Mineral Content Conversion by Piecewise Polynomial Truncated Singular Value Decomposition Algorithm in the Context of Formation Element Logging

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Abstract. In spite of diverse types of elements and minerals in the stratum, there are only a few kinds they are mainly concentrated, thus the key to element-mineral conversion lies in the quantitative relationship between main elements and main minerals, which task, however, is challenged in practical logging. Firstly, the element types detected by logging tools are fixed, while the mineral types vary in different regions, which makes it difficult to determine the mineral type merely from logging data accurately. Secondly, the mineral types are generally more than the element types detected in the stratum, leading to a multiplicity of the conversion results. Therefore aiming to solve such challenges, this paper establishes a reasonable conversion relationship between the element and mineral, and ultimately attains relatively precise results through certain mathematical method, i.e. piecewise polynomial truncated singular value decomposition (PP-TSVD) algorithm that eliminates “small” singular values of the ill-conditioned conversion coefficients matrix, and meanwhile makes a superimposition of the effective components in the “small” singular value spectrum in the solution of the TSVD method, which greatly reduces the mean square error of the solution, so as to improve the accuracy and reliability of the solution. In addition, PP-TSVD method can determine either the mineral content of single mineral or diversified types, on condition that the known element types are not less than the mineral types to seek. When mineral types are numerous, the integration of some types into one mineral is imperative in order to establish suitable conversion coefficients. In this paper, based on previous studies and the #JD1 well data measured by ECS logging tool, the PP-TSVD method is employed to study the calculation and conversion between the element content and mineral content.

1. Introduction

It has been far more difficult for conventional logging series, currently, to evaluate reservoirs of complex lithology, since the types of complex mineral elements are too hard to measure – since there is not a unique solution for mineral content conversion¹⁻². None one-to-one correspondence between the elemental content and the mineral content of the certain rock³⁻⁴, makes it impossible to directly determine the main rock-forming minerals by using the detected elemental content. ECS logging, a remarkable case of formation element logging, has become one of the key technologies to accomplish this determination of rock mineral content.

In accordance with experiments, analyses, statistics and researches of a large number of cores throughout the world by Herron and other scholars⁵, the element-mineral conversion is proposed:
where, $E_i$ is the content of the $i$-th element, $i = 1, 2, \ldots, m$; $C_{ij}$, the conversion coefficient, is the content of the $i$-th element in the $j$-th mineral, $j = 1, 2, 3, \ldots, n$; $M_j$ is the content of the $j$-th mineral to be determined.

Since mineral types in different regions are not the same, the element-mineral conversion coefficients will thus be slightly different, which can be obtained by analysis and statistics of considerable core samples in one region, with heavy workload and high costs yet. Therefore, Li and Wang (1998) have proposed that conversion relationship selection be the key work in element-mineral conversion\cite{6}, especially in those regions without such relationship, and either the globally “universal” relationship proposed by Herron et al. (1990) (Table 1) or conversion coefficients of areas with similar geological backgrounds be chosen to accomplish the conversion initially, with further practical revise and modification\cite{7}.

Table 1. “Universal” element-mineral conversion coefficients\cite{7}

| Mineral   | Al  | Si  | Fe  | K   | Ti  | S   | Ca  | XS Fe\textsuperscript{a} | W(H2O)_{\text{min}}\textsuperscript{b} |
|-----------|-----|-----|-----|-----|-----|-----|-----|--------------------------|---------------------------------------|
| Feldspar  | 10  | 30  | 0   | 10  | 0   | 0   | 1   | 0                        | 0                                    |
| Quartz    | 0   | 46.7| 0   | 0   | 0   | 0   | 0   | 0                        | 0                                    |
| Calcite   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 40                       | 0                                    |
| Kaolinite | 19  | 22  | 0.8 | 0.9 | 0   | 0   | 0   | 0                        | 14                                   |
| Illite    | 12  | 24  | 8   | 4   | 0.8 | 0   | 0   | 0                        | 8                                    |
| Smectite  | 8.5 | 21.1| 1   | 0.5 | 0.2 | 0   | 0.2 | 0                        | 32                                   |
| Pyrite    | 0   | 0   | 47  | 0   | 0   | 53  | 0   | 0                        | 0                                    |
| Rutile    | 0   | 0   | 0   | 60  | 0   | 0   | 0   | 0                        | 0                                    |
| Siderite  | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 48                       | 0                                    |

\textsuperscript{a} XS Fe – the residual iron content;

\textsuperscript{b} W(H2O)_{\text{min}} – the minimum water content of the minerals

Nevertheless, the large condition number of the conversion coefficient matrix brings about ill-conditioned equations, and general numerical solutions may result in serious errors and even severe distortion. In other words, the coefficient matrix $C$ is overdetermined or underdetermined rather than a square one. Given the alterable complexity of the coefficient matrix $C$, the PP-TSVD method is introduced in this paper, in order to solve such problems more efficiently.

2. Methodology

As a regularization algorithm based on truncated singular value decomposition (TSVD)\cite{8}, the PP-TSVD algorithm, is first proposed by Hansen and Mosegaard in the application of non-continuous density recognition\cite{9}, whose main advantage is that it can complete the computation of the piecewise polynomial solution without any a priori knowledge of the location of the break points. This method is specially suitable for the analysis of those rough data, embracing step changes and discontinuity, particularly in geophysical image restoration and formation parameters calculation\cite{10-13}.

The mathematical relation between the element and mineral, in the context of ECS logging, can be briefly described as:

$$Ax = b$$  \hspace{1cm} (2)

where, matrix $A \in R^{m \times n}$ and matrix $b \in R^m$ are given, while $x \in R^n$ is the target. The least square solution for Equation (2) can be written as

$$X_{ls} = (A^\prime A)^{-1} A^\prime b$$  \hspace{1cm} (3)

While the PP-TSVD method is efficient for solving the following problem\cite{14}:

$$\min \| L_D x \|_1 \text{ subject to } \| A_k x - b \|_2 = \min$$  \hspace{1cm} (4)
where, \( L_D \) is a discrete approximation that represents \( \zeta \)-th derivative operator, while \( \zeta \) usually equals to 1 or 2. Then the bidiagonal matrix \( L_1 \) and the tridiagonal matrix \( L_2 \) can thus be obtained:

\[
L_1 = \begin{bmatrix}
1 & -1 & \cdots & \\
& 1 & -1 & \\
& & \ddots & -1 \\
& & & 1
\end{bmatrix} \quad (5)
\]

\[
L_2 = \begin{bmatrix}
1 & -2 & -1 & \\
& 1 & -2 & \\
& & \ddots & -1 \\
& & & 1
\end{bmatrix} \quad (6)
\]

SVD for matrix \( A \) takes the following form:

\[
A = U\Sigma V^T = \sum_{i=1}^{n} u_i \sigma_i v_i^T \quad (7)
\]

where, \( U \) and \( V \) are respectively square matrixes carrying \( m \times m \) and \( n \times n \) dimensional size, whose rows are orthogonal eigenvectors of \( A^T A \); \( u_i, v_i \) are respectively the \( i \)-th row of matrix \( U \) and matrix \( V \); \( \Sigma = \text{diag}(\sigma_1, \sigma_2, \sigma_3, \ldots, \sigma_n) \) is a diagonal matrix with diagonal elements being \( \sigma_i (i = 1, 2, 3, \ldots, n) \) that is the singular value of matrix \( A \), whose condition number is \( \frac{\sigma_1}{\sigma_n} \).

Then solve Equations (3) and (4):

\[
X_{1r} = V(S^T S)^{-1} S^T U^T b = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i \quad (8)
\]

If there are \( n-k \) singular values close to 0 obtained by decomposition of \( A \), only first \( k \) larger singular values are retained, and the solution for truncated singular value decomposition (TSVD) algorithm is obtained:

\[
X_{TSVD} = \sum_{i=1}^{k} \frac{u_i^T b}{\sigma_i} v_i \quad (9)
\]

The most critical point in PP-TSVD method lies in how to extract valid information from the spectrum of small-medium singular values and then superimpose them together. In the truncated small-medium singular value spectrum, submatrix \( V_n \) contains the effective information required for calculating mineral content. Assume \( V_n \) is composed of row vectors, namely \( V_k, V_{k+1}, \ldots, V_n \), it can be noted as follows:

\[
V_n = [V_k \ V_{k+1} \ V_{k+2} \ \cdots \ V_n] \quad (10)
\]

Generally speaking, the process of extracting effective information can be taken as solving the issue of linear \( l_1 \), which can be expressed as

\[
\min \| (L \bar{V}_n) w - L \bar{x}_k \|_1 \quad (11)
\]

whose solution is

\[
\bar{x}_{l_1,k} = \bar{x}_k - \bar{V}_n \bar{w}_k \quad (12)
\]

Note that \( k \) is the truncation number in the PP-TSVD algorithm that plays a vital role as a regularization parameter controlling the stabilization of the solution. Therefore, the \( k \) should be carefully determined in order that useful information can be retained at most when its value shall be as small as possible. In accordance with the method of generalized cross-validation (GCV) [15], the optimal regularization parameter \( k^* \) is the minimizer of \( f(k) \) given by

\[
f(k^*) = \min f(k) = \frac{\|A\bar{x}_k - b\|_2^2}{\text{Trace}(I - AM_k A^T)} \quad (13)
\]

where \( M_k = A^T A + k^2 I \); \( \text{Trace} \) means the trace of matrix \( A \). Then the GCV can be further simplified with Sherman–Morrison formula, that is

\[
k^2(AA^T + k^2 I)^{-1} = I - A(A^T A + k^2 I)^{-1} A^T \quad (14)
\]

Therefore Equation (13) can be written as
Meanwhile an effective method for calculation of trace is expected to employ, which Eldén (1984) proposes\cite{16}:

\[
\text{Trace} \left( I - AM^{-1}_A \right) = m - \text{Trace} \left( AM^{-1}_A \right)
\]

\[
= m - \text{Trace} \left( I - k^2 M^{-1}_A \right)
\]

\[
= m - n + k^2 \text{Trace} \left( M^{-1}_A \right)
\]

whose valid content takes the form of

\[
\text{Trace} \left[ I - A(A^T A + k^2 I)^{-1} A^T \right] = m - n + k^2 \text{Trace} \left[ (\Psi_k^T \Psi_k)^{-1} \right]
\]

where \(\Psi_k\) can be marked as

\[
\Psi_k = \begin{pmatrix}
\psi_{11} & \psi_{12} & 0 & 0 & 0 \\
0 & \psi_{22} & \psi_{23} & 0 & 0 \\
0 & 0 & \ddots & \ddots & 0 \\
0 & 0 & 0 & \psi_{n-1,n-1} & \psi_{n-1,n} \\
0 & 0 & 0 & 0 & \psi_{nn}
\end{pmatrix}
\]

Assume \(s_i\) as the \(l_2\) trace of the \(i\)-th row in \(\Psi_k^{-1}\) (\(i = 1, 2, 3, \ldots, n\)), then

\[
\text{Trace} \left[ (\Psi_k^T \Psi_k)^{-1} \right] = s_1^2 + s_2^2 + s_3^2 + \cdots + s_n^2
\]

The whole calculation procedures by the PP-TSVD algorithm are briefly shown in Figure 1.

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**Figure 1.** A flow diagram of the PP-TSVD algorithm applied to the conversion calculation

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3. **Results and Discussion**

On the basis of X-ray diffraction core analysis results, with the “universal” mineral conversion
coefficients referenced, the mineral types in the target region are confirmed so that the conversion coefficients can be further modified (shown in Table 2), which makes the element-mineral relationship more suitable and appropriate, and the conversion calculation more precisely, while the PP-TSVD method is implemented in the conversion with the aid of MATLAB that facilitates the calculation model establishment and follow-up analyses, and then the mineral content curves are being compared with Schlumberger interpretation results and core analysis data.

Table 2. Modified element-mineral conversion coefficients

| Mineral       | Element (%) | Al | Si | Fe | K | Ti | S | Ca |
|---------------|-------------|----|----|----|---|----|---|----|
| Quartz        |             | 0  | 46.7 | 0 | 0 | 0 | 0 | 0  |
| Potassium Feldspar |         | 9.7 | 30 | 0 | 12 | 0 | 0 | 0  |
| Sodium Feldspar          |      | 10.3 | 31.3 | 0 | 0 | 0 | 0 | 0  |
| Kaolinite      |             | 21 | 22 | 0.8 | 0 | 0.9 | 0 | 0  |
| Illite         |             | 13.2 | 24 | 7.6 | 4 | 0.8 | 0 | 0  |
| Smectite       |             | 8  | 20 | 1 | 0.5 | 0.2 | 0 | 1  |
| Calcite        |             | 0  | 0 | 0 | 0 | 0 | 0 | 40 |
| Pyrite         |             | 0  | 0 | 47 | 0 | 0 | 54 | 0  |

What is depicted below, from Figure 2a to Figure 2e, is a series of correlation analyses, between the calculation result of mineral content and the X-ray diffraction core analysis, with presence of each individual regression equation and coefficient of determination, which characterize these results of quartz, feldspar (potassium & sodium), clay, carbonate and pyrite. It is apparent that such correlations between the calculation result and the core analysis, with $R^2$ ranging from 0.8463 to 0.9278, are generally good enough to maintain a strong consistency, excluding the pyrite content which bias is led by its small portion.

![Figure 2(a) Calculation result and lab test of quartz content of #JD1 well](image)

![Figure 2(b) Calculation result and lab test of feldspar content of #JD1 well](image)

![Fig. 2c Calculation result and lab test of clay content of #JD1 well](image)

![Fig. 2d Calculation result and lab test of carbonate content of #JD1 well](image)
Meanwhile, the mineral content curves of #JD1 well have been shown in Figure 3. The red curves, represent the mineral content curves of #JD1 well derived by the PP-TSVD method, where the feldspar is composed by potassium feldspar and sodium feldspar, the clay content is the sum of Kaolinite, Illite and Smectite, and the carbonate content is merely the calcite content, with dolomite left out owing to its little portion; and the black curves, are the results interpreted by Schlumberger, along with the dark blue diamond-shaped scatters. Obviously, the mineral content curves, derived by such method, are consistent with the change trend of mineral content overall interpreted by Schlumberger, and are in perfect agreement with the core analysis data, especially those with high content, such as Quartz+Feldspar and Clay, despite of a relatively low standard deviation of pyrite. In order to weaken and even eliminate the impact of the conversion calculation models, the next task is expected to be fixed on modification of the pertinent oxide factors. In a nutshell, the PP-TSVD method is particularly suitable for the element-mineral conversion.
The MRE analysis of the conversion calculation for major mineral contents is then conducted, as is illustrated in Table 3, the Quartz+Feldspar and clay whose contents are over 20%, of which the MSE is 4.7% and 9.9%, respectively, both less than 10%, notwithstanding greater MSEs of carbonate and pyrite resulted from their little portion, which is reasonably acceptable. By comparison, the MSEs of the calculation content by PP-TSVD in this study are either less than or approximate to the ones of the Schlumberger interpretation, which demonstrates that the PP-TSVD algorithm can conspicuously meet the demands of the element-mineral conversion calculations.

Table 3. MRE$^a$ analysis of the mineral content

| Sample | Quartz+Feldspar (%) | Clay (%) | Carbon (%) | Pyrite (%) |
|--------|---------------------|----------|------------|-----------|
| Lab$^b$ | Calc.$^c$ | Schlum.$^d$ | Lab | Calc. | Schlum. | Lab | Calc. | Schlum. | Lab | Calc. | Schlum. |
| 1 | 49.1 | 46.3 | 47.8 | 40.5 | 44 | 46.2 | 2 | 2.5 | 3.1 | 8.4 | 7.2 | 2.9 |
| 2 | 62.3 | 64 | 63.2 | 17.9 | 14.8 | 15.8 | 10.8 | 12.4 | 12.7 | 9 | 8.8 | 8.3 |
| 4 | 57.7 | 65 | 65.8 | 28 | 23.1 | 24.7 | 7.3 | 6.5 | 5.6 | 7 | 5.4 | 3.9 |
| 5 | 60 | 56.5 | 62.4 | 21.4 | 24.5 | 26.1 | 8.9 | 9.5 | 9.2 | 9.7 | 9.5 | 2.3 |
| 7 | 64.4 | 63 | 68.7 | 11.2 | 11.7 | 12.3 | 15.4 | 16.9 | 15.5 | 9 | 8.4 | 3.5 |
| 11 | 55.4 | 57.4 | 52 | 34.9 | 36.7 | 37.4 | 4.8 | 4.5 | 3.9 | 4.9 | 1.4 | 6.7 |
| 14 | 55.4 | 57 | 50.1 | 34.9 | 36 | 32 | 5.6 | 5.2 | 9.3 | 4.1 | 1.8 | 8.6 |
| 16 | 61.5 | 60.4 | 64.9 | 20.8 | 26 | 18.6 | 9.6 | 8.6 | 7.4 | 8.1 | 5 | 9.1 |
| 17 | 54.5 | 57 | 50.6 | 37.2 | 37 | 40.5 | 3.2 | 4 | 5.7 | 5.1 | 2 | 3.2 |
| 19 | 56.9 | 59.8 | 61.3 | 30.9 | 30 | 27.4 | 6.5 | 5.1 | 5.8 | 5.7 | 5.1 | 5.5 |

MRE$^b$ (%) / 4.7 6.5 / 9.9 11.6 / 13.8 29.7 / 28.5 45.5

$^a$ MRE – Mean relative error.
$^b$ Lab – Lab test by X-ray diffraction core analysis;
$^c$ Calc. – Mineral content calculated by PP-TSVD method;
$^d$ Schlum. – Schlumberger interpretation results;

4. Summary and Conclusions

(1) The PP-TSVD method based on mathematical theories to accurately describe the conversion relationship between the elemental content and the mineral content, can achieve optimization of mineral content calculation;

(2) The scatter plots and the mineral content curves, derived by the PP-TSVD method, are all very much in good agreement with experimental results of X-ray diffraction core analysis, meanwhile the MSE analysis reveals that the fruits of such algorithm enjoy a better accuracy compared with the Schlumberger interpretation results, which indicate that such method is, in a substantial way, eminently adaptable and practical;

(3) Further revision and adjustment of the element related oxide factors need supplementary considerations, in order to diminish the impact of the conversion calculation models.

(4) Additionally, a combination of other approaches to element-mineral content conversion is proposed, such as the oxide closure model, the artificial neural network method, the nonlinear multiple regression method and the like, aiming to achieve more satisfactory multialgorithms and multimethods.

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