Modeling of geochemical processes

Numeric Algorithm Refreshment

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Modeling of geochemical processes

Numeric mathematics

Numerical Algorithms

Taylor Series

$$f(x+h) = f(x) + \frac{h}{1!} f'(x) + \frac{h^2}{2!} f''(x) + \ldots + \frac{h^n}{n!} f^{(n)}(x) + \ldots + R_n \quad \text{(a remainder term)}$$

The terms of higher orders are often neglected!

Newton method algoithm:

$$f(x+h) = f(x) + h f'(x) = 0$$

$$-f(x) = \Delta x \; f'(x)$$

$$-f(x) = (x^{k+1} - x^k) \; f'(x)$$

$$x^{k+1} = x^k - \frac{f(x)}{f'(x)}$$

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Taylor Series of the Function of two Variables:

$$f(x_1+h_1, x_2+h_2) = f(x_1,x_2) + h_1\frac{\partial f(x_1,x_2)}{\partial x_1} + h_2\frac{\partial f(x_1,x_2)}{\partial x_2} +$$

$$+\frac{1}{2}\left\{h_1^2\frac{\partial^2 f(x_1,x_2)}{\partial x_1^2} + 2\,h_1h_2\frac{\partial^2 f(x_1,x_2)}{\partial x_1\,\partial x_2} + h_2^2\frac{\partial^2 f(x_1,x_2)}{\partial x_2^2}\right\} + \ldots + R_n\,(\text{remainder})$$

$$f(x_1+h_1, x_2+h_2) = f(x_1,x_2) + h_1\frac{\partial f(x_1,x_2)}{\partial x_1} + h_2\frac{\partial f(x_1,x_2)}{\partial x_2} +$$

$$+\frac{1}{2}h_1^2\frac{\partial^2 f(x_1,x_2)}{\partial x_1^2} + \frac{1}{2}h_1h_2\frac{\partial^2 f(x_1,x_2)}{\partial x_1\,\partial x_2} + \frac{1}{2}h_1h_2\frac{\partial^2 f(x_1,x_2)}{\partial x_1\,\partial x_2} + \frac{1}{2}h_2^2\frac{\partial^2 f(x_1,x_2)}{\partial x_2^2} + \ldots + R_n$$

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A vector form:

gradient

$$f(x_1+h_1, x_2+h_2) = f(x_1,x_2) + \begin{bmatrix} h_1 & h_2 \end{bmatrix} \begin{bmatrix} \dfrac{\partial f(x_1,x_2)}{\partial x_1} \\ \dfrac{\partial f(x_1,x_2)}{\partial x_2} \end{bmatrix} +$$

$$+ \begin{bmatrix} \dfrac{1}{2} h_1 \dfrac{\partial^2 f(x_1,x_2)}{\partial x_1^2} + \dfrac{1}{2} h_2 \dfrac{\partial^2 f(x_1,x_2)}{\partial x_1\,\partial x_2} & \dfrac{1}{2} h_1 \dfrac{\partial^2 f(x_1,x_2)}{\partial x_1\,\partial x_2} + \dfrac{1}{2} h_2 \dfrac{\partial^2 f(x_1,x_2)}{\partial x_2^2} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

$$f(x_1+h_1, x_2+h_2) = f(x_1,x_2) + \begin{bmatrix} h_1 & h_2 \end{bmatrix} \begin{bmatrix} \dfrac{\partial f(x_1,x_2)}{\partial x_1} \\ \dfrac{\partial f(x_1,x_2)}{\partial x_2} \end{bmatrix} +$$

Hessian

$$+ \frac{1}{2} \begin{bmatrix} h_1 & h_2 \end{bmatrix} \begin{bmatrix} \dfrac{\partial^2 f(x_1,x_2)}{\partial x_1^2} & \dfrac{\partial^2 f(x_1,x_2)}{\partial x_1\,\partial x_2} \\ \dfrac{\partial^2 f(x_1,x_2)}{\partial x_1\,\partial x_2} & \dfrac{\partial^2 f(x_1,x_2)}{\partial x_2^2} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

$$f(x_1+h_1, x_2+h_2) = f(x_1,x_2) + \mathbf{h}^T \mathbf{grad}\, f(x_1,x_2) + \frac{1}{2} \mathbf{h}^T \mathbf{H}\, \mathbf{h}$$

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Taylor Series of the System of the Functions of more Variables

Two functions of two variables (only the first order terms; the first derivations)

$$f_1(x_1+h_1,\, x_2+h_2) = f_1(x_1,x_2) + h_1\frac{\partial f_1(x_1,x_2)}{\partial x_1} + h_2\frac{\partial f_1(x_1,x_2)}{\partial x_2}$$

$$f_2(x_1+h_1,\, x_2+h_2) = f_2(x_1,x_2) + h_1\frac{\partial f_2(x_1,x_2)}{\partial x_1} + h_2\frac{\partial f_2(x_1,x_2)}{\partial x_2}$$

In vectors: *Jakobian*

$$\begin{bmatrix} f_1(x_1+h_1,\, x_2+h_2) \\ f_2(x_1+h_1,\, x_2+h_2) \end{bmatrix} = \begin{bmatrix} f_1(x_1,x_2) \\ f_2(x_1,x_2) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1(x_1,x_2)}{\partial x_1} & \frac{\partial f_1(x_1,x_2)}{\partial x_2} \\ \frac{\partial f_2(x_1,x_2)}{\partial x_1} & \frac{\partial f_2(x_1,x_2)}{\partial x_2} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

$$\mathbf{f}(\mathbf{x}+\mathbf{h}) = \mathbf{f}(\mathbf{x}) + \mathbf{J}\,\mathbf{h}$$

alternatively $\mathbf{f}(\mathbf{x}+\mathbf{h}) = \mathbf{f}(\mathbf{x}) + \mathbf{D}\,\mathbf{h}$

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Newton-Raphson methods

Equation system: $\mathbf{f}_i\,(x_1,x_2...x_n) = 0$ $\quad\quad$ $\mathbf{f}\,(\mathbf{x}) = 0$

Taylor Series (first order terms only):

$$f_i\left(\mathbf{x}^{k+1}\right) = f_i\left(\mathbf{x}^{k}\right) + \mathbf{grad}\, f_i\left(\mathbf{x}^{k}\right)\Delta\mathbf{x}$$

In matrix form (some matrix elements are vectors), it is:

$$\begin{bmatrix} f_1\left(\mathbf{x}^{k+1}\right) \\ f_2\left(\mathbf{x}^{k+1}\right) \\ \vdots \\ f_n\left(\mathbf{x}^{k+1}\right) \end{bmatrix} = \begin{bmatrix} f_1\left(\mathbf{x}^{k}\right) \\ f_2\left(\mathbf{x}^{k}\right) \\ \vdots \\ f_n\left(\mathbf{x}^{k}\right) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1\left(\mathbf{x}^{k}\right)}{\partial x_1} & \cdots & \frac{\partial f_1\left(\mathbf{x}^{k}\right)}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n\left(\mathbf{x}^{k}\right)}{\partial x_1} & \cdots & \frac{\partial f_n\left(\mathbf{x}^{k}\right)}{\partial x_n} \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \vdots \\ \Delta x_n \end{bmatrix}$$

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For $\mathbf{f}(\mathbf{x}^{k+1}) = 0$, then it is:

$$\begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} f_1(\mathbf{x}^k) \\ f_2(\mathbf{x}^k) \\ \vdots \\ f_n(\mathbf{x}^k) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1(\mathbf{x}^k)}{\partial x_1} & \cdots & \frac{\partial f_1(\mathbf{x}^k)}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n(\mathbf{x}^k)}{\partial x_1} & \cdots & \frac{\partial f_n(\mathbf{x}^k)}{\partial x_n} \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \vdots \\ \Delta x_n \end{bmatrix}$$

in vectors: $\mathbf{0} = \mathbf{f}(\mathbf{x}^k) + \mathbf{D}\,\Delta\mathbf{x}$ After rearranging: $\mathbf{0} = \mathbf{D}^{-1}\,\mathbf{f}(\mathbf{x}^k) + \mathbf{D}^{-1}\,\mathbf{D}\,\Delta\mathbf{x}$

$-\Delta\mathbf{x} = \mathbf{D}^{-1}\,\mathbf{f}(\mathbf{x}^k)$ where $\mathbf{x}^{k+1} = \mathbf{x}^k + \Delta\mathbf{x}$ and $\Delta\mathbf{x} = \mathbf{x}^{k+1} - \mathbf{x}^k$

Rearranging gives the algorithm: $\boxed{\mathbf{x}^{k+1} = \mathbf{x}^k - \mathbf{D}^{-1}\,\mathbf{f}(\mathbf{x}^k)}$