Research Article

Study on the Effect of Fractional Derivative on the Hyperspectral Data of Soil Organic Matter Content in Arid Region

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Discussion on the application of fractional derivative algorithm in monitoring organic matter content in field soil is scarce. This study is aimed at improving the accuracy of soil organic matter (SOM) content estimation in arid region, and the undesirable model precision caused by the missing information associated with the larger discrepancy between conventional integer-order, i.e., first order and second order, derivative, and raw spectral data. We utilized fractional derivative (of zeroth order to second order in 0.2-order interval) processing on the field spectral reflectance \( R \) of the salinized soil sample from Fukang, Xinjiang, and its square root-transformed \( \sqrt{R} \), log-transformed \( \log(R) \), inverse-transformed \( 1/R \), and inverse log-transformed \( 1/\log(R) \) values. The correlation coefficient of each fractional derivative of transformed value with SOM content was calculated. The simulation showed the derivative reflectance value approximates zero. When increasing from zeroth order to first order, the derivative curve gradually aligns to the first-order curve, and the destination alignment was also seen while increasing from first order to second order. The significance test of 0.05 showed initial increase and later decay of bands in the five spectral transformations as the order increases. For specific bands, the derivative algorithm clearly justifies the correlation between soil spectra and organic matter content, and all of the absolute highest correlation coefficient values were obtained at fractional orders. When compared with integer-order derivative, fractional derivative is significantly better in improving correlation, showing overall superiority. The result supports the application of fractional derivative in the hyperspectral remote monitor of SOM in arid zone, which may in turn realize the timely and accurate SOM monitor in arid zone, and provides the basis for ecological restoration.

1. Introduction

Soil organic matter (SOM) refers to all carbon-containing organic matter found in soil, including animal and plant debris, microorganisms, and the organic products resulted from biological activities; it helps improve soil structure and maintain porosity and is an important indicator of fertility [1–3]. Soil fertility has major effect on plant growth rate, which in turn determines biodiversity and ecological stability. Therefore, soil organic matter content is a key parameter in agriculture, forestry, and ecological balance. Conventional field sampling in combination with lab chemical analysis is unable to satisfy the demand of efficient and dynamic mass-scale SOM monitor and evaluation [6–9]. The hyperspectral method as an advanced remote sensor technology provides a possible solution for being efficient, convenient, economic, and lossless. Soil reflectance has some degree of relationship with SOM [10–14], and provides the basis for efficient remote monitor of SOM in vast wasteland.

In arid and semi-arid desert areas, the overall level of SOM content is very low. When SOM mass fraction is less than 2%, because of the absorption of spectral reflectance of organic matter is greatly reduced, there is a big challenge to accurately determine the response band of SOM. However, the spectral response band determination is the key to estimate SOM content accurately and effectively. At present, there are few studies on the hyperspectral estimation of organic matter in desert soil, and the traditional integer-order derivative algorithm has been widely applied in studies building models for hyperspectral monitoring SOM. For instance, Tian et al. [15] applied infrared photoacoustic spectra in SOM estimation and
revealed that the spectral model smoothened with first-order derivative show higher precision. Hou et al. [16] combined the lab SOM content and hyperspectral data to compare the modeling precision of simple linear regression, multiple linear stepwise regression, and PLSR; they confirmed that second-order derivative PLSR is the optimal model, and the best sensitivity bands were found at 640–790 nm. Studies showed that first- and second-order derivatives have greater discrepancy from the raw data and are prone to missing data that impacts model precision. Meanwhile, fractional-order derivative as the derived concept of integer-order derivative is widely applied in the control system, signal smoothening, biological engineering, and image processing [17–21]. Its wide applicability is due to the fact that integer-order derivative models lack the precision when presenting the wide applicability is due to the fact that integer-order derivative lacks the precision when presenting the model precision. Meanwhile, fractional-order derivative show higher precision. Hou et al. [16] combined spectral derivative with first-order derivative to smoothen the spectra. However, fractional differential. Results showed that fractional derivative into any order [29–31]. the uniform expression of fractional derivative for a single-variable function is expressed as follows:

\[
d^\alpha f(x) = \lim_{h \to 0} \frac{1}{h^\alpha} \sum_{m=0}^{(l-\alpha)/h} (-1)^m \Gamma(\alpha + 1) \frac{m!}{\Gamma(\alpha - m + 1)} f(x - mh),
\]

(1)

where \(\alpha\) is any order, \(h\) is the step size, \(t\) and \(a\) are the upper and lower extreme values, respectively, and gamma function \(\Gamma(\alpha) = \int_0^\infty \exp(-u)u^{\alpha-1} du = (\alpha - 1)\). Consider that the resampling interval of spectrometer is 1 nm and \(h = 1\), the derived difference in the fractional-order derivative of single-variable function \(f(x)\) is expressed as follows:

\[
\frac{d^\alpha f(x)}{dx^\alpha} = f(x) + (-\alpha) f(x - 1) + \frac{(-\alpha)(-\alpha + 1)}{2} \cdot f(x - 2) + \cdots + \frac{\Gamma(-\alpha + 1)}{n!(-\alpha + n + 1)} f(x - n).
\]

2. Fractional-Order Derivative Algorithm

Fractional-order derivative refers to derived integer-order derivative into any order [29–31]. The uniform expression of fractional-order derivative is unavailable. The best known models are Riemann–Liouville, Grünwald–Letnikov, and Caputo [32–37]. The Grünwald–Letnikov model is mostly expressed as

\[
d^\alpha f(x) = \lim_{h \to 0} \frac{1}{h^\alpha} \sum_{m=0}^{(l-\alpha)/h} (-1)^m \Gamma(\alpha + 1) \frac{m!}{\Gamma(\alpha - m + 1)} f(x - mh),
\]

where \(\alpha\) is any order, \(h\) is the step size, \(t\) and \(a\) are the upper and lower extreme values, respectively, and gamma function \(\Gamma(\alpha) = \int_0^\infty \exp(-u)u^{\alpha-1} du = (\alpha - 1)\). Consider that the resampling interval of spectrometer is 1 nm and \(h = 1\), the derived difference in the fractional-order derivative of single-variable function \(f(x)\) is expressed as follows:

\[
\frac{d^\alpha f(x)}{dx^\alpha} = f(x) + (-\alpha) f(x - 1) + \frac{(-\alpha)(-\alpha + 1)}{2} \cdot f(x - 2) + \cdots + \frac{\Gamma(-\alpha + 1)}{n!(-\alpha + n + 1)} f(x - n).
\]

3. Experiment Design and Operation

3.1. The Study Site. The study site locates between the Northern Foothill of Tianshan Mountain and the southern border of Junggar Basin (87°42′–88°46′E, 43°29′–45°45′N), which is at the downstream area of Xinjiang Fukang 500 Reservoir. This temperate region features arid continental climate with drastic day-night temperature gradients and a seasonal pattern of long winters, nondefinitive springs and autumns, and scorching summers. With mean annual temperature at 6.7°C, it has the highest temperature of 42.6°C and the lowest temperature of −41.6°C. Precipitation is scarce and spatially uneven. The mean annual precipitation is 164 mm, with 3–29 cm snow in the winter. The mean annual evaporation potential is about 2000 mm. The soil structure comprises gray desert soil, cracked soil, and sandy soil. The primary vegetation includes Haloxylon ammodendron, salt cedar, weed, and artificial Haloxylon ammodendron or elm forest, or farmed saplings.

3.2. Soil Sampling. Five sampling lines, each 600–800 m apart, were assigned northward at the left of the waterway at the study site, and six sampling lines, each 800–1000 m apart, were assigned northward at the right of the waterway at the study site. Depending on the field condition, five sampling points, each 300–500 m apart, were chosen on each line to collect the soil sample to define regional background. A total of 55 sampling points were chosen and located with GPS. The samples were collected in mid-May 2017. The samples were collected from sampling holes of 1 m × 1 m × 1 m. Since the soil spectra primarily reflect the nature of top soil, the spectra were analyzed with the SOM content in soil at
0–10 cm. The soil samples were subject to preprocessing of grinding and sieving before being submitted to Xinjiang Institute of Ecology and Geography, Chinese Academy of Sciences for soil organic matter content testing.

3.3. Field Spectral Test. The spectrum of top soil from each sampling point was obtained in mid-May 2017 using the portable FieldSpec®3 Hi-Res (ASD, United States) powered by ASD View Spec Pro. The spectral test was conducted at 11:00–15:00 (local time) on calm sunny days of little cloud cover to avoid undesirable effects of the elements. Before each spectral collection, white calibration was conducted to eliminate the dark current effect. The probe was placed at 15 cm above the sampling point. To avoid the possible interference from surface cracking and surrounding vegetation, each sampling point is kept as far away from possible source of interference as possible, and spectral curves were collected in ten replicas at 5 spots (within 1 m) around the sampling point showing similar background. A total of 50 curves were obtained, and the mean was used as the spectral data of the point to minimize the environmental effect.

3.4. Data Processing. Spectral data processing is used to reduce high-frequency noises, abnormal values, and the interference from internal and external spectra as well as environmental factors to provide accurate and reliable spectral signals, which are crucial for quantitative analysis and studies and the accuracy of models created.

The collected spectral digital signals contain noise “spikes” arising from the band differences in responsiveness. Smoothening preprocessing was conducted on spectral data to provide smoother change profile. In this study, Savitzky–Golay filter smoothing was applied on the hyperspectral reflectance data of 55 soil samples. The spectral reflectance data were removed of the low signal-noise bands of 350–399 nm and 2401–2500 nm, and the water absorption bands of 1355–1410 nm and 1820–1942 nm should be excluded for the greater impact on the accuracy of organic matter content determined using spectral inversion. Lastly, fractional derivative (of zeroth order to second order in 0.2-order steps) processing was applied on the spectral reflectance (R) and its square root-transformed (R), log-transformed (logR), inverse-transformed (1/R), and inverse log-transformed (1/logR) values. The correlation coefficient of each fractional derivative of transformed value with SOM content was calculated. The calculation was done with Matlab2015a software.

4. Simulation Results

4.1. Spectral Reflectance Curve of Different Organic Matter Content. Spectral feature refers to the overall physical and chemical properties, while the curve to some degree indicates the soil composition. Of these 55 sampling points, the organic matter content is the highest at point 1 (17.181 g/kg), the lowest at point 29 (4.168 g/kg), and the median value is at point 52 (9.503 g/kg) (see Figure 1 for the maximal, minimal, and median values and their corresponding sampling points in the spectral curve). As SOM content increases, the soil reflectance decreases and the spectral curves relative to SOM content show smoother and consistent trend with three significant absorption troughs of water at around 1400 nm, 1900 nm, and 2200 nm. The hyperspectral curve was analyzed with the seven bands of Landsat 8 satellite. The result shows steeper inclination at 433 nm–453 nm, suggesting greater reflectance change in this band. The curve shows slow increase at 450 nm–515 nm, rapid increase at 525 nm–600 nm, smoothness around 600 nm, then slow increase at 630 nm–680 nm, and insignificant change at 845 nm–885 nm. At 1560 nm–1600 nm, slow increase was observed with increasing spectral reflectance difference between content levels. At 2100 nm–2300 nm, an initial increase followed by decay is observed.

4.2. Simulation Result of Fractional-Order Derivative Algorithm. The 11-step fractional-order derivative calculations of the mean spectra of 55 sampling points are shown in Figure 2. The 1100 nm–1300 nm band was chosen as the difference in derivative-processed reflectance (the longitudinal axis) is small. The simulation showed the value approximates zero. When increasing from zeroth order to first order, the derivative curve gradually aligns with the first-order curve, and the destination alignment was also seen while increasing from first order to second order. This is due to the fact that fractional-order derivative is derived from integer-order derivative; integer-order derivative has better-defined physical and geometric significance: the first-order derivative of displacement relative to time is speed and the slope of tangent for curves. The second-order derivative of displacement relative to time is acceleration and curvature (change of slope) for curves. These clear definitions facilitate its research and
applications. Much effort has been addressed on the physical and geometric significance of fractional derivative. While the result remained obscure due to the complicated nature of the underlying issue, its application and development was unaffected. Spectral analysis studies showed that while fractional derivative lacks well-defined physical significance, fractional orders show the sensitivity to the slope, the first-order derivative, and curvature, the second-order derivative, of the spectral curve as they indicate inflection points and extreme values, respectively. That is, increasing from zeroth order to first order, the derivative result decreases the spectral reflectance sensitivity and increases the curve slope sensitivity, and derivative result decreases the slope sensitivity of curve and increases the curvature sensitivity of curve when increasing from first order to second order.

4.3. Full-Band Correlation Coefficient Change Trend. The higher correlation between spectral reflectance and surface parameters suggests better sensitivity of spectral response, and the bands showing high correlation are considered for modeling. As an example, the correlation coefficient between fractional derivative values of raw spectral reflectance \( R \) and soil salt content was tested at 0.05 significance level (* \( P = 0.26561 \)), as shown in Figure 3. Many bands in the raw spectral reflectance data passed the test: in the bands of decreasing correlation coefficient (500 nm–600 nm, 1850 nm–1900 nm), the decrease is more apparent at higher orders, and a similar trend was observed in the bands of increasing correlation coefficient (800 nm–900 nm, 2150 nm–2200 nm). This shows that fractional-order derivative presents more details about the trending of correlation coefficient curve, and the degree of change increases with order.

The number of bands passing the significance test of 0.05 on the correlation coefficient of raw reflectance data and each fractional order is not shown in Figure 3, so statistical effort was done to define mentioned number on processed \( R, 1/R, \lg R, \sqrt{R}, \text{and } 1/\lg R \) with each fractional order. The result is presented in Table 1. The significance test (of 0.05) showed initial increase and later decrease of band quantity in the five spectral transformations as the order increases.

4.4. Bands with the Highest Absolute Correlation Coefficient Value in Each Spectral Transformation. The bands with the highest absolute correlation coefficient value in each fractional order and spectral transformation are defined in Table 2. At zeroth- and 0.2-order derivative transformation, \( 1/\lg R \) increases the correlation between spectral reflectance \( R \) and SOM content, while \( 1/R, \lg R, \text{and } \sqrt{R} \) decreases the correlation. At 0.4 order and 0.8 order, \( 1/R \) and \( 1/\lg R \) reduce correlation, while \( \sqrt{R} \) and \( \lg R \) increase it. At 0.6 order, correlation reduction is only seen with \( \sqrt{R} \) and the others increase the correlation. At first order, \( \sqrt{R} \) is the only transformation increasing correlation and the others decrease correlation. At 1.2 order, correlation decrease is observed in all of the four transformations. At 1.4-, 1.6-, 1.8-, and second-order, \( 1/\lg R \) is the only transformation showing increase of correlation, while it is decreased for the others. In each mathematical transformation, the maximal absolute correlation coefficient value shows initial increase followed by decay as the order increases. The absolute correlation coefficient value of \( \lg R \) reaches maximum at 634 nm of 1.2-order derivative, and it is 667 nm of 0.8-order for \( 1/R \) and 623 nm of 1.2-order for \( R, \sqrt{R}, \text{and } 1/\lg R \).
Figure 3: Continued.
Figure 3: Correlation coefficient of fractional derivative-processed raw spectral reflectance data and SOM content. (a) Zeroth order. (b) 0.2 order. (c) 0.4 order. (d) 0.6 order. (e) 0.8 order. (f) First order. (g) 1.2 order. (h) 1.4 order. (i) 1.6 order. (j) 1.8 order. (k) Second order.

Table 1: Number of bands passing the significance test of 0.05.

<table>
<thead>
<tr>
<th>Order</th>
<th>( R )</th>
<th>( \sqrt{R} )</th>
<th>( 1/R )</th>
<th>( \lg R )</th>
<th>( 1/\lg R )</th>
</tr>
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<tr>
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<td>36</td>
<td>0</td>
<td>12</td>
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<td>15</td>
<td>61</td>
<td>87</td>
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<td>225</td>
<td>262</td>
<td>252</td>
<td>270</td>
<td>163</td>
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<td>333</td>
<td>313</td>
<td>269</td>
</tr>
<tr>
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<td>313</td>
<td>376</td>
<td>323</td>
<td>304</td>
</tr>
<tr>
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<td>320</td>
<td>351</td>
<td>297</td>
<td>367</td>
<td>324</td>
</tr>
<tr>
<td>1.2</td>
<td>277</td>
<td>285</td>
<td>184</td>
<td>256</td>
<td>272</td>
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<tr>
<td>1.6</td>
<td>133</td>
<td>124</td>
<td>99</td>
<td>116</td>
<td>132</td>
</tr>
<tr>
<td>1.8</td>
<td>98</td>
<td>92</td>
<td>70</td>
<td>82</td>
<td>108</td>
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<td>2</td>
<td>79</td>
<td>72</td>
<td>64</td>
<td>75</td>
<td>83</td>
</tr>
</tbody>
</table>

Table 2: Bands with the highest absolute correlation coefficient value in each spectral transformation.

<table>
<thead>
<tr>
<th>Order</th>
<th>( R )</th>
<th>( \sqrt{R} )</th>
<th>( 1/R )</th>
<th>( \lg R )</th>
<th>( 1/\lg R )</th>
</tr>
</thead>
<tbody>
<tr>
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<td>2310</td>
<td>0.2767</td>
<td>2310</td>
<td>0.2608</td>
</tr>
<tr>
<td>0.2</td>
<td>0.3036</td>
<td>2395</td>
<td>0.2958</td>
<td>2309</td>
<td>0.2780</td>
</tr>
<tr>
<td>0.4</td>
<td>0.3533</td>
<td>2395</td>
<td>0.3425</td>
<td>2395</td>
<td>0.4302</td>
</tr>
<tr>
<td>0.6</td>
<td>0.4147</td>
<td>2327</td>
<td>0.4116</td>
<td>2258</td>
<td>0.4702</td>
</tr>
<tr>
<td>0.8</td>
<td>0.4629</td>
<td>2064</td>
<td>0.4778</td>
<td>667</td>
<td>0.5335</td>
</tr>
<tr>
<td>1</td>
<td>0.5564</td>
<td>648</td>
<td>0.5717</td>
<td>648</td>
<td>0.5238</td>
</tr>
<tr>
<td>1.2</td>
<td>0.5966</td>
<td>623</td>
<td>0.5928</td>
<td>623</td>
<td>0.4747</td>
</tr>
<tr>
<td>1.4</td>
<td>0.5323</td>
<td>580</td>
<td>0.5127</td>
<td>580</td>
<td>0.4685</td>
</tr>
<tr>
<td>1.6</td>
<td>0.4947</td>
<td>570</td>
<td>0.4924</td>
<td>620</td>
<td>0.4814</td>
</tr>
<tr>
<td>1.8</td>
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<td>579</td>
<td>0.4337</td>
<td>619</td>
<td>0.4361</td>
</tr>
<tr>
<td>2</td>
<td>0.4483</td>
<td>2272</td>
<td>0.4412</td>
<td>2272</td>
<td>0.4034</td>
</tr>
</tbody>
</table>
Figure 4: Continued.
Figure 4: Continued.
4.5. Correlation Coefficient Chang Trend at Specific Bands.
As shown in Table 2, the bands showing the highest absolute correlation coefficient value in zeroth order, 0.2 order, 0.6 order, 0.8 order, first order, 1.2 order, 1.4 order, 1.6 order, and 1.8 order and second-order derivatives are at 2310 nm, 2395 nm, 2327 nm, 667 nm, 648 nm, 623 nm, 681 nm, 570 nm, 579 nm, and 2272 nm, respectively. The correlation coefficient trending with fractional order in these ten bands is shown in Figure 4. For each mathematical transformation, derivative processing greatly increases the absolute correlation coefficient value with organic matter content at these bands. For example, by applying 1.8-order derivative and taking zeroth order in comparison, the absolute correlation coefficient value of spectral reflectance with organic matter content is increased from 0.08539 to 0.50777 and 0.08440 to 0.49339 for square-root transformation, 0.079938 to 0.426081 for inverse transformation, 0.083140 to 0.47189 for log transformation, and 0.085726 to 0.501937 for inverse log transformation.

5. Discussion
Fractional differentiation is one of the ways the concept of the integer differential can be expanded. The aim is to fit the noninteger differential behavior to a physical system. In the selection of order, it breaks the limitations of integer orders in general dynamic systems and has wider application and better fitting. Moreover, the choices are not limited to integers, and this expands the calculation order possibilities. Fractional differentiation offers a wider order selection range and more freedom than the integer differential. Although, it increases the complexity of implementation, suitable software calculation routines already exist that easily overcome this problem. Studies have shown that the behavior of many real physical systems is fractional. The use of fractional differentials for hyperspectral quantitative inversion allows the physical model of soil organic matter to be clearly explained and described. This improves inversion accuracy and extends the scope of application of the model.

During the soil organic matter hyperspectral inversion model building process, the feature band is often confirmed by correlation analysis of organic matter and spectral reflectance. The higher correlation will induce more sensitivity into the band response. According to the results of this study, fractional differentiation has a wider order selection range. It can refine the changes in correlation coefficient between spectral reflectance (and the curve after mathematical transformation), the first-order differential, second-order differential, and soil organic matter. The fractional differential can also significantly increase the features of certain bands and can provide more feature band choices.

6. Conclusion
Salinization is significant in the arid region of Xinjiang; this factor, along with soil content, texture, and degree of compaction, may impact the precision of SOM content derived from hyperspectral inversion. The fractional-order derivative as a preprocessing technique provides detailed trending of correlation between SOM and spectral reflectance. At bands of 500 nm–600 nm, 1850 nm–1900 nm, 800 nm–900 nm, and 2150 nm–2200 nm, increased and decreased fluctuations of correlation coefficient with increasing order were observed and may have more implications. The number of bands with preprocessed correlation coefficient passing the significance test of 0.05 shows an overall trend of initial increase followed by decay, but the order with the highest number of bands remained
inconsistent between transformations. This study explored the applicability of fractional-order derivative algorithm in monitoring field hyperspectral SOM content, shedding new light on the projection of such data.

Data Availability
The data used to support the findings of this study will be available from the corresponding author upon request after this project has been finished in 2021.

Conflicts of Interest
The authors declare that they have no conflicts of interest.

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