} & a_{32} & a_{33} - \lambda \end{bmatrix} = 0$$

Modeling of geochemical processes
Dynamic models

The example: $$\det\begin{bmatrix} -1-\lambda & -6 \\ 1 & 4-\lambda \end{bmatrix} = 0$$

characteristic equation is $$(-1-\lambda)(4-\lambda)-(-6).1=0$$

rewriting gives $(-1-\lambda)(4-\lambda)+6=0$; solution is $\lambda_1 = 1, \lambda_2 = 2$

Diagonal matrix of eigen values is $$\mathbf{\Lambda} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

Substituting of the eigen values yields the equation set

$$\begin{bmatrix} -1 & -6 \\ 1 & 4 \end{bmatrix}\begin{bmatrix} u_{11} \\ u_{21} \end{bmatrix} = 1\begin{bmatrix} u_{11} \\ u_{21} \end{bmatrix} \qquad \begin{bmatrix} -1 & -6 \\ 1 & 4 \end{bmatrix}\begin{bmatrix} u_{12} \\ u_{22} \end{bmatrix} = 2\begin{bmatrix} u_{12} \\ u_{22} \end{bmatrix}$$

Modeling of geochemical processes
Dynamic models

A decomposition gives

$$- u_{11} - 6\,u_{21} = u_{11} \qquad u_{11} = -3\,u_{21}$$

$$u_{11} + 4\,u_{21} = u_{21} \qquad u_{11} = -3\,u_{21}$$ both equations are depended

and

$$- u_{12} - 6\,u_{22} = 2\,u_{12} \qquad u_{12} = -2\,u_{22}$$

$$u_{12} + 4\,u_{22} = 2\,u_{22} \qquad u_{12} = -2\,u_{22}$$ both equations are depended

If it is chosen $u_{21} = -1$, then $u_{11} = 3$. If $u_{22} = -1$, then $u_{12} = 2$!

$$\mathbf{U} = \begin{bmatrix} 3 & 2 \\ -1 & -1 \end{bmatrix} \qquad \mathbf{u}_1 = \begin{bmatrix} 3 \\ -1 \end{bmatrix} \qquad \mathbf{u}_2 = \begin{bmatrix} 2 \\ -1 \end{bmatrix}$$

Modeling of geochemical processes
Dynamic models

The equations give only **direction** of the eigen vectors; they give not coordinates of end point. Therefore, **unitary lengths of vectors** are often chosen:

$$u_{11}^2 + u_{21}^2 = 1, \qquad \text{and} \qquad u_{12}^2 + u_{22}^2 = 1$$

It results from the former example

$$u_{11}^2 = 9\,u_{21}^2 \qquad \text{and} \qquad 10\,u_{21}^2 = 1$$

The substituting yields $u_{21} = \sqrt{\frac{1}{10}}$ and $u_{11} = -\sqrt{\frac{9}{10}}$

It results from the second equation set $u_{12}^2 = 4\,u_{22}^2$

The substituting yields $u_{22} = \sqrt{\frac{1}{5}}$ and $u_{12} = -\sqrt{\frac{4}{5}}$

The matrix of eigen vectors $\mathbf{U} = \begin{bmatrix} -\sqrt{\frac{9}{10}} & -\sqrt{\frac{4}{5}} \\ \sqrt{\frac{1}{10}} & \sqrt{\frac{1}{5}} \end{bmatrix} = \begin{bmatrix} -0.94868 & -0.89443 \\ 0.31622 & 0.44721 \end{bmatrix}$

Modeling of geochemical processes
Dynamic models

Inverse matrix can be find, e.g., under using of MS Excel

$$\mathbf{U}^{-1} = \begin{bmatrix} -3.16228 & -6.32456 \\ 2.23607 & 6.70820 \end{bmatrix}$$

Verifying

$$\mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^{-1} = \begin{bmatrix} -0.94868 & -0.89443 \\ 0.31622 & 0.44721 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -3.16228 & -6.32456 \\ 2.23607 & 6.70820 \end{bmatrix}$$

$$\mathbf{U}\,\mathbf{\Lambda} = \begin{bmatrix} -0.94868 & -1.78885 \\ 0.31623 & 0.89443 \end{bmatrix}$$

$$\mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^{-1} = \begin{bmatrix} -1 & -6 \\ 1 & 4 \end{bmatrix}$$