

Technical Note

Equivalence of modified Gaussian model (MGM) in wavenumber and Gaussian in wavelength for deconvolution of hyperspectral reflectance spectra

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A modified Gaussian model (MGM) is used to separate overlapping absorption features into their fundamental bands in mineral reflectance spectra; it is widely used in the planetary remote sensing community. To facilitate its use for earth-observation studies where it has not been widely adopted, we show that the MGM analysis in wavenumber is numerically equivalent to Gaussian analysis in wavelength, improving access to software that is capable of the analysis. The two approaches were tested on a synthetic spectrum and a measured mineral spectrum. Results for the two methods are as close to identical as computationally possible, confirming their equivalency.

1. Introduction

The modified Gaussian model (MGM) (Sunshine *et al.* 1990) is a method for deconvolving overlapping absorption features in hyperspectral reflectance spectra. The method is valuable because the band centre, width and strength of absorption features may vary if influenced by more than one absorption band. The ability to identify materials and their relative proportions in mixtures from reflectance spectra is improved by reducing overlapping features to their fundamental bands (Sunshine *et al.* 1993).

The MGM method is widely used in the lunar and planetary remote sensing communities. It has been used successfully to characterize compositional or abundance information in minerals or mineral mixtures (Sunshine and Pieters 1990, 1993, 1998, Mustard 1992, Mustard and Sunshine 1995, Hiroi *et al.* 2000, de Leon *et al.* 2004, Combe *et al.* 2005, Vernazza *et al.* 2005, to name but a few) with the ability to estimate modal abundances within 5%–10% for specific minerals and assemblages (Sunshine and Pieters 1993). Despite these successes, the MGM has not made inroads into the environmental and earth science literature. Cloutis (1996) identified the MGM as an important technique for use in earth-based geological remote sensing, but the technique may also have potential for the remote sensing of other materials, from such widespread applications as the biochemical content of

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vegetation, which, in turn, may be linked to vegetation classification (Martin *et al.* 1998), to more specific applications such as the makeup and concentration of bitumen in oil sands. The lack of acceptance of this method within the broader remote sensing community can be attributed to two principal causes: a lack of familiarity with the MGM model and the lack of user-friendly fully supported software to implement it.

The original development of the MGM by Sunshine *et al.* (1990) was based on the observation that absorbance features seen in reflectance spectra of minerals, measured in wavenumbers, were not well modelled by a Gaussian distribution, i.e.

$$\text{Absorbance}(x) = A_G \exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right), \quad (1)$$

where A_G is the amplitude of the feature, x is its position, μ is its mean and σ is its standard deviation. This was contrary to expectations where it was believed that absorbance should be directly proportional to bond energy (Burns 1970) and hence should be Gaussian when spectra are viewed in wavenumbers. Furthermore, they noted that a better fit was obtained by fitting a 'modified' Gaussian of the form:

$$\text{Absorbance}(x) = A_{\text{MGM}} \exp\left(\frac{-\left(\frac{1}{x} - \frac{1}{\mu}\right)^2}{2\sigma^2}\right), \quad (2)$$

where A_{MGM} is again an amplitude parameter. The argument put forward justifying this equation was that absorbance was related to bond length rather than bond energy.

Wavelength is, by definition, the reciprocal of wavenumber. Thus, it appears that equation (2) might be equivalent to the Gaussian equation (equation (1)), provided that the spectra were in wavelength rather than wavenumber. Sunshine *et al.* (1990) worked only in wavenumber and showed that the MGM performed better than the Gaussian, but what if you work in wavelength? Is the MGM in wavenumber equal to the Gaussian in wavelength? This is an accepted interpretation in some of the literature, although it is always presented without proof (see, for example, Hiroi *et al.* 2000, Hiroi and Sasaki 2001). The fundamental problem with proving the equivalence of the two systems lies in the statistical properties of the two equations. In the case of the Gaussian distribution the moments, i.e. mean, variance, kurtosis, etc., may be easily found by integrating equation (1) with the appropriate normalization (the integral represents a probability density function and must be equal to one). In the case of the MGM equation (equation (2)), a closed form solution of the integral does not exist. Hence, one is left to show the equivalence of these two equations by other means, i.e. by their numerical equivalence.

Given that the equivalence of the MGM in wavenumber versus the Gaussian in wavelength must be established numerically, the problem still remains to implement a solution. Many researchers have access to free or commercial programs that are well supported, which can fit Gaussian distributions and which have user-friendly visual and interactive formats. The details of how such programs work in regards to such things as the optimization scheme they employ, terminating conditions, etc., are not central to our discussion with the proviso that we use the same set up and approach in all analyses. Within such a framework, we will show that the MGM

approach of fitting Modified Gaussian distributions in wavenumbers (MGM/wN) is numerically equivalent to fitting Gaussian distributions in wavelength (G/wL), thus enabling the use of many readily available software programs. We think it is important to establish the equivalence of the MGM in wavenumbers to Gaussians in wavelength, and to communicate it clearly to the non-planetary remote sensing community, with the goal of facilitating investigation of such methods for earth-observation applications.

2. Approach

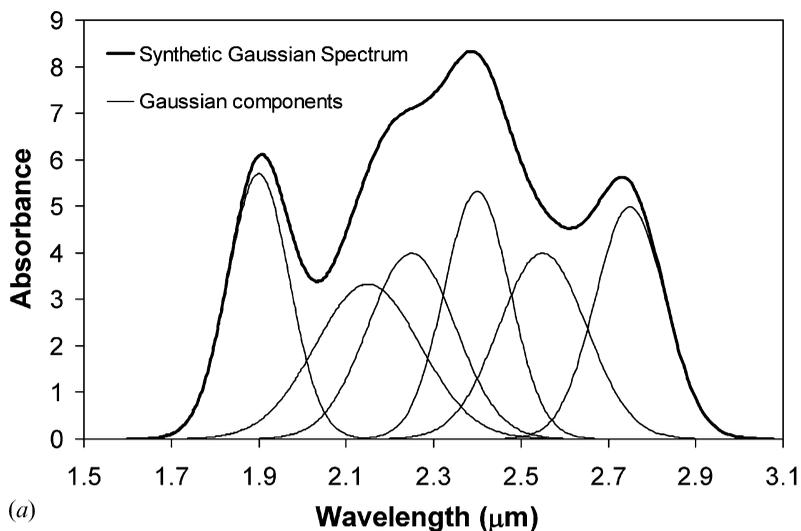
We have addressed the question of the numerical equivalence of the MGM/wN with the G/wL by comparing the MGM and Gaussian solutions using first a synthetic spectrum and then a measured spectrum (clinopyroxene: PP-CMP-022 from the RELAB spectral catalogue at <http://lf314-rlds.geo.brown.edu/>). The synthetic spectrum provides a test case for which we know with complete confidence the contributing components that make up the observed features. The measured spectrum provides a real-world mineral spectrum, one that is well known to the remote sensing community and whose contributing components are well understood physically (Burns 1970, Sunshine *et al.* 1990).

A synthetic Gaussian spectrum was created by combining six individual Gaussian distributions, each generated at discrete sampling points over the desired wavelength range (see figure 1(a) and table 1). The synthetic Gaussian spectrum was then transformed to wavenumbers, which will produce a synthetic MGM spectrum provided that the MGM distribution in wavenumbers equals the Gaussian distribution in wavelength (figure 1(b)). We then fit the MGM distributions to the synthetic spectrum in wavenumbers, and the Gaussian distributions to the synthetic Gaussian spectrum in wavelength, with a constant baseline in both cases. Fitting was carried out using PeakFit V4.12 (SeaSolve Software Inc.) with the noise tolerance and degree of smoothing set to zero. The Levenburg–Marquardt algorithm (Press *et al.* 1982) was chosen to find the minimum least squares difference between the calculated and input spectra. Because the solution is found using an optimization process, there is no guarantee that a stable solution will be found, or even identical solutions will be found, each time a spectrum is fitted. Therefore, 30 trials were conducted for each case, using slightly varying starting guesses with the mean residual being reported. Since the input spectra are synthetic, we expect a perfect fit for both approaches if the two cases are equivalent.

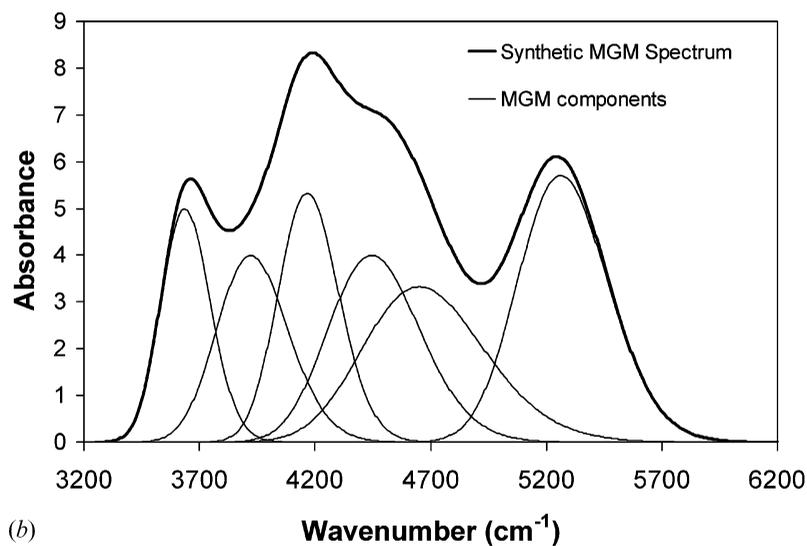
The measured clinopyroxene spectrum was processed in the same way, except that the spectrum was inverted by taking the natural log of $1/R$, where R is reflectance, to convert reflectance troughs to absorbance peaks. Because it is a measured spectrum, the MGM/wN fit and the G/wL fit will not be perfect. However, the test of whether the two approaches are equivalent is not whether the fit is perfect or even good, but whether the two fits are the same. If the MGM/wN equals the G/wL, the two approaches should produce identical results.

3. Results and discussion

The Gaussian solution for the synthetic Gaussian spectrum in wavelength correctly found a baseline of zero, and six components whose moments exactly match those used to generate the spectrum to eight decimal places. As expected, the overall fit, as measured by the residual between the calculated and input spectra, is as close to zero



(a)



(b)

Figure 1. (a) Synthetic Gaussian spectrum formed from six synthetic Gaussian components, and (b) the same spectrum displayed in wavenumber rather than wavelength, which converts it to an MGM spectrum if equations (1) and (2) are equal. The MGM components are slightly asymmetrical compared to the Gaussian components in (a).

as the precision of the calculations allow, of the order of 10^{-15} at all wavelengths in this case (see figure 2). The MGM solution in wavenumbers also found a baseline of zero and six components, but since their moments cannot be found analytically, we rely on the residuals to compare results with the Gaussian case (figure 2). The MGM residuals ($\mu=6.51 \times 10^{-17}$, $\sigma=3.25 \times 10^{-15}$) are noisier than the Gaussian residuals ($\mu=2.82 \times 10^{-17}$, $\sigma=1.44 \times 10^{-15}$), reaching an order of 10^{-14} , which we attribute to rounding errors that occur in the divisions performed by the MGM. There is an apparent systematic error in the residuals (figure 2). We attribute this to the way PeakFit works, in which it resamples the discrete input spectrum before optimization and then resamples the calculated spectrum back into the original

Table 1. Parameters of Gaussian components used for construction of the synthetic Gaussian spectrum in wavelength. Units are μm .

Construction	Peak 1	Peak 2	Peak 3	Peak 4	Peak 5	Peak 6
Mean μ	1.900	2.150	2.250	2.400	2.550	2.750
Std. dev. σ	0.070	0.120	0.100	0.075	0.100	0.080

abscissa values before output. Nevertheless, we conclude that the two results are as close to identical as computationally possible, and that the two cases are equivalent.

We also briefly considered the problem of the robustness and uniqueness of the derived solutions by allowing for extremes in the initial guess of peak locations and amplitudes. Trials were conducted whereby peaks were initially set outside of the spectral range of coverage, clustered within the spectral range of coverage and where the initial amplitudes were widely varied. Both methods did not obtain the correct solution when a peak was set outside of the spectral range of coverage, with the outlier's contribution to the spectra being essentially set to zero. In the case of peaks clustered within the spectral range, both methods obtained the correct solution, provided that the amplitudes of the clustered peaks were not set too large. If the amplitudes of the clustered peaks were large, in some cases the optimization found a local minimum in its decision criteria; this stopped better solutions from being found. In all cases, for both methods, the behaviour and results of the algorithms were the same. The only notable exception was that the MGM method took considerably more iterations than the Gaussian solution, although this may be attributed to better optimization of the Gaussian method within PeakFit.

We also tested for equivalence using a measured spectrum. In this case, we expect the fits for both the G/wL and the MGM/wN to be significantly poorer, since we are

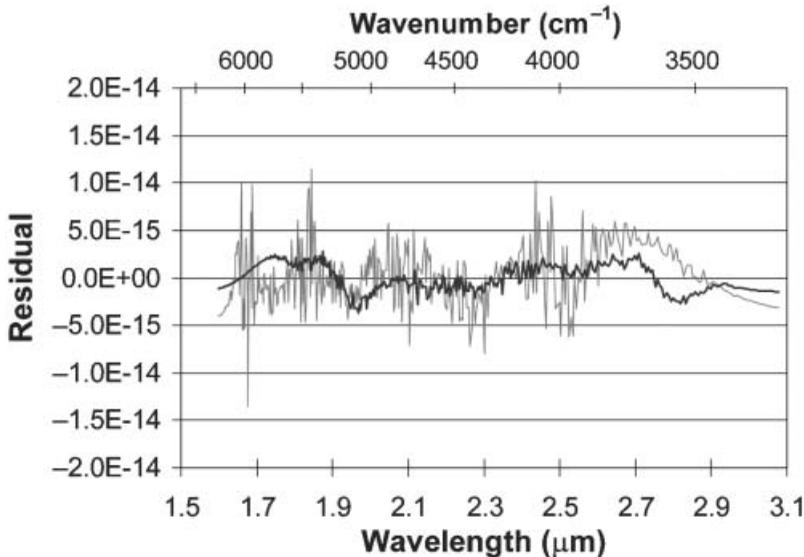


Figure 2. Average residuals for 30 trials for the G/wL fitting of the synthetic Gaussian spectrum in wavelength (black), and for the MGM/wN fitting of the synthetic spectrum in wavenumbers (grey). The MGM/wN residuals were transformed into wavelength for ease of comparison.

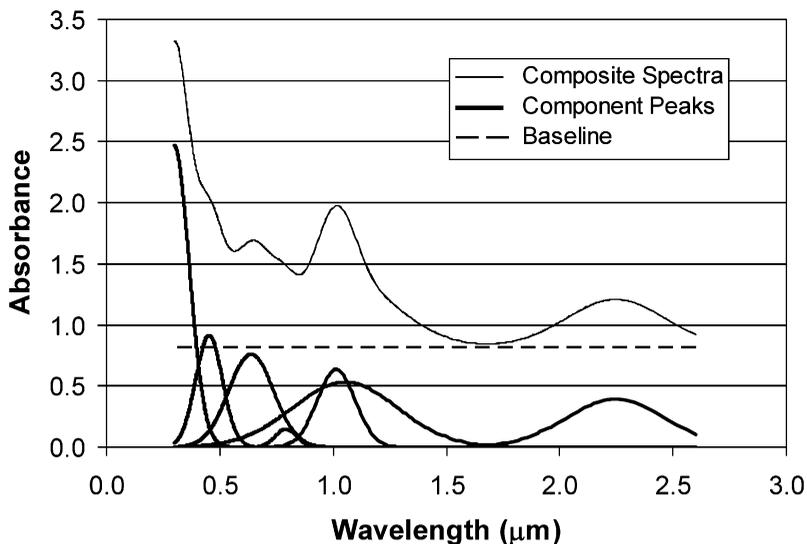


Figure 3. The G/wL best-fit solution for a clinopyroxene spectrum overlaid on the MGM/wN best-fit solution (fitted in wavenumbers, but presented in wavelength for ease of comparison) for the same mineral spectrum. The two solutions are so similar that each result appears as a single line. The data are presented in absorbance, which inverts the usual reflectance view.

dealing with real data. However, the test of equivalence is whether the two approaches produce identical results, not good results. The results for the two cases are so similar that when the results are plotted on top of each other, only a single line is visible for the composite, background and individual peaks (figure 3). There are differences in the two solutions, this time of the order of 10^{-6} to 10^{-7} , but this is again at the level of the floating-point precision reported by PeakFit. Therefore, we again conclude that the two results are as close to identical as computationally possible, and that the two cases are equivalent. As an aside, the solutions also match those in the literature (Sunshine *et al.* 1990) judged to be physically meaningful in terms of the expected optical behaviour of the mineral.

The original MGM paper (Sunshine *et al.* 1990) showed that a modified Gaussian distribution is preferred to a Gaussian distribution, when spectra are in wavenumbers. In the literature, however, there are references to the MGM as Gaussian fitting, without indicating whether spectra are in wavelength or wavenumbers (Lucey 1998, Lucey *et al.* 1998, Schade and Wasch 1999, Combe *et al.* 2005, Pinet *et al.* 2006). Even if the authors mean Gaussian in wavelength, such terminology is unclear, apparently in contradiction to the intent of Sunshine *et al.* (1990), and could lead to the misconception that the MGM work of Sunshine *et al.* (1990) is Gaussian fitting in wavenumbers (Craig 1994, Brown 2006). We have shown that the G/wL fitting produces the same results as the MGM/wN. For users who adopt the G/wL approach to implement what is widely known as MGM analysis, we strongly recommend that they specify the spectral units used in the actual fitting process. Furthermore, using the term 'MGM' for G/wL fitting is potentially confusing and it may be better to simply refer to the process as Gaussian fitting in wavelength.

4. Conclusions

Deconvolving spectra into fundamental absorbance features has proved to be of great value in the analysis of planetary minerals. We have shown that the MGM approach used widely in the planetary remote sensing community can be implemented by using spectra in wavelength and the Gaussian distribution. We do not claim to be the first to recognize this, but we think it is important to demonstrate and communicate it to encourage other researchers to adopt the approach. Optimization analysis needs to be undertaken with suitable caution to ensure that physically meaningful results are found, but by opening the road to the use of many software packages, some of them with easy user interfaces and multiple tools to evaluate results, we think others will find it a useful method for understanding reflectance spectra in a range of environmental and earth science applications.

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