A New Method for Gas Continuous Spectra Description Invariant to Environment Changes

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Abstract: Spectra play an increasingly important role in object detection, recognition, and identification. A key challenge in object identification using infrared spectroscopy is that spectral profiles change with variations in temperature and pressure, making robust feature extraction difficult. Thus, a stable descriptor for infrared spectra is essential for invariant feature extraction under varying environmental conditions. In this paper, we propose a novel spectral descriptor grounded in the concept of curvature. The fundamental insight is that the relative curvature across different scales remains unchanged despite environmental perturbations. The Curvature Scale Space (CSS) method is adopted as the foundation, upon which we develop the Normalized Curvature Scale Space (NCSS) descriptor for invariant spectral representation.

Keywords: Gas spectral recognition; Invariant feature extraction; Curvature Scale Space; Spectral descriptor

1. Introduction

Spectral feature extraction plays a pivotal role in object recognition across a wide range of applications [1-3], including remote sensing, infrared gas identification, and chemical analysis. Among these, gas identification presents particular challenges when physical conditions vary. On one hand, gas spectra become sharper as temperature increases, as illustrated in Figure 1(a). On the other hand, spectra become narrower as pressure increases, as shown in Figure 1(b). When both temperature and pressure change simultaneously, the combined effect produces more complex spectral deformations, as depicted in Figure 1(c). Consequently, a stable and robust representation of gas spectra is crucial for reliable object identification.

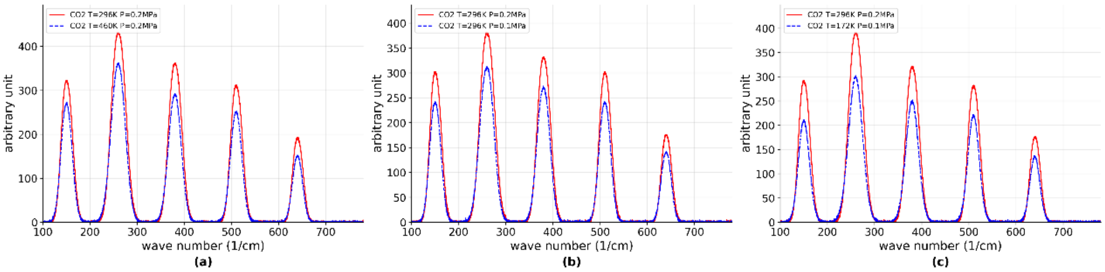

Figure 1: Gas Spectra in Different Temperature and Pressure.

It is well established in physics that high pressure reduces molar volume and generally brings atoms closer together. Changes in temperature alter intermolecular distances, which in turn affect hydrogen bond strengths, resulting in frequency shifts toward lower wavenumbers. These physical mechanisms lead to abrupt and sometimes unpredictable changes in spectral profiles, making spectral identification considerably more difficult [4, 5].

The hydrogen bonding effect provides a general physical explanation for how temperature and pressure influence spectral profiles. The evolution of spectra under changing conditions manifests primarily as shifts in frequency and amplitude. Understanding this mechanism is the first step toward designing a robust spectral descriptor.

This paper addresses the spectral recognition problem in complex and dynamically changing environments, with particular focus on conditions involving varying temperature and pressure. After carefully examining the underlying physical principles governing spectral changes, we propose an anti-change strategy for spectral feature extraction. Since the primary spectral changes manifest as frequency and amplitude shifts, one key property remains relatively stable: the relative curvature of spectral peaks. This assumption is supported by physical and chemical evidence from the literature [6].

Infrared spectra typically appear as combinations of peaks that may differ in height and width. Regardless of how physical conditions change (e.g. temperature, pressure) the mathematical consequence is a change in the curvature of individual peaks. Importantly, if the environmental changes affect all spectral bands equally, the curvature of all peaks within the same spectrum changes at the same rate. This observation motivates our proposal of a novel algorithm based on relative curvature analysis of spectra.

To summarize, the evolution of spectra under environmental changes can be characterized in terms of curvature variation. Under the simplifying assumption that hydrogen bonding effects act equally on all spectral bands, the curvature of each peak changes at the same pace. Consequently, the relative curvature among peaks remains unchanged. This invariance property forms the theoretical foundation of our algorithm for invariant spectral feature extraction.

2. Algorithm

In this section, we address the spectral representation problem from a signal processing perspective. The proposed method is specifically designed to handle spectral changes arising from varying physical conditions. We first review the Curvature Scale Space (CSS) framework and then introduce the NCSS (Normalized Curvature Scale Space) descriptor, which aims to extract more stable and discriminative spectral features.

2.1 Curvature

The CSS approach was a shape representation method for planar curves. Spectral curves are naturally represented as one-dimensional planar curves that do not self-intersect. This method is based on identifying inflection points on the curve at varying levels of smoothing scale. The curvature k of a spectral curve at a given point is defined as the instantaneous rate of change of the tangent slope with respect to arc length, and can be expressed as:

$$k(t) = \frac{x'(t)y''(t) - y'(t)x''(t)}{(x'(t)^2 + y'(t)^2)^{3/2}}$$

where x'(t), x''(t), y'(t), and y''(t) are the first and second derivatives of x(t) and y(t) respectively, and (x(t), y(t)) is the parametric representation of the curve.

To compute the curvature at varying levels of detail, x(t) and y(t) are convolved with a Gaussian function g(t, σ). The smoothed curvature k_\sigma(t) can then be expressed as:

$$k_\sigma(t) = \frac{X_t(t,\sigma)\, Y_{tt}(t,\sigma) - Y_t(t,\sigma)\, X_{tt}(t,\sigma)}{(X_t(t,\sigma)^2 + Y_t(t,\sigma)^2)^{3/2}}$$

where X_t, X_{tt}, Y_t, Y_{tt} denote the first and second partial derivatives of the Gaussian-smoothed versions of x(t) and y(t) with respect to t.

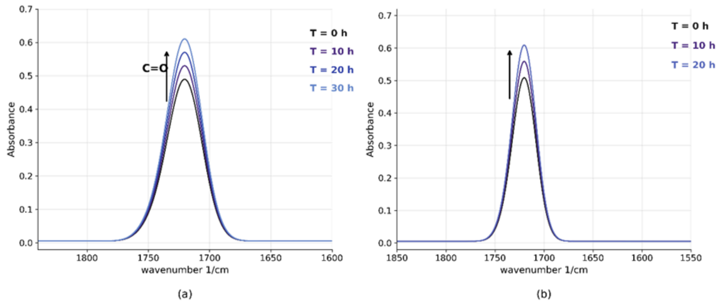

Figure 2: ATR-FTIR of Cross Lined PEGDA Treated in N2 and in Air After Different Exposure Times.

(a) Spectra of crosslinked PEGDA without particles treated in dry air and dry nitrogen. After irradiation the changes in the samples are different. In the sample treated in N2 the OH-band (~3500 cm^{-1}) increases in intensity while for the samples treated in air the same band is subject to an extensive broadening; (b) In the area of the C=O band (1700 cm^{-1}) there is the appearance of shoulders at both samples treated in nitrogen or air. In the sample treated in air there is also a pronounced shift of the maximum of the C=O to lower wavelengths. The two different behaviors are related with the possible reactions involved in the different conditions.

As illustrated in Figure 2, certain spectral regions are particularly susceptible to environmental perturbations. Regions with small curvature (typically the flanks and baseline regions of peaks) are more easily affected by changes in temperature, pressure, or chemical environment. In contrast, regions with high curvature, such as peak apices and inflection points, tend to preserve their relative positions more robustly. We therefore identify local curvature maxima as shape specification points (see Step 2 in Figure 3), which serve as the key feature descriptors for spectral data. The arrows in Figure 2 indicate spectral regions that are most susceptible to environmental influence, further motivating the use of curvature-based features.

2.2 NCSS Feature Graphic

In the standard CSS feature graphic, the locations of curvature maxima across different scale levels are treated as key features representing the spectral shape. However, when physical conditions change, the two CSS feature graphics of the same substance may not appear identical, due to shifts in peak positions and widths. To address this, we introduce a normalization procedure that maps the observed spectral features into a canonical coordinate frame aligned with the reference spectrum. This normalized representation is referred to as the NCSS (Normalized Curvature Scale Space) feature graphic.

The NCSS normalization procedure operates as follows. Given the CSS feature graphics of a reference spectrum and an observed spectrum, the shape specification points extracted at each scale level are aligned by normalizing the spatial extent of the observed feature set to match that of the reference. Specifically, let p_j^r and p_j^o denote the shape specification point locations of the reference and observed spectra at a given scale\sigma. The normalized observed point locations $\hat{p}_j^o$ are computed as:

$$\hat{p}_j^o = \frac{p_j^o - \min(\{p^o\})}{\max(\{p^o\}) - \min(\{p^o\})} \cdot (\max(\{p^r\}) - \min(\{p^r\})) + \min(\{p^r\})$$

This normalization effectively removes the effect of global frequency shifts and scale changes, allowing the intrinsic shape structure of the spectrum to be compared directly. The matching procedure between NCSS feature graphics is performed using a best-first search algorithm.

The complete NCSS feature graphic generation pipeline is illustrated in Figure 3. The red color indicates the reference spectrum stored in the database, while the blue color indicates the observed spectrum acquired under real-world conditions. As shown in the figure, the raw CSS feature graphics of the two spectra exhibit noticeable discrepancies due to environmental changes. After applying the NCSS normalization, the shape specification points become significantly closer and nearly overlapping, demonstrating the effectiveness of the proposed normalization in achieving environment-invariant spectral representation.

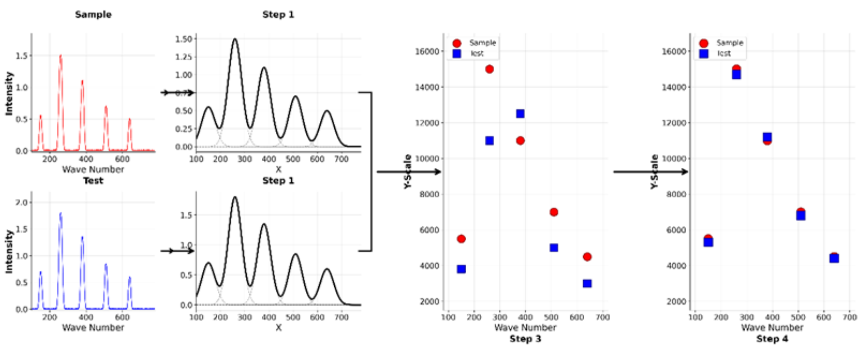

Figure 3: NCSS Feature Graphic Generation.

3. Results and Discussion

To validate the proposed NCSS algorithm, we collected spectral data from published literature covering multiple gas species and environmental conditions. The sample dataset includes spectral emission and absorbance measurements of CO_2, CO, and H_2O. Experimental results demonstrate that the proposed NCSS algorithm outperforms traditional methods in both stability and discriminability across all tested conditions.

3.1 Comparison Between CSS and NCSS

We conducted four experiments to systematically evaluate the performance of the proposed NCSS algorithm in comparison with the standard CSS approach.

Experiment 1 simulated a constant-pressure environment. The target gas was CO_2 at a constant pressure of 0.2 MPa, with temperature varying from 296 K to 460 K.

Experiment 2 simulated a constant-temperature environment. The target gas was CO_2 at a constant temperature of 296 K, with pressure varying from 0.1 MPa to 0.2 MPa.

Experiment 3 simulated an environment with simultaneous changes in both temperature and pressure. The target gas was CO_2, with temperature varying from 296 K to 172 K and pressure from

0.1 MPa to 0.2 MPa.

Experiment 4 evaluated the discriminative capability of the proposed algorithm by collecting spectral data from different gas categories.

The experimental results are presented in Figure 4. From the top row to the bottom row, the results correspond to Experiments 1 through 4. In Experiments 1 to 3, where spectral data from the same gas category are subject to varying physical conditions, the NCSS algorithm consistently yields more stable features compared to the standard CSS approach. The shape specification points extracted by CSS alone exhibit more dispersed distributions, resulting in higher matching costs. In contrast, since the relative curvatures of spectral peaks remain invariant under environmental changes, the NCSS algorithm is able to uncover an intrinsically stable pattern in the locations of curvature maxima. This leads to a more compact and consistent distribution of shape specification points, which better reflects the intrinsic spectral attributes of the gas.

In Experiment 4, the proposed algorithm demonstrates strong discriminative capability. Both CSS and NCSS features clearly distinguish between spectra from different gas categories, confirming that the normalization procedure does not compromise inter-class separability.

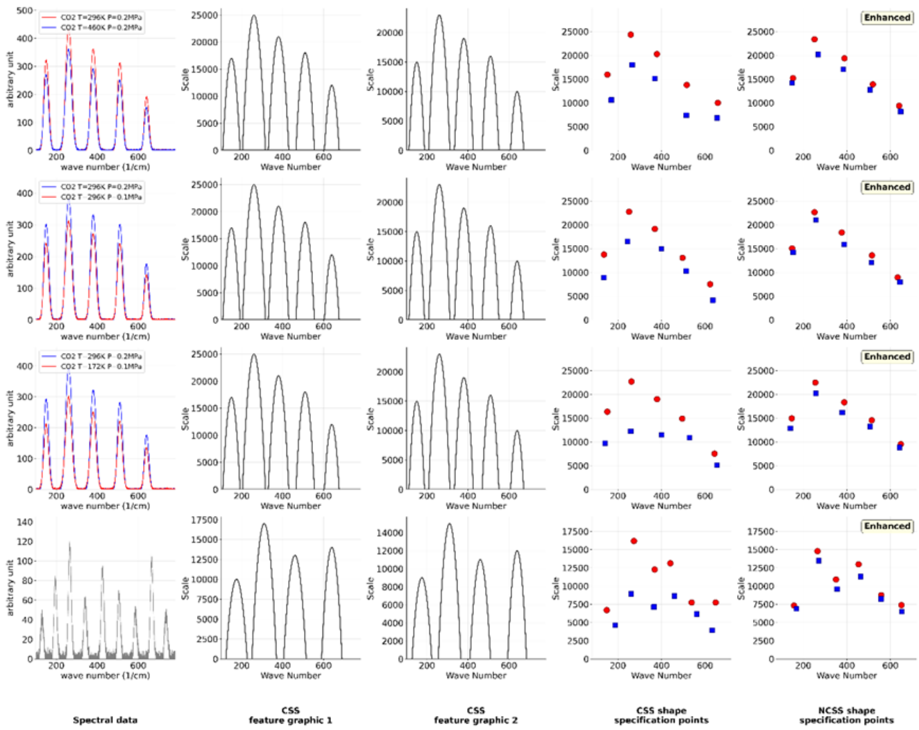

Figure 4: Comparisons Between CSS and NCSS.

3.2 Stability Under Different Conditions

The first part of the experiments focuses on stability evaluation. The test data (see Table 1) consist of spectra from the same substance measured under different conditions, including varying temperature, pressure, relative humidity (RH), and exposure time in air.

Table 1: Spectra in Different Conditions.

Substance Condition	CO_2	SO_3H	C=O band	–C=O band

Pressure	0.1 MPa – 0.2 MPa	\	\	\
Temperature	296 K-460 K	\	\	\
RH	\	0% – 100%	\	\
Exposure Time	\	\	0 -30 h	0 -20 h

Cross-validation is adopted as the evaluation protocol. Stability is quantified by the average intra-class difference, defined as:

$$\text{stability} = \text{ave}\left(\text{Diff}(s_i, s_j)\right), i \neq j, i, j = 1, \dots, N$$

where s denotes a spectral sample, s∈S, ave represents the average operator, and Diff denotes the dissimilarity measure between spectra s_i and s_j. A lower stability value indicates that the algorithm produces more consistent feature representations across different environmental conditions, which is desirable for robust recognition.

For comparison, we evaluate four algorithms: EDM (Euclidean Distance Matching), ASM (Active Shape Model), CC (Cross-Correlation), and the proposed NCSS. The stability results are shown in Figure 5. The proposed NCSS method achieves the lowest intra-class difference across all tested substances and conditions, demonstrating superior stability compared to all baseline methods. This result confirms that the curvature-based normalization effectively suppresses the influence of environmental variations on spectral features.

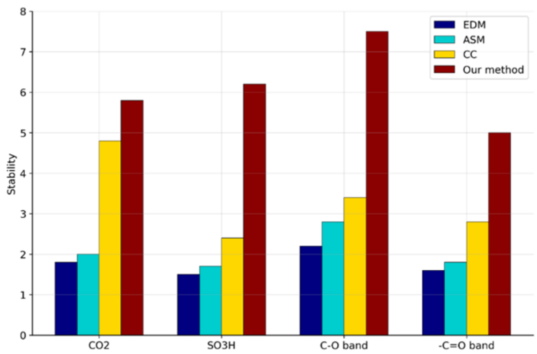

Figure 5: Stability Performance.

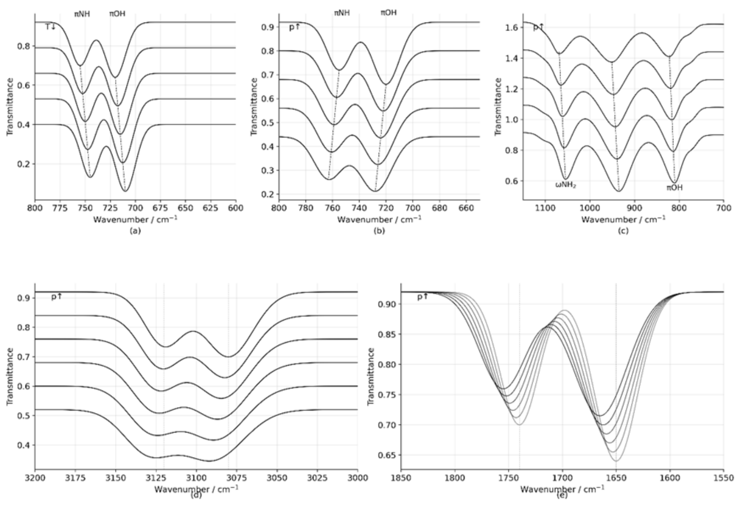

Figure 6: Frequency Shifts.

3.3 Dealing with Frequency Shifts

Frequency shifts are a common phenomenon in gas spectroscopy, particularly when pressure changes. Representative examples of frequency-shifted spectra are shown in Figure 6 [5]. Such shifts pose a significant challenge for spectral matching algorithms that rely on absolute peak positions.

The proposed NCSS algorithm handles frequency shifts effectively through the introduction of the multiscale analysis framework. By analyzing spectral curvature across a range of smoothing scales, the algorithm captures structural features that are robust to minor positional displacements. Small frequency shifts therefore have minimal impact on the extracted NCSS features. Furthermore, the normalization step explicitly compensates for global frequency offsets by aligning the spatial extent of the observed feature set to that of the reference.

Experimental results confirming the robustness of the proposed algorithm to frequency shifts are presented in Figure 7. The NCSS method maintains consistently good performance across a range of frequency shift magnitudes, while the performance of baseline methods degrades more rapidly as the shift increases. These results validate the effectiveness of the multiscale curvature approach in handling real-world spectral variability.

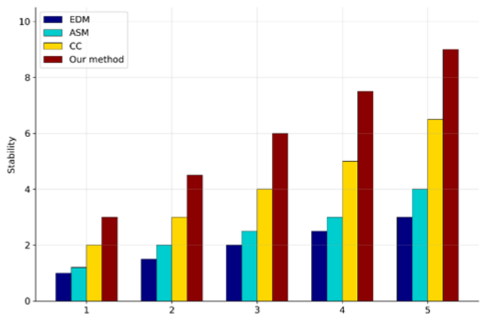

Figure 7: Stability Performance in Frequency Shifts.

4. Conclusions

In this paper, we have proposed a novel algorithm for invariant feature extraction from gas spectra, enabling robust spectral recognition that is unaffected by environmental changes in temperature, pressure, humidity, and exposure conditions. The core insight is that the relative curvature of spectral peaks across different scales remains invariant under environmental perturbations. Building on this observation, we adopted the Curvature Scale Space (CSS) framework and extended it with a normalization procedure to develop the NCSS (Normalized Curvature Scale Space) descriptor.

The proposed NCSS algorithm was validated on spectral data from multiple gas species under a wide range of physical conditions. Experimental results demonstrate that NCSS achieves superior stability (as measured by intra-class difference) compared to traditional methods including EDM, ASM, and CC, while maintaining strong discriminative capability for inter-class separation. The algorithm also exhibits robust performance in the presence of frequency shifts, which are common in real-world gas spectroscopy applications.

Despite these encouraging results, further work is needed to enhance the discriminative capability of the algorithm when test spectra exhibit high intra-class similarity. Future research directions include the incorporation of additional spectral features beyond curvature, the development of adaptive normalization strategies for more complex environmental conditions, and the extension of the framework to handle multi-component gas mixtures.

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References

[1] G. A. F. Buersgens and R. Kersting, "Millimeter wave probing of the acoustic phase for concealed object detection," Optics Express 15 (2017).

[2] S. Y. Dong-Su Lee, Jung-Young Son, Shin-Hwan Kim, "Automatic image segmentation for concealed object detection using the expectation-maximization algorithm," Optics Express 18 (2020).

[3] D.-S. L. Seokwon Yeom, Jung-Young Son, Min-Kyoo, "Real-time outdoor concealed-object detection with passive millimeter wave imaging," Optics Express 19, 7 (2021).

[4] A. C. Flora Boccuzzi, Maela Manzoli, "Au/TiO_2 nanostructured catalyst: pressure and temperature effects on the FTIR spectra of CO adsorbed at 90 K," Surface Science 6 (2022).

[5] K. C. H. O. Desseyn, R. Keuleers, R. Miao, V. E. Van Doren, and N. Blaton, "The effect of pressure and temperature on the vibrational spectra of different hydrogen bonded systems," Spectrochimica Acta Part A 57, 16 (2021).

[6] S. W. Jun Liu, Dapeng Cao and Liqun Zhang, "Effects of pressure on structure and dynamics of model elastomers: A molecular dynamics study," THE JOURNAL OF CHEMICALPHYSICS 129(2018).